# STATA MULTIVARIATE STATISTICS REFERENCE MANUAL RELEASE 14



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# **Cross-referencing the documentation**

When reading this manual, you will find references to other Stata manuals. For example,

- [U] 26 Overview of Stata estimation commands
- [R] regress
- [D] reshape

The first example is a reference to chapter 26, Overview of Stata estimation commands, in the User's Guide; the second is a reference to the regress entry in the Base Reference Manual; and the third is a reference to the reshape entry in the Data Management Reference Manual.

All the manuals in the Stata Documentation have a shorthand notation:

[GSM] [GSU] [GSW]	Getting Started with Stata for Mac Getting Started with Stata for Unix Getting Started with Stata for Windows
[U]	Stata User's Guide
[R]	Stata Base Reference Manual
[BAYES]	Stata Bayesian Analysis Reference Manual
[D]	Stata Data Management Reference Manual
[FN]	Stata Functions Reference Manual
[G]	Stata Graphics Reference Manual
[IRT]	Stata Item Response Theory Reference Manual
[XT]	Stata Longitudinal-Data/Panel-Data Reference Manual
[ME]	Stata Multilevel Mixed-Effects Reference Manual
[MI]	Stata Multiple-Imputation Reference Manual
[MV]	Stata Multivariate Statistics Reference Manual
[PSS]	Stata Power and Sample-Size Reference Manual
[P]	Stata Programming Reference Manual
[SEM]	Stata Structural Equation Modeling Reference Manual
[SVY]	Stata Survey Data Reference Manual
[ST]	Stata Survival Analysis Reference Manual
[TS]	Stata Time-Series Reference Manual
[TE]	Stata Treatment-Effects Reference Manual: Potential Outcomes/Counterfactual Outcomes
[1]	Stata Glossary and Index
[M]	Mata Reference Manual

## **Title**

**intro** — Introduction to multivariate statistics manual

# **Description**

This manual documents Stata's multivariate analysis features and is referred to as the [MV] manual in cross-references.

Following this entry, [MV] multivariate provides an overview of the multivariate analysis features in Stata and Stata's multivariate analysis commands. The other parts of this manual are arranged alphabetically.

Stata is continually being updated, and Stata users are always writing new commands. To find out about the latest multivariate analysis features, type search multivariate analysis after installing the latest official updates; see [R] update.

#### Also see

- [U] 1.3 What's new
- [R] intro Introduction to base reference manual

multivariate — Introduction to multivariate commands

Description Remarks and examples Also see

# **Description**

The Multivariate Reference Manual organizes the commands alphabetically, which makes it easy to find individual command entries if you know the name of the command. This overview organizes and presents the commands conceptually, that is, according to the similarities in the functions that they perform. The table below lists the manual entries that you should see for additional information.

## Cluster analysis.

These commands perform cluster analysis on variables or the similarity or dissimilarity values within a matrix. An introduction to cluster analysis and a description of the cluster and clustermat subcommands is provided in [MV] cluster and [MV] clustermat.

## Discriminant analysis.

These commands provide both descriptive and predictive linear discriminant analysis (LDA), as well as predictive quadratic discriminant analysis (QDA), logistic discriminant analysis, and *k*th-nearest-neighbor (KNN) discriminant analysis. An introduction to discriminant analysis and the discrim command is provided in [MV] discrim.

#### Factor analysis and principal component analysis.

These commands provide reliability analysis using Cronbach's alpha, factor analysis of a correlation matrix, and principal component analysis (PCA) of a correlation or covariance matrix. The correlation or covariance matrix can be provided directly or computed from variables.

#### Rotation.

These commands provide methods for rotating a factor or PCA solution or for rotating a matrix. Also provided is Procrustean rotation analysis for rotating a set of variables to best match another set of variables.

#### Multivariate analysis of variance and related techniques.

These commands provide canonical correlation analysis, multivariate regression, multivariate analysis of variance (MANOVA), and comparison of multivariate means. Also provided are multivariate tests on means, covariances, and correlations, and tests for multivariate normality.

#### Structural equation modeling.

These commands provide multivariate linear models that can include observed and latent variables. These models include confirmatory factor analysis, multivariate regression, path analysis, mediator analysis, and more; see the *Stata Structural Equation Modeling Reference Manual*.

#### Multidimensional scaling and biplots.

These commands provide classic and modern (metric and nonmetric) MDS and two-dimensional biplots. MDS can be performed on the variables or on proximity data in a matrix or as proximity data in long format.

#### Correspondence analysis.

These commands provide simple correspondence analysis (CA) on the cross-tabulation of two categorical variables or on a matrix and multiple correspondence analysis (MCA) and joint correspondence analysis (JCA) on two or more categorical variables.

#### Bayesian analysis.

These commands provide Bayesian estimation of multivariate linear models, including multivariate normal regression; see the Stata Bayesian Analysis Reference Manual.

#### Item response theory.

These commands fit item response theory models to binary, ordinal, and nominal items, and their combinations. Postestimation features include graphical tools to plot characteristic curves and information functions; see the Stata Item Response Theory Reference Manual.

#### Cluster analysis

[MV] cluster	Introduction to cluster-analysis commands
[MV] clustermat	Introduction to clustermat commands

[MV] matrix dissimilarity Compute similarity or dissimilarity measures; may be

used by clustermat

#### Discriminant analysis

[MV] discrim	Introduction to discriminant-analysis commands
[MV] discrim lda	Linear discriminant analysis (LDA)
[MV] discrim lda postestimation	Postestimation tools for discrim Ida
[MV] candisc	Canonical (descriptive) linear discriminant analysis
[MV] discrim qda	Quadratic discriminant analysis (QDA)
[MV] discrim qda postestimation	Postestimation tools for discrim qda
[MV] discrim logistic	Logistic discriminant analysis
[MV] discrim logistic postestimation	Postestimation tools for discrim logistic
[MV] discrim knn	kth-nearest-neighbor (KNN) discriminant analysis
[MV] discrim knn postestimation	Postestimation tools for discrim knn
[MV] discrim estat	Postestimation tools for discrim

#### Factor analysis and principal component analysis

[MV] alpha	Compute interitem correlations (covariances) and Cronbach's alpha
[MV] factor	Factor analysis
[MV] factor postestimation	Postestimation tools for factor and factormat
[MV] pca	Principal component analysis
[MV] pca postestimation	Postestimation tools for pca and pcamat
[MV] rotate	Orthogonal and oblique rotations after factor and pca
[MV] screeplot	Scree plot
[MV] scoreplot	Score and loading plots

#### Rotation

[MV] rotate	Orthogonal and oblique rotations after factor and pca
[MV] rotatemat	Orthogonal and oblique rotation of a Stata matrix
[MV] procrustes	Procrustes transformation

[MV] procrustes postestimation Postestimation tools for procrustes

#### Multivariate analysis of variance and related techniques

[MV] canon Canonical correlations

[MV] canon postestimation Postestimation tools for canon

[MV] mvreg Multivariate regression

[MV] **mvreg postestimation** Postestimation tools for mvreg

[MV] manova Multivariate analysis of variance and covariance

[MV] manova postestimation Postestimation tools for manova

[MV] **hotelling** Hotelling's T-squared generalized means test

[MV] **mytest** Multivariate tests on means, covariances, correlations,

and of normality

#### Structural equation modeling

[SEM] Stata Structural Equation Modeling Reference Manual

#### Multidimensional scaling and biplots

[MV] mds Multidimensional scaling for two-way data

[MV] mds postestimation Postestimation tools for mds, mdsmat, and mdslong Postestimation plots Postestimation plot

[MV] mdslong Multidimensional scaling of proximity data in long format Multidimensional scaling of proximity data in a matrix

[MV] **biplot** Biplots

#### Correspondence analysis

[MV] ca Simple correspondence analysis

[MV] ca postestimation Postestimation tools for ca and camat
[MV] ca postestimation plots
[MV] mca Postestimation plots for ca and camat
Multiple and joint correspondence analysis

[MV] mca postestimation Postestimation tools for mca [MV] mca postestimation plots Postestimation plots Postestimation plots

#### Bayesian analysis

[BAYES] Stata Bayesian Analysis Reference Manual

#### Item response theory

[IRT] Stata Item Response Theory Reference Manual

# Remarks and examples

Remarks are presented under the following headings:

Cluster analysis

Discriminant analysis

Factor analysis and principal component analysis

Rotation

Multivariate analysis of variance and related techniques

Structural equation modeling

Multidimensional scaling and biplots

Correspondence analysis

Bayesian analysis

Item response theory

## Cluster analysis

Cluster analysis is concerned with finding natural groupings, or clusters. Stata's cluster-analysis commands provide several hierarchical and partition clustering methods, postclustering summarization methods, and cluster-management tools. The hierarchical clustering methods may be applied to the data with the cluster command or to a user-supplied dissimilarity matrix with the clustermat command. See [MV] cluster for an introduction to cluster analysis and the cluster and clustermat suite of commands.

A wide variety of similarity and dissimilarity measures are available for comparing observations; see [MV] *measure\_option*. Dissimilarity matrices, for use with clustermat, are easily obtained using the matrix dissimilarity command; see [MV] *matrix dissimilarity*. This provides the building blocks necessary for clustering variables instead of observations or for clustering using a dissimilarity not automatically provided by Stata; [MV] *clustermat* provides examples.

## Discriminant analysis

Discriminant analysis may be used to describe differences between groups and to exploit those differences in allocating (classifying) observations to the groups. These two purposes of discriminant analysis are often called descriptive discriminant analysis and predictive discriminant analysis.

discrim has both descriptive and predictive LDA; see [MV] discrim lda. The candisc command computes the same thing as discrim lda, but with output tailored for the descriptive aspects of the discrimination; see [MV] candisc.

The remaining discrim subcommands provide alternatives to linear discriminant analysis for predictive discrimination. [MV] **discrim qda** provides quadratic discriminant analysis. [MV] **discrim logistic** provides logistic discriminant analysis. [MV] **discrim knn** provides kth-nearest-neighbor discriminant analysis.

Postestimation commands provide classification tables (confusion matrices), error-rate estimates, classification listings, and group summarizations. In addition, postestimation tools for LDA and QDA include display of Mahalanobis distances between groups, correlations, and covariances. LDA postestimation tools also include discriminant-function loading plots, discriminant-function score plots, scree plots, display of canonical correlations, eigenvalues, proportion of variance, likelihood-ratio tests for the number of nonzero eigenvalues, classification functions, loadings, structure matrix, standardized means, and ANOVA and MANOVA tables. See [MV] discrim estat, [MV] discrim lda postestimation, and [MV] discrim qda postestimation.

## Factor analysis and principal component analysis

Cronbach's alpha is a measure of reliability often used as a preliminary step before factor analysis. Though not literally correct, alpha is sometimes conceptualized as the average correlation among all possible pairwise combinations of a group of variables. A value of alpha greater than 0.7 (sometimes 0.8) indicates high intracorrelation among a group of variables and is typically used as a criterion to determine that a subsequent factor analysis is appropriate. See [MV] alpha for details.

Factor analysis and principal component analysis (PCA) have dual uses. They may be used as a dimension-reduction technique, and they may be used in describing the underlying data.

In PCA, the leading eigenvectors from the eigen decomposition of the correlation or covariance matrix of the variables describe a series of uncorrelated linear combinations of the variables that contain most of the variance. For data reduction, a few of these leading components are retained. For describing the underlying structure of the data, the magnitudes and signs of the eigenvector elements are interpreted in relation to the original variables (rows of the eigenvector).

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pca uses the correlation or covariance matrix computed from the dataset. pcamat allows the correlation or covariance matrix to be directly provided. The vce(normal) option provides standard errors for the eigenvalues and eigenvectors, which aids in their interpretation. See [MV] pca for details.

Factor analysis finds a few common factors that linearly reconstruct the original variables. Reconstruction is defined in terms of prediction of the correlation matrix of the original variables, unlike PCA, where reconstruction means minimum residual variance summed across all variables. Factor loadings are examined for interpretation of the structure of the data.

factor computes the correlation from the dataset, whereas factormat is supplied the matrix directly. They both display the eigenvalues of the correlation matrix, the factor loadings, and the "uniqueness" of the variables. See [MV] factor for details.

To perform factor analysis or PCA on binary data, compute the tetrachoric correlations and use these with factormat or pcamat. Tetrachoric correlations are available with the tetrachoric command; see [R] tetrachoric.

After factor analysis and PCA, a suite of commands are available that provide for rotation of the loadings; generation of score variables; graphing of scree plots, loading plots, and score plots; display of matrices and scalars of interest such as anti-image matrices, residual matrices, Kaiser–Meyer–Olkin measures of sampling adequacy, squared multiple correlations; and more. See [MV] factor postestimation, [MV] pca postestimation, [MV] rotate, [MV] screeplot, and [MV] scoreplot for details.

## **Rotation**

Rotation provides a modified solution that is rotated from an original multivariate solution such that interpretation is enhanced. Rotation is provided through three commands: rotate, rotatemat, and procrustes.

rotate works directly after pca, pcamat, factor, and factormat. It knows where to obtain the component- or factor-loading matrix for rotation, and after rotating the loading matrix, it places the rotated results in e() so that all the postestimation tools available after pca and factor may be applied to the rotated results. See [MV] rotate for details.

Perhaps you have the component or factor loadings from a published source and want to investigate various rotations, or perhaps you wish to rotate a loading matrix from some other multivariate command. rotatemat provides rotations for a specified matrix. See [MV] rotatemat for details.

A large selection of orthogonal and oblique rotations are provided for rotate and rotatemat. These include varimax, quartimax, equamax, parsimax, minimum entropy, Comrey's tandem 1 and 2, promax power, biquartimax, biquartimin, covarimin, oblimin, factor parsimony, Crawford—Ferguson family, Bentler's invariant pattern simplicity, oblimax, quartimin, target, and weighted target rotations. Kaiser normalization is also available.

The procrustes command provides Procrustean analysis. The goal is to transform a set of source variables to be as close as possible to a set of target variables. The permitted transformations are any combination of dilation (uniform scaling), rotation and reflection (orthogonal and oblique transformations), and translation. Closeness is measured by the residual sum of squares. See [MV] **procrustes** for details.

A set of postestimation commands are available after procrustes for generating fitted values and residuals; for providing fit statistics for orthogonal, oblique, and unrestricted transformations; and for providing a Procrustes overlay graph. See [MV] procrustes postestimation for details.

## Multivariate analysis of variance and related techniques

The first canonical correlation is the maximum correlation that can be obtained between a linear combination of one set of variables and a linear combination of another set of variables. The second canonical correlation is the maximum correlation that can be obtained between linear combinations of the two sets of variables subject to the constraint that these second linear combinations are orthogonal to the first linear combinations, and so on.

canon estimates these canonical correlations and provides the loadings that describe the linear combinations of the two sets of variables that produce the correlations. Standard errors of the loadings are provided, and tests of the significance of the canonical correlations are available. See [MV] canon for details.

Postestimation tools are available after canon for generating the variables corresponding to the linear combinations underlying the canonical correlations. Various matrices and correlations may also be displayed. See [MV] canon postestimation for details.

In canonical correlation, there is no real distinction between the two sets of original variables. In multivariate regression, however, the two sets of variables take on the roles of dependent and independent variables. Multivariate regression is an extension of regression that allows for multiple dependent variables. See [MV] **mvreg** for multivariate regression, and see [MV] **mvreg postestimation** for the postestimation tools available after multivariate regression.

Just as analysis of variance (ANOVA) can be formulated in terms of regression where the categorical independent variables are represented by indicator (sometimes called dummy) variables, multivariate analysis of variance (MANOVA), a generalization of ANOVA that allows for multiple dependent variables, can be formulated in terms of multivariate regression where the categorical independent variables are represented by indicator variables. Multivariate analysis of covariance (MANCOVA) allows for both continuous and categorical independent variables.

The manova command fits MANOVA and MANCOVA models for balanced and unbalanced designs, including designs with missing cells, and for factorial, nested, or mixed designs, or designs involving repeated measures. Four multivariate test statistics—Wilks's lambda, Pillai's trace, the Lawley—Hotelling trace, and Roy's largest root—are computed for each term in the model. See [MV] manova for details.

Postestimation tools are available after manova that provide for univariate Wald tests of expressions involving the coefficients of the underlying regression model and that provide for multivariate tests involving terms or linear combinations of the underlying design matrix. Linear combinations of the dependent variables are also supported. Also available are marginal means, predictive margins, marginal effects, and average marginal effects. See [MV] manova postestimation for details.

Related to MANOVA is Hotelling's T-squared test of whether a set of means is zero or whether two sets of means are equal. It is a multivariate test that reduces to a standard t test if only one variable is involved. The hotelling command provides Hotelling's T-squared test; see [MV] hotelling, but also see [MV] mytest means for more extensive multivariate means testing.

A suite of mvtest commands perform assorted multivariate tests. mvtest means performs one-sample and multiple-sample multivariate tests on means, assuming multivariate normality. mvtest covariances performs one-sample and multiple-sample multivariate tests on covariances, assuming multivariate normality. mvtest correlations performs one-sample and multiple-sample tests on correlations, assuming multivariate normality. mvtest normality performs tests for univariate, bivariate, and multivariate normality. See [MV] mvtest.

#### Ω

## Structural equation modeling

Structural equation modeling (SEM) is a flexible estimation method for fitting a variety of multivariate models, and it allows for latent (unobserved) variables. See [SEM] intro 5.

#### Multidimensional scaling and biplots

Multidimensional scaling (MDS) is a dimension-reduction and visualization technique. Dissimilarities (for instance, Euclidean distances) between observations in a high-dimensional space are represented in a lower-dimensional space (typically two dimensions) so that the Euclidean distance in the lower-dimensional space approximates the dissimilarities in the higher-dimensional space.

The mds command provides classical and modern (metric and nonmetric) MDS for dissimilarities between observations with respect to the variables; see [MV] mds. A wide variety of similarity and dissimilarity measures are allowed (the same ones available for the cluster command); see [MV] measure\_option.

mdslong and mdsmat provide MDS directly on the dissimilarities recorded either as data in long format (mdslong) or as a dissimilarity matrix (mdsmat); see [MV] mdslong and [MV] mdsmat.

Postestimation tools available after mds, mdslong, and mdsmat provide MDS configuration plots and Shepard diagrams; generation of the approximating configuration or the disparities, dissimilarities, distances, raw residuals and transformed residuals; and various matrices and scalars, such as Kruskal stress (loss), quantiles of the residuals per object, and correlations between disparities or dissimilarities and approximating distances. See [MV] mds postestimation and [MV] mds postestimation plots.

Biplots are two-dimensional representations of data. Both the observations and the variables are represented. The observations are represented by marker symbols, and the variables are represented by arrows from the origin. Observations are projected to two dimensions so that the distance between the observations is approximately preserved. The cosine of the angle between arrows approximates the correlation between the variables. A biplot aids in understanding the relationship between the variables, the observations, and the observations and variables jointly. The biplot command produces biplots; see [MV] biplot.

## Correspondence analysis

Simple correspondence analysis (CA) is a technique for jointly exploring the relationship between rows and columns in a cross-tabulation. It is known by many names, including dual scaling, reciprocal averaging, and canonical correlation analysis of contingency tables.

ca performs CA on the cross-tabulation of two integer-valued variables or on two sets of crossed (stacked) integer-valued variables. camat performs CA on a matrix with nonnegative entries—perhaps from a published table. See [MV] ca for details.

A suite of commands are available following ca and camat. These include commands for producing CA biplots and dimensional projection plots; for generating fitted values, row coordinates, and column coordinates; and for displaying distances between row and column profiles, individual cell inertia contributions,  $\chi^2$  distances between row and column profiles, and the fitted correspondence table. See [MV] ca postestimation and [MV] ca postestimation plots.

mca performs multiple (MCA) or joint (JCA) correspondence analysis on two or more categorical variables and allows for crossing (stacking). See [MV] mca.

Postestimation tools available after mca provide graphing of category coordinate plots, dimensional projection plots, and plots of principal inertias; display of the category coordinates, optionally with column statistics; the matrix of inertias of the active variables after JCA; and generation of row scores. See [MV] mca postestimation and [MV] mca postestimation plots.

## Bayesian analysis

Bayesian analysis provides a flexible framework for fitting a variety of Bayesian models, including multivariate models. See Stata Bayesian Analysis Reference Manual.

## Item response theory

Item response theory (IRT) is used in the design, analysis, scoring, and comparison of tests and similar instruments whose purpose is to measure unobservable characteristics of the respondents; see Stata Item Response Theory Reference Manual.

## Also see

[R] intro — Introduction to base reference manual [MV] Glossary

#### Title

alpha — Compute interitem correlations (covariances) and Cronbach's alpha

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

Acknowledgment References Also see

# **Description**

alpha computes the interitem correlations or covariances for all pairs of variables in *varlist* and Cronbach's  $\alpha$  statistic for the scale formed from them. At least two variables must be specified with alpha.

#### **Quick start**

Cronbach's alpha and the average interitem covariance of 6 variables

alpha v1 v2 v3 v4 v5 v6

As above, but standardize the variables to give average interitem correlation

alpha v1 v2 v3 v4 v5 v6, std

As above, and show table of item-test and item-rest correlations and the effect of removing each variable from the scale

alpha v1 v2 v3 v4 v5 v6, std item

As above, and also list each interitem correlation

alpha v1 v2 v3 v4 v5 v6, std item detail

As above, but force v2 and v5 to enter with reversed sign

alpha v1 v2 v3 v4 v5 v6, std item detail reverse(v2 v5)

As above, and generate scalevar with the summative score (scale)

alpha v1 v2 v3 v4 v5 v6, std item detail reverse(v2 v5) ///
 generate(scalevar)

#### Menu

Statistics > Multivariate analysis > Cronbach's alpha

# **Syntax**

alpha varlist [if] [in] [, options]

options	Description
Options	
<u>a</u> sis	take sign of each item as is
<u>c</u> asewise	delete cases with missing values
$\underline{\mathtt{d}}\mathtt{etail}$	list individual interitem correlations and covariances
<pre>generate(newvar)</pre>	save the generated scale in newvar
<u>i</u> tem	display item-test and item-rest correlations
<u>l</u> abel	include variable labels in output table
$\underline{\mathtt{m}}\mathtt{in}(\#)$	must have at least # observations for inclusion
<u>r</u> everse( <i>varlist</i> )	reverse signs of these variables
<u>s</u> td	standardize items in the scale to mean 0, variance 1

by is allowed; see [D] by.

# **Options**

Options )

asis specifies that the sense (sign) of each item be taken as presented in the data. The default is to determine the sense empirically and reverse the scorings for any that enter negatively.

casewise specifies that cases with missing values be deleted listwise. The default is pairwise computation of covariances and correlations.

detail lists the individual interitem correlations and covariances.

generate(newvar) specifies that the scale constructed from varlist be saved in newvar. Unless asis is specified, the sense of items entering negatively is automatically reversed. If std is also specified, the scale is constructed by using standardized (mean 0, variance 1) values of the individual items. Unlike most Stata commands, generate() does not use casewise deletion. A score is created for every observation for which there is a response to at least one item (one variable in varlist is not missing). The summative score is divided by the number of items over which the sum is calculated.

item specifies that item-test and item-rest correlations and the effects of removing an item from the scale be displayed. item is valid only when more than two variables are specified in varlist.

label requests that the detailed output table be displayed in a compact format that enables the inclusion of variable labels.

min(#) specifies that only cases with at least # observations be included in the computations. casewise is a shorthand for min(k), where k is the number of variables in varlist.

reverse(varlist) specifies that the signs (directions) of the variables (items) in varlist be reversed. Any variables specified in reverse() that are not also included in alpha's varlist are ignored.

std specifies that the items in the scale be standardized (mean 0, variance 1) before summing.

# Remarks and examples

Cronbach's alpha (Cronbach 1951) assesses the reliability of a summative rating (Likert 1932) scale composed of the variables (called items) specified. The set of items is often called a test or battery. A scale is simply the sum of the individual item scores, reversing the scoring for statements that have negative correlations with the factor (for example, attitude) being measured. Scales can be formed by using the raw item scores or standardized item scores.

The reliability  $\alpha$  is defined as the square of the correlation between the measured scale and the underlying factor. If you think of a test as being composed of a random sample of items from a hypothetical domain of items designed to measure the same thing,  $\alpha$  represents the expected correlation of one test with an alternative form containing the same number of items. The square root of  $\alpha$  is the estimated correlation of a test with errorless true scores (Nunnally and Bernstein 1994, 235).

In addition to reporting  $\alpha$ , alpha generates the summative scale from the items (variables) specified and automatically reverses the sense of any when necessary. Stata's decision can be overridden by specifying the reverse(varlist) option.

Because it concerns reliability in measuring an unobserved factor,  $\alpha$  is related to factor analysis. The test should be designed to measure one factor, and, because the scale will be composed of an unweighted sum, the factor loadings should all contribute roughly equal information to the score. Both of these assumptions can be verified with factor; see [MV] factor. Equality of factor loadings can also be assessed by using the item option.

#### Example 1

To illustrate alpha, we apply it, first without and then with the item option, to the automobile dataset after randomly introducing missing values:

```
. use http://www.stata-press.com/data/r14/automiss
(1978 Automobile Data)
. alpha price headroom rep78 trunk weight length turn displ, std
Test scale = mean(standardized items)
Reversed item: rep78
Average interitem correlation:
                                    0.5251
Number of items in the scale:
                                         8
Scale reliability coefficient:
                                    0.8984
```

The scale derived from our somewhat arbitrarily chosen automobile items (variables) appears to be reasonable because the estimated correlation between it and the underlying factor it measures is  $\sqrt{0.8984} \approx 0.9478$  and the estimated correlation between this battery of eight items and all other eight-item batteries from the same domain is 0.8984. Because the "items" are not on the same scale, it is important that std was specified so that the scale and its reliability were based on the sum of standardized variables. We could obtain the scale in a new variable called sc with the gen(sc) option.

Though the scale appears reasonable, we include the item option to determine if all the items fit the scale:

	alpha	price	headroom	rep78	trunk	weight	length	turn	displ,	std	item
Т	est sc	ale = r	nean(stand	dardize	ed iter	ns)					

Item	Obs	Sign	item-test correlation	item-rest correlation	average interitem correlation	alpha
price	70	+	0.5260	0.3719	0.5993	0.9128
headroom	66	+	0.6716	0.5497	0.5542	0.8969
rep78	61	-	0.4874	0.3398	0.6040	0.9143
trunk	69	+	0.7979	0.7144	0.5159	0.8818
weight	64	+	0.9404	0.9096	0.4747	0.8635
length	69	+	0.9382	0.9076	0.4725	0.8625
turn	66	+	0.8678	0.8071	0.4948	0.8727
displacement	63	+	0.8992	0.8496	0.4852	0.8684
Test scale					0.5251	0.8984

"Test" denotes the additive scale; here 0.5251 is the average interitem correlation, and 0.8984 is the alpha coefficient for a test scale based on all items.

"Obs" shows the number of nonmissing values of the items; "Sign" indicates the direction in which an item variable entered the scale; "-" denotes that the item was reversed. The remaining four columns in the table provide information on the effect of one item on the scale.

Column four gives the item-test correlations. Apart from the sign of the correlation for items that entered the scale in reversed order, these correlations are the same numbers as those computed by the commands

- . alpha price headroom rep78 trunk weight length turn displ, std gen(sc)
- . pwcorr sc price headroom rep78 trunk weight length turn displ

Typically, the item-test correlations should be roughly the same for all items. Item-test correlations may not be adequate to detect items that fit poorly because the poorly fitting items may distort the scale. Accordingly, it may be more useful to consider item-rest correlations (Nunnally and Bernstein 1994), that is, the correlation between an item and the scale that is formed by all other items. The average interitem correlations (covariances if std is omitted) of all items, excluding one, are shown in column six. Finally, column seven gives Cronbach's  $\alpha$  for the test scale, which consists of all but the one item.

Here neither the price item nor the rep78 item seems to fit well in the scale in all respects. The item-test and item-rest correlations of price and rep78 are much lower than those of the other items. The average interitem correlation increases substantially by removing either price or rep78; apparently, they do not correlate strongly with the other items. Finally, we see that Cronbach's  $\alpha$ coefficient will increase from 0.8984 to 0.9128 if the price item is dropped, and it will increase from 0.8984 to 0.9143 if rep78 is dropped. For well-fitting items, we would of course expect that  $\alpha$  decreases by shortening the test.

## Example 2

The variable names for the automobile data are reasonably informative. This may not always be true; items in batteries commonly used to measure personality traits, attitudes, values, etc., are usually named with indexed names, for example, item12a, item12b, item12c. The label option forces alpha to produce the same statistical information in a more compact format that leaves room to include variable (item) labels. In this compact format, alpha excludes the number of nonmissing values of the items, displays the statistics using fewer digits, and uses somewhat cryptic headers:

. alpha price headroom rep78 trunk weight length turn disp1, std item label detail Test scale = mean(standardized items)

Items	S	it-cor	ir-cor	ii-cor	alpha	label
price	+	0.526	0.372	0.599	0.913	Price
headroom	+	0.672	0.550	0.554	0.897	Headroom (in.)
rep78	-	0.487	0.340	0.604	0.914	Repair Record 1978
trunk	+	0.798	0.714	0.516	0.882	Trunk space (cu. ft.)
weight	+	0.940	0.910	0.475	0.863	Weight (lbs.)
length	+	0.938	0.908	0.473	0.862	Length (in.)
turn	+	0.868	0.807	0.495	0.873	Turn Circle (ft.)
displacement	+	0.899	0.850	0.485	0.868	Displacement (cu. in.)
				0 505		
Test scale				0.525	0.898	mean(standardized items)

Interitem cor	relations (revers	e applied)	(obs=pairwise,	see below)	
	price	headroom	rep78	trunk	
price	1.0000				
headroom	0.1174	1.0000			
rep78	-0.0479	0.1955	1.0000		
trunk	0.2748	0.6841	0.2777	1.0000	
weight	0.5093	0.5464	0.3624	0.6486	
length	0.4511	0.5823	0.3162	0.7404	
turn	0.3528	0.4067	0.4715	0.5900	
displacement	0.5537	0.5166	0.3391	0.6471	
	weight	length	turn	displacement	
weight	1.0000				
length	0.9425	1.0000			
turn	0.8712	0.8589	1.0000		
displacement	0.8753	0.8422	0.7723	1.0000	
-	er of observation	5			
-	er of observation	s headroom	rep78	trunk	
-			rep78	trunk	
Pairwise numb	price		rep78	trunk	
Pairwise numb	price 70 62 59	headroom 66 54	rep78 61	trunk	
Pairwise numb	price 70 62 59 65	headroom 66 54 61	61 59	69	
Pairwise numb	price 70 62 59	headroom 66 54 61 56	61		
Pairwise numb  price headroom rep78 trunk	price 70 62 59 65	headroom 66 54 61	61 59	69 60 64	
Pairwise numb  price headroom rep78 trunk weight	price 70 62 59 65 60 66 62	headroom  66 54 61 56 61 58	61 59 52 58 56	69 60 64 62	
Pairwise numb  price headroom rep78 trunk weight length	price 70 62 59 65 60 66	headroom 66 54 61 56 61	61 59 52 58	69 60 64	
Pairwise numb  price headroom rep78 trunk weight length turn displacement	price 70 62 59 65 60 66 62 59 weight	headroom  66 54 61 56 61 58	61 59 52 58 56	69 60 64 62	
Pairwise numb  price headroom rep78 trunk weight length turn displacement  weight	price 70 62 59 65 60 66 62 59 weight 64	headroom  66 54 61 56 61 58 58 length	61 59 52 58 56 51	69 60 64 62 58	
Pairwise numb  price headroom rep78 trunk weight length turn displacement	price 70 62 59 65 60 66 62 59 weight 64 60	headroom  66 54 61 56 61 58 58 length	61 59 52 58 56 51 turn	69 60 64 62 58	
Pairwise numb  price headroom rep78 trunk weight length turn displacement  weight	price 70 62 59 65 60 66 62 59 weight 64	headroom  66 54 61 56 61 58 58 length	61 59 52 58 56 51	69 60 64 62 58	

Because the detail option was also specified, the interitem correlation matrix was printed, together with the number of observations used for each entry (because these varied across the matrix). Note the negative sign attached to rep78 in the output, indicating the sense in which it entered the scale.

4

Better-looking output with less-cryptic headers is produced if the linesize is set to a value of at least 100:

- . set linesize 100
- . alpha price headroom rep78 trunk weight length turn disp1, std item label

Test scale = mean(standardized items)

Item	Obs	Sign	item-test corr.	item-rest corr.	interitem corr.	alpha	Label
price	70	+	0.5260	0.3719	0.5993	0.9128	Price
headroom	66	+	0.6716	0.5497	0.5542	0.8969	Headroom (in.)
rep78	61	-	0.4874	0.3398	0.6040	0.9143	Repair Record 1978
trunk	69	+	0.7979	0.7144	0.5159	0.8818	Trunk space (cu. ft.)
weight	64	+	0.9404	0.9096	0.4747	0.8635	Weight (lbs.)
length	69	+	0.9382	0.9076	0.4725	0.8625	Length (in.)
turn	66	+	0.8678	0.8071	0.4948	0.8727	Turn Circle (ft.)
displacement	63	+	0.8992	0.8496	0.4852	0.8684	Displacement (cu. in.)
Test scale					0.5251	0.8984	mean(standardized items)

Users of alpha require some standard for judging values of  $\alpha$ . We paraphrase Nunnally and Bernstein (1994, 265): In the early stages of research, modest reliability of 0.70 or higher will suffice; values in excess of 0.80 often waste time and funds. In contrast, where measurements on individuals are of interest, a reliability of 0.80 may not be nearly high enough. Even with a reliability of 0.90, the standard error of measurement is almost one-third as large as the standard deviation of test scores; a reliability of 0.90 is the minimum that should be tolerated, and a reliability of 0.95 should be considered the desirable standard.

#### Stored results

alpha stores the following in r():

```
Scalars
                                 scale reliability coefficient
    r(alpha)
    r(k)
                                 number of items in the scale
    r(cov)
                                 average interitem covariance
    r(rho)
                                 average interitem correlation if std is specified
Matrices
    r(Alpha)
                                 scale reliability coefficient
    r(ItemTestCorr)
                                 item-test correlation
    r(ItemRestCorr)
                                 item-rest correlation
    r(MeanInterItemCov)
                                 average interitem covariance
    r(MeanInterItemCorr)
                                 average interitem correlation if std is specified
```

If the item option is specified, results are stored as row matrices for the k subscales when one variable is removed.

## Methods and formulas

Let  $x_i$ , i = 1, ..., k, be the variables over which  $\alpha$  is to be calculated. Let  $s_i$  be the sign with which  $x_i$  enters the scale. If asis is specified,  $s_i = 1$  for all i. Otherwise, principal-factor analysis is performed on  $x_i$ , and the first factor's score is predicted; see [MV] factor.  $s_i$  is -1 if correlation of the  $x_i$  and the predicted score is negative and +1 otherwise.

Let  $r_{ij}$  be the correlation between  $x_i$  and  $x_j$ ,  $c_{ij}$  be the covariance, and  $n_{ij}$  be the number of observations used in calculating the correlation or covariance. The average correlation is

$$\overline{r} = \frac{\sum_{i=2}^{k} \sum_{j=1}^{i-1} s_i s_j n_{ij} r_{ij}}{\sum_{i=2}^{k} \sum_{j=1}^{i-1} n_{ij}}$$

and the average covariance similarly is

$$\overline{c} = \frac{\sum_{i=2}^{k} \sum_{j=1}^{i-1} s_i s_j n_{ij} c_{ij}}{\sum_{i=2}^{k} \sum_{j=1}^{i-1} n_{ij}}$$

Let  $c_{ii}$  denote the variance of  $x_i$ , and define the average variance as

$$\overline{v} = \frac{\sum_{i=1}^{k} n_{ii} c_{ii}}{\sum_{i=1}^{k} n_{ii}}$$

If std is specified, the scale reliability  $\alpha$  is calculated as defined by the general form of the Spearman-Brown Prophecy Formula (Nunnally and Bernstein 1994, 232; Allen and Yen 1979, 85–88):

$$\alpha = \frac{k\overline{r}}{1 + (k-1)\overline{r}}$$

This expression corresponds to  $\alpha$  under the assumption that the summative rating is the sum of the standardized variables (Nunnally and Bernstein 1994, 234). If std is not specified,  $\alpha$  is defined (Nunnally and Bernstein 1994, 232 and 234) as

$$\alpha = \frac{k\overline{c}}{\overline{v} + (k-1)\overline{c}}$$

Let  $x_{ij}$  reflect the value of item i in the jth observation. If std is specified, the jth value of the scale computed from the k  $x_{ij}$  items is

$$S_j = \frac{1}{k_j} \sum_{i=1}^k s_i S(x_{ij})$$

where S() is the function that returns the standardized (mean 0, variance 1) value if  $x_{ij}$  is not missing and returns zero if  $x_{ij}$  is missing.  $k_j$  is the number of nonmissing values in  $x_{ij}$ ,  $i = 1, \ldots, k$ . If std is not specified, S() is the function that returns  $x_{ij}$  or returns missing if  $x_{ij}$  is missing.

Lee Joseph Cronbach (1916–2001) was an American psychometrician and educational psychologist who worked principally on measurement theory, program evaluation, and instruction. He taught and researched at the State College of Washington, the University of Chicago, the University of Illinois, and Stanford University. Cronbach's initial paper on alpha led to a theory of test reliability.

# Acknowledgment

This improved version of alpha was written by Jeroen Weesie of the Department of Sociology at Utrecht University, The Netherlands.

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#### Also see

[MV] **factor** — Factor analysis

[R] icc — Intraclass correlation coefficients

## **Title**

## **biplot** — Biplots

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

Acknowledgment References Also see

# **Description**

biplot displays a two-dimensional biplot of a dataset. A biplot simultaneously displays the observations (rows) and the relative positions of the variables (columns). Marker symbols (points) are displayed for observations, and arrows are displayed for variables. Observations are projected to two dimensions such that the distance between the observations is approximately preserved. The cosine of the angle between arrows approximates the correlation between the variables.

## **Quick start**

Biplot of v1, v2, v3, and v4

biplot v1 v2 v3 v4

As above, but use standardized instead of centered variables

biplot v1 v2 v3 v4, std

As above, but graph dimension 3 versus 1 instead of 2 versus 1

biplot v1 v2 v3 v4, std dim(3 1)

Biplot with separate row and column plots

biplot v1 v2 v3 v4, separate

Only graph the column plot

biplot v1 v2 v3 v4, norow

Biplot with different color row markers for each category of catvar

biplot v1 v2 v3 v4, rowover(catvar)

Label row observations using the values in variable mylabel

biplot v1 v2 v3 v4, rowlabel(mylabel)

Store biplot coordinates in new variables x and y

biplot v1 v2 v3 v4, generate(x y)

#### Menu

Statistics > Multivariate analysis > Biplot

# **Syntax**

$\texttt{biplot} \ \textit{varlist} \ \left[\textit{if}\ \right] \ \left[\textit{in}\ \right]$	[, options]
options	Description
Main	
rowover(varlist)	identify observations from different groups of <i>varlist</i> ; may not be combined with separate or norow
dim(# #)	two dimensions to be displayed; default is dim(2 1)
std	use standardized instead of centered variables
<pre>alpha(#)</pre>	row weight = $\#$ ; column weight = $1 - \#$ ; default is 0.5
<u>st</u> retch(#)	stretch the column (variable) arrows
<u>mah</u> alanobis	approximate Mahalanobis distance; implies alpha(0)
<u>xneg</u> ate	negate the data relative to the $x$ axis
ynegate	negate the data relative to the $y$ axis
<u>auto</u> aspect	adjust aspect ratio on the basis of the data; default aspect ratio is 1
<u>sep</u> arate	<pre>produce separate plots for rows and columns; may not be combined with rowover()</pre>
${f nograph}$	suppress graph
<u>tab</u> le	display table showing biplot coordinates
Rows	
<pre>rowopts(row_options)</pre>	affect rendition of rows (observations)
row#opts(row_options)	affect rendition of rows (observations) in the # group of varlist defined in rowover(); available only with rowover()
rowlabel(varname)	specify label variable for rows (observations)
norow	suppress row points; may not be combined with rowover()
$\underline{\underline{\mathtt{gen}}}\mathtt{erate}(\mathit{newvar}_x\ \mathit{newvar}_y)$	store biplot coordinates for observations in variables $newvar_x$ and $newvar_y$
Columns	
<pre>colopts(col_options)</pre>	affect rendition of columns (variables)
negcol	include negative column (variable) arrows
negcolopts(col_options)	affect rendition of negative columns (variables)
nocolumn	suppress column arrows
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by() documented in [G-3] twoway_options
	, opening once and of (, occurrence in [o o] occurry <b></b>
row_options	Description
marker_options	change look of markers (color, size, etc.)
marker_label_options	change look or position of marker labels
nolabel	remove the default row (variable) label from the graph
name(name)	override the default name given to rows (observations)

#### 20 biplot — Biplots

col_options	Description
<pre>pcarrow_options nolabel name(name)</pre>	affect the rendition of paired-coordinate arrows remove the default column (variable) label from the graph override the default name given to columns (variables)

See [G-2] graph twoway pcarrow.

# **Options**

Main

rowover(varlist) distinguishes groups among observations (rows) by highlighting observations on
the plot for each group identified by equal values of the variables in varlist. By default, the graph
contains a legend that consists of group names. rowover() may not be combined with separate
or norow.

dim(##) identifies the dimensions to be displayed. For instance, dim(3 2) plots the third dimension (vertically) versus the second dimension (horizontally). The dimension numbers cannot exceed the number of variables. The default is dim(2 1).

std produces a biplot of the standardized variables instead of the centered variables.

alpha(#) specifies that the variables be scaled by  $\lambda^{\#}$  and the observations by  $\lambda^{(1-\#)}$ , where  $\lambda$  are the singular values. It is required that  $0 \le \# \le 1$ . The most common values are 0, 0.5, and 1. The default is alpha(0.5) and is known as the symmetrically scaled biplot or symmetric factorization biplot. The result with alpha(1) is the principal-component biplot, also called the row-preserving metric (RPM) biplot. The biplot with alpha(0) is referred to as the column-preserving metric (CPM) biplot.

stretch(#) causes the length of the arrows to be multiplied by #. For example, stretch(1) would leave the arrows the same length, stretch(2) would double their length, and stretch(0.5) would halve their length.

mahalanobis implies alpha(0) and scales the positioning of points (observations) by  $\sqrt{n-1}$  and positioning of arrows (variables) by  $1/\sqrt{n-1}$ . This additional scaling causes the distances between observations to change from being approximately proportional to the Mahalanobis distance to instead being approximately equal to the Mahalanobis distance. Also, the inner products between variables approximate their covariance.

xnegate specifies that dimension-1 (x axis) values be negated (multiplied by -1).

ynegate specifies that dimension-2 (y axis) values be negated (multiplied by -1).

autoaspect specifies that the aspect ratio be automatically adjusted based on the range of the data to be plotted. This option can make some biplots more readable. By default, biplot uses an aspect ratio of one, producing a square plot. Some biplots will have little variation in the y-axis direction, and using the autoaspect option will better fill the available graph space while preserving the equivalence of distance in the x and y axes.

As an alternative to autoaspect, the  $twoway\_option$  aspectratio() can be used to override the default aspect ratio. biplot accepts the aspectratio() option as a suggestion only and will override it when necessary to produce plots with balanced axes; that is, distance on the x axis equals distance on the y axis.

twoway\_options, such as xlabel(), xscale(), ylabel(), and yscale(), should be used with caution. These axis\_options are accepted but may have unintended side effects on the aspect ratio. See [G-3] twoway\_options.

separate produces separate plots for the row and column categories. The default is to overlay the plots. separate may not be combined with rowover().

nograph suppresses displaying the graph.

table displays a table with the biplot coordinates.

Rows

rowopts (row\_options) affects the rendition of the points plotting the rows (observations). This option may not be combined with rowover(). The following row\_options are allowed:

*marker\_options* affect the rendition of markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] *marker\_options*.

marker\_label\_options specify the properties of marker labels; see [G-3] marker\_label\_options. mlabel() in rowopts() may not be combined with the rowlabel() option.

nolabel removes the default row label from the graph.

name (name) overrides the default name given to rows.

row#opts(row\_options) affects rendition of the points plotting the rows (observations) in the #th group
identified by equal values of the variables in varlist defined in rowover(). This option requires
specifying rowover(). See rowopts() above for the allowed row\_options, except mlabel() is
not allowed with row#opts().

rowlabel(varname) specifies label variable for rows (observations).

norow suppresses plotting of row points. This option may not be combined with rowover().

generate( $newvar_x$   $newvar_y$ ) stores biplot coordinates for rows in variables  $newvar_x$  and  $newvar_y$ .

Columns

colopts (col\_options) affects the rendition of the arrows and points plotting the columns (variables). The following col\_options are allowed:

pcarrow\_options affect the rendition of paired-coordinate arrows; see [G-2] graph twoway pcarrow.

nolabel removes the default column label from the graph.

name(name) overrides the default name given to columns.

negcol includes negative column (variable) arrows on the plot.

negcolopts (col\_options) affects the rendition of the arrows and points plotting the negative columns (variables). The col\_options allowed are given above.

nocolumn suppresses plotting of column arrows.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option). See autoaspect above for a warning against using options such as xlabel(), xscale(), ylabel(), and yscale().

# Remarks and examples

The biplot command produces what Cox and Cox (2001) refer to as the "classic biplot". Biplots were introduced by Gabriel (1971); also see Gabriel (1981). Gower and Hand (1996) discuss extensions and generalizations to biplots and place many of the well-known multivariate techniques into a generalized biplot framework extending beyond the classic biplot implemented by Stata's biplot command. Cox and Cox (2001), Jolliffe (2002), Gordon (1999), Jacoby (1998), Rencher and Christensen (2012), and Seber (1984) discuss the classic biplot. Kohler (2004) provides a Stata implementation of biplots.

Let X be the centered (or standardized if the std option is specified) data. A biplot splits the information in X into a portion related to the observations (rows of X) and a portion related to the variables (columns of X)

$$\mathbf{X} pprox (\mathbf{U}_2 \; \mathbf{\Lambda}_2^{lpha}) (\mathbf{V}_2 \; \mathbf{\Lambda}_2^{1-lpha})'$$

where  $0 \le \alpha \le 1$ ; see *Methods and formulas* for details.  $\mathbf{U}_2 \ \mathbf{\Lambda}_2^{\alpha}$  contains the plotting coordinates corresponding to observations (rows), and  $\mathbf{V}_2 \ \mathbf{\Lambda}_2^{1-\alpha}$  contains the plotting coordinates corresponding to variables (columns). In a biplot, the row coordinates are plotted as symbols, and the column coordinates are plotted as arrows from the origin.

The commonly used values for  $\alpha$  are 0, 0.5, and 1. The default is 0.5. The alpha() option allows you to set  $\alpha$ .

Biplots with an  $\alpha$  of 1 are also called principal-component biplots because  $U_2 \Lambda_2$  contains the principal-component scores and  $V_2$  contains the principal-component coefficients. Euclidean distance between points in this kind of biplot approximates the Euclidean distance between points in the original higher-dimensional space.

Using an  $\alpha$  of 0, Euclidean distances in the biplot are approximately proportional to Mahalanobis distances in the original higher-dimensional space. Also, the inner product of the arrows is approximately proportional to the covariances between the variables.

When you set  $\alpha$  to 0 and specify the mahalanobis option, the Euclidean distances are not just approximately proportional but are approximately equal to Mahalanobis distances in the original space. Likewise, the inner products of the arrows are approximately equal (not just proportional) to the covariances between the variables. This means that the length of an arrow is approximately equal to the standard deviation of the variable it represents. Also, the cosine of the angle between two arrows is approximately equal to the correlation between the two variables.

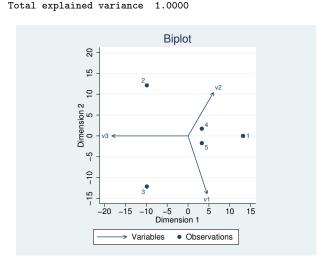
A biplot with an  $\alpha$  of 0.5 is called a symmetric factorization biplot or symmetrically scaled biplot. It often produces reasonable looking biplots where the points corresponding to observations and the arrows corresponding to variables are given equal weight. Using an  $\alpha$  of 0 (or 1) causes the points (or the arrows) to be bunched tightly around the origin while the arrows (or the points) are predominant in the graph. Here many authors recommend picking a scaling factor for the arrows to bring them back into balance. The stretch() option allows you to do this.

Regardless of your choice of  $\alpha$ , the position of a point in relation to an arrow indicates whether that observation is relatively large, medium, or small for that variable. Also, although the special conditions mentioned earlier may not strictly hold for all  $\alpha$ , the biplot still aids in understanding the relationship between the variables, the observations, and the observations and variables jointly.

#### Example 1

Gordon (1999, 176) provides a simple example of a biplot based on data having five rows and three columns.

```
. input v1 v2 v3
             v1
                        v2
                                    v3
  1.
       60
            80 -240
  2.
     -213
            66
                 180
      123 -186
                 180
       -9
            38
                 -60
  5.
       39
             2
                 -60
  6. end
. biplot v1 v2 v3
Biplot of 5 observations and 3 variables
    Explained variance by component 1
    Explained variance by component 2
```



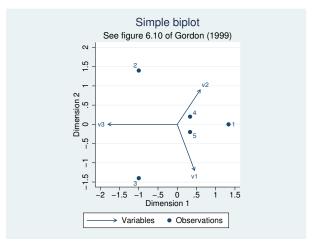
The first component accounts for 63% of the variance, and the second component accounts for the remaining 37%. All the variance is accounted for because, here, the 5-by-3 data matrix is only of rank 2.

Gordon actually used an  $\alpha$  of 0 and performed the scaling to better match Mahalanobis distance. We do the same using the options alpha(0) and mahalanobis. (We could just use mahalanobis because it implies alpha(0).) With an  $\alpha$  of 0, Gordon decided to scale the arrows by a factor of 0.01. We accomplish this with the stretch() option and add options to provide a title and subtitle in place of the default title obtained previously.

```
. biplot v1 v2 v3, alpha(0) mahalanobis stretch(.01) title(Simple biplot) > subtitle(See figure 6.10 of Gordon (1999))
Biplot of 5 observations and 3 variables

Explained variance by component 1 0.6283
Explained variance by component 2 0.3717

Total explained variance 1.0000
```



The outcome is little changed between the first and second biplot except for the additional titles and the scale of the x and y axes.

biplot allows you to highlight observations belonging to different groups by using option rowover(). Suppose our data come from two groups defined by variable group, group=1 and group=2.

- . generate byte group =  $cond(_n<3, 1, 2)$
- . list

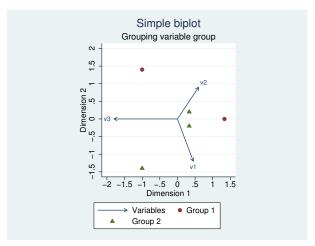
	v1	v2	v3	group
1.	60	80	-240	1
2.	-213	66	180	1
3.	123	-186	180	2
4.	-9	38	-60	2
5.	39	2	-60	2

Here is the previous biplot with group-specific markers:

- . biplot v1 v2 v3, alpha(0) mahalanobis stretch(.01) title(Simple biplot)
- > subtitle(Grouping variable group) rowover(group)
- > rowlopts(name("Group 1") msymbol(0) nolabel)
- > row2opts(name("Group 2") msymbol(T) nolabel)

Biplot of 5 observations and 3 variables

Explained variance by component 1 0.6283 Explained variance by component 2 0.3717 Total explained variance 1.0000



In the above example, groups are defined by a single variable group but you can specify multiple variables with rowover(). The rendition of group markers is controlled by options row1opts() and row2opts(). The marker labels are disabled by using the nolabel option.

4

# ▶ Example 2

Table 7.1 of Cox and Cox (2001) provides the scores of 10 Renaissance painters on four attributes using a scale from 0 to 20, as judged by Roger de Piles in the 17th century.

- . use http://www.stata-press.com/data/r14/renpainters, clear (Scores by Roger de Piles for Renaissance Painters)
- . list, abbrev(12)

	painter	composition	drawing	colour	expression
1.	Del Sarto	12	16	9	8
2.	Del Piombo	8	13	16	7
3.	Da Udine	10	8	16	3
4.	Giulio Romano	15	16	4	14
5.	Da Vinci	15	16	4	14
6.	Michelangelo	8	17	4	8
7.	Fr. Penni	0	15	8	0
8.	Perino del Vaga	15	16	7	6
9.	Perugino	4	12	10	4
10.	Raphael	17	18	12	18

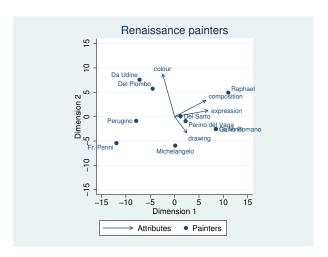
- . biplot composition-expression, alpha(1) stretch(10) table
- > rowopts(name(Painters)) rowlabel(painter) colopts(name(Attributes))
- > title(Renaissance painters)

Biplot of 10 painters and 4 attributes

Explained variance by component 1 0.6700 Explained variance by component 2 0.2375 Total explained variance 0.9075

Biplot coordinates

Painters	dim1	dim2
Del Sarto	1.2120	0.0739
Del Piombo	-4.5003	5.7309
Da Udine	-7.2024	7.5745
Giulio Rom~o	8.4631	-2.5503
Da Vinci	8.4631	-2.5503
Michelangelo	0.1284	-5.9578
Fr Penni	-11.9449	-5.4510
Perino del~a	2.2564	-0.9193
Perugino	-7.8886	-0.8757
Raphael	11.0131	4.9251
Attributes	dim1	dim2
composition	6.4025	3.3319
drawing	2.4952	-3.3422
colour	-2.4557	8.7294
expression	6.8375	1.2348

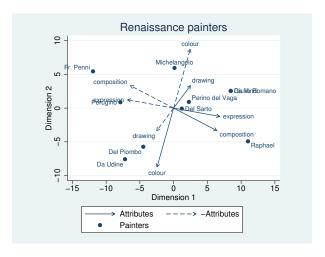


alpha(1) gave us an  $\alpha$  of 1. stretch(10) made the arrows 10 times longer. table requested that the biplot coordinate table be displayed. rowopts() and colopts() affected the rendition of the rows (observations) and columns (variables). The name() suboption provided a name to use instead of the default names "Observations" and "Variables" in the graph legend and in the biplot coordinate table. The rowlabel(painter) option requested that the variable painter be used to label the row points (observations) in both the graph and table. The title() option was used to override the default title.

The default is to produce a square graphing region. Because the x axis containing the first component has more variability than the y axis containing the second component, there are often

no observations or arrows appearing in the upper and lower regions of the graph. The autoaspect option sets the aspect ratio and the x-axis and y-axis scales so that more of the graph region is used while maintaining the equivalent interpretation of distance for the x and y axes.

Here is the previous biplot with the omission of the table option and the addition of the autoaspect option. We also add the ynegate option to invert the orientation of the data in the y-axis direction to match the orientation shown in figure 7.1 of Cox and Cox (2001). We add the negcol option to include column (variable) arrows pointing in the negative directions, and the rendition of these negative columns (variables) is controlled by negcolopts().



# Stored results

biplot stores the following in r():

```
Scalars
    r(rho1)
                    explained variance by component 1
    r(rho2)
                    explained variance by component 2
    r(rho)
                    total explained variance
    r(alpha)
                    value of alpha() option
Matrices
    r(U)
                    biplot coordinates for the observations; stored only if the row dimension
                       does not exceed Stata's maximum matrix size; as an alternative, use
                       generate() to store biplot coordinates for the observations in variables
    r(V)
                    biplot coordinates for the variables
    r(Vstretch)
                    biplot coordinates for the variables times stretch() factor
```

4

#### Methods and formulas

Let X be the centered (standardized if std is specified) data with N rows (observations) and p columns (variables). A biplot splits the information in X into a portion related to the observations (rows of X) and a portion related to the variables (columns of X). This task is done using the singular value decomposition (SVD).

$$\mathbf{X} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}'$$

The biplot formula is derived from this SVD by first splitting  $\Lambda$ , a diagonal matrix, into

$$\Lambda = \Lambda^{\alpha} \Lambda^{1-\alpha}$$

and then retaining the first two columns of U, the first two columns of V, and the first two rows and columns of  $\Lambda$ . Using the subscript 2 to denote this, the biplot formula is

$$\mathbf{X} \approx \mathbf{U}_2 \, \mathbf{\Lambda}_2^{\alpha} \, \mathbf{\Lambda}_2^{1-\alpha} \, \mathbf{V}_2'$$

where  $0 \le \alpha \le 1$ . This is then written as

$$\mathbf{X} \approx (\mathbf{U}_2 \, \mathbf{\Lambda}_2^{\alpha}) (\mathbf{V}_2 \, \mathbf{\Lambda}_2^{1-\alpha})'$$

 $\mathbf{U}_2$   $\mathbf{\Lambda}_2^{\alpha}$  contains the plotting coordinates corresponding to observations (rows) and  $\mathbf{V}_2$   $\mathbf{\Lambda}_2^{1-\alpha}$  contains the plotting coordinates corresponding to variables (columns). In a biplot, the row coordinates are plotted as symbols and the column coordinates are plotted as arrows from the origin.

Let  $\lambda_i$  be the *i*th diagonal of  $\Lambda$ . The explained variance for component 1 is

$$\rho_1 = \left\{ \sum_{i=1}^p \lambda_i^2 \right\}^{-1} \lambda_1^2$$

and for component 2 is

$$\rho_2 = \left\{ \sum_{i=1}^p \lambda_i^2 \right\}^{-1} \lambda_2^2$$

The total explained variance is

$$\rho = \rho_1 + \rho_2$$

# Acknowledgment

Several biplot options were based on the work of Ulrich Kohler (2004) of Methoden der Empirischen Sozialforschung at Universität Potsdam, Germany, and coauthor of the Stata Press book Data Analysis Using Stata.

Kuno Ruben Gabriel (1929–2003) was born in Germany, raised in Israel, and studied at the London School of Economics and the Hebrew University of Jerusalem, earning a doctorate in demography in 1957. After several years on the faculty at the Hebrew University, he moved to the University of Rochester in 1975. His wide-ranging statistical interests spanned applications in meteorology, including weather-modification experiments, and medicine. Gabriel's best-known contribution is the biplot.

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## Also see

[MV] ca — Simple correspondence analysis

[MV] mds — Multidimensional scaling for two-way data

[MV] **pca** — Principal component analysis

#### **Title**

**ca** — Simple correspondence analysis

Description

Quick start

Menu

Syntax

Options References Remarks and examples Also see Stored results

Methods and formulas

# **Description**

ca performs a simple correspondence analysis (CA) and optionally creates a biplot of two categorical variables or multiple crossed variables. camat is similar to ca but is for use with a matrix containing cross-tabulations or other nonnegative values with strictly increasing margins.

#### **Quick start**

Simple correspondence analysis of two categorical variables

Correspondence analysis of the cross-tabulation with rows catvar1 and columns catvar2

ca catvar1 catvar2

Also produce the correspondence analysis biplot

ca catvar1 catvar2, plot

Increase the number of dimensions from 2 to 3

ca catvar1 catvar2, dimensions(3)

Use row and column principal coordinate normalization

ca catvar1 catvar2, normalize(principal)

Simple correspondence analysis with crossed (stacked) variables

Correspondence analysis of the cross-tabulation of rows catvar1 and crossed columns mycol from the crossed variables catvar2 and catvar3

```
ca catvar1 (mycol: catvar2 catvar3)
```

As above, but display compact tables and produce the correspondence analysis biplot

```
ca catvar1 (mycol: catvar2 catvar3), compact plot
```

Simple correspondence analysis of a matrix

Correspondence analysis of the cross-tabulations contained in matrix M

camat M

Also produce the correspondence analysis biplot

camat M, plot

## Menu

са

Statistics > Multivariate analysis > Correspondence analysis > Two-way correspondence analysis (CA)

#### camat

Statistics > Multivariate analysis > Correspondence analysis > Two-way correspondence analysis of a matrix

# **Syntax**

Simple correspondence analysis of two categorical variables

```
ca rowvar colvar [if] [in] [weight] [, options]
```

Simple correspondence analysis with crossed (stacked) variables

```
ca row\_spec\ col\_spec\ [if]\ [in]\ [weight]\ [,\ options]
```

Simple correspondence analysis of an  $n_r \times n_c$  matrix

```
camat matname [, options]
```

where  $spec = varname \mid (newvar : varlist)$ 

and matname is an  $n_r \times n_c$  matrix with  $n_r$ ,  $n_c \ge 2$ .

options	Description
Model 2	
<pre>dimensions(#)</pre>	number of dimensions (factors, axes); default is dim(2)
<pre>normalize(nopts)</pre>	normalization of row and column coordinates
$\underline{\mathtt{rows}}\mathtt{upp}(\mathit{matname}_r)$	matrix of supplementary rows
$\underline{\mathtt{cols}}\mathtt{upp}(\mathit{matname}_c)$	matrix of supplementary columns
rowname(string)	label for rows
<pre>colname(string)</pre>	label for columns
missing	treat missing values as ordinary values (ca only)
Codes (ca only)	
$report(\underline{v}ariables)$	report coding of crossing variables
report( <u>c</u> rossed)	report coding of crossed variables
report( <u>a</u> ll)	report coding of crossing and crossed variables
length(min)	use minimal length unique codes of crossing variables
length(#)	use # as coding length of crossing variables
Reporting	
ddimensions(#)	number of singular values to be displayed; default is ddim(.)
norowpoints	suppress table with row category statistics
nocolpoints	suppress table with column category statistics
compact	display tables in a compact format
plot	plot the row and column coordinates
<pre>maxlength(#)</pre>	maximum number of characters for labels; default is maxlength(12)

nopts	Description
symmetric	symmetric coordinates (canonical); the default
<u>st</u> andard	row and column standard coordinates
<u>ro</u> w	row principal, column standard coordinates
<u>co</u> lumn	column principal, row standard coordinates
principal	row and column principal coordinates
#	power $0 \le \# \le 1$ for row coordinates; seldom used

bootstrap, by, jackknife, rolling, and statsby are allowed with ca; see [U] 11.1.10 Prefix commands. However, bootstrap and jackknife results should be interpreted with caution; identification of the ca parameters involves data-dependent restrictions, possibly leading to badly biased and overdispersed estimates (Milan and Whittaker 1995).

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

fweights, aweights, and iweights are allowed with ca; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

## **Options**

Model 2

- dimensions (#) specifies the number of dimensions (= factors = axes) to be extracted. The default is dimensions(2). If you may specify dimensions(1), the row and column categories are placed on one dimension. # should be strictly smaller than the number of rows and the number of columns, counting only the active rows and columns, excluding supplementary rows and columns (see options rowsupp() and colsupp()).
  - CA is a hierarchical method, so extracting more dimensions does not affect the coordinates and decomposition of inertia of dimensions already included. The percentages of inertia accounting for the dimensions are in decreasing order as indicated by singular values. The first dimension accounts for the most inertia, followed by the second dimension, and then the third dimension, etc.
- normalize(nopt) specifies the normalization method, that is, how the row and column coordinates are obtained from the singular vectors and singular values of the matrix of standardized residuals. See Normalization and interpretation of correspondence analysis in Remarks and examples for a discussion of these different normalization methods.
  - symmetric, the default, distributes the inertia equally over rows and columns, treating the rows and columns symmetrically. The symmetric normalization is also known as the standard, or canonical, normalization. This is the most common normalization when making a biplot. normalize(symmetric) is equivalent to normalize(0.5). canonical is a synonym for symmetric.
  - standard specifies that row and column coordinates should be in standard form (singular vectors divided by the square root of mass). This normalization method is not equivalent to normalize(#) for any #.
  - row specifies principal row coordinates and standard column coordinates. This option should be chosen if you want to compare row categories. Similarity of column categories should not be interpreted. The biplot interpretation of the relationship between row and column categories is appropriate. normalize(row) is equivalent to normalize(1).
  - column specifies principal column coordinates and standard row coordinates. This option should be chosen if you want to compare column categories. Similarity of row categories should not be interpreted. The biplot interpretation of the relationship between row and column categories is appropriate. normalize(column) is equivalent to normalize(0).
  - principal is the normalization to choose if you want to make comparisons among the row categories and among the column categories. In this normalization, comparing row and column points is not appropriate. Thus a biplot in this normalization is best avoided. In the principal normalization, the row and column coordinates are obtained from the left and right singular vectors, multiplied by the singular values. This normalization method is not equivalent to normalize(#) for any #.
  - #,  $0 \le \# \le 1$ , is seldom used; it specifies that the row coordinates are obtained as the left singular vectors multiplied by the singular values to the power #, whereas the column coordinates equal the right singular vectors multiplied by the singular values to the power 1 #.
- rowsupp ( $matname_r$ ) specifies a matrix of supplementary rows.  $matname_r$  should have  $n_c$  columns. The row names of  $matname_r$  are used for labeling. Supplementary rows do not affect the computation of the dimensions and the decomposition of inertia. They are, however, included in the plots and in the table with statistics of the row points. Because supplementary points do not contribute to the dimensions, their entries under the column labeled contrib are left blank.

- colsupp( $matname_c$ ) specifies a matrix of supplementary columns.  $matname_c$  should have  $n_r$  rows. The column names of  $matname_c$  are used for labeling. Supplementary columns do not affect the computation of the dimensions and the decomposition of inertia. They are, however, included in the plots and in the table with statistics of the column points. Because supplementary points do not contribute to the dimensions, their entries under the column labeled contrib are left blank.
- rowname(string) specifies a label to refer to the rows of the matrix. The default is rowname(rowvar) for ca and rowname(rows) for camat.
- colname(string) specifies a label to refer to the columns of the matrix. The default is colname(colvar) for ca and colname(columns) for camat.
- missing, allowed only with ca, treats missing values of *rowvar* and *colvar* as ordinary categories to be included in the analysis. Observations with missing values are omitted from the analysis by default.

Codes

- report(opt) displays coding information for the crossing variables, crossed variables, or both. report() is ignored if you do not specify at least one crossed variable.
  - report(variables) displays the coding schemes of the crossing variables, that is, the variables used to define the crossed variables.
  - report(crossed) displays a table explaining the value labels of the crossed variables.
  - report(all) displays the codings of the crossing and crossed variables.
- length(opt) specifies the coding length of crossing variables.
  - length(min) specifies that the minimal-length unique codes of crossing variables be used.
  - length(#) specifies that the coding length # of crossing variables be used, where # must be between 4 and 32.

Reporting

- ddimensions(#) specifies the number of singular values to be displayed. The default is ddimensions(.), meaning all.
- norowpoints suppresses the table with row point (category) statistics.
- nocolpoints suppresses the table with column point (category) statistics.
- compact specifies that the table with point statistics be displayed multiplied by 1,000 as proposed by Greenacre (2007), enabling the display of more columns without wrapping output. The compact tables can be displayed without wrapping for models with two dimensions at line size 79 and with three dimensions at line size 99.
- plot displays a plot of the row and column coordinates in two dimensions. With row principal normalization, only the row points are plotted. With column principal normalization, only the column points are plotted. In the other normalizations, both row and column points are plotted. You can use cabiplot directly if you need another selection of points to be plotted or if you want to otherwise refine the plot; see [MV] ca postestimation plots.
- maxlength(#) specifies the maximum number of characters for row and column labels in plots. The default is maxlength(12).

Note: The reporting options may be specified during estimation or replay.

## Remarks and examples

Remarks are presented under the following headings:

Introduction
A first example
How many dimensions?
Statistics on the points
Normalization and interpretation of correspondence analysis
Plotting the points
Supplementary points
Matrix input
Crossed variables

#### Introduction

Correspondence analysis (CA) offers a geometric representation of the rows and columns of a two-way frequency table that is helpful in understanding the similarities between the categories of variables and the association between the variables. CA is formally equivalent to various other geometric approaches, including dual scaling, reciprocal averaging, and canonical correlation analysis of contingency tables (Greenacre 1984, chap. 4). For an informal introduction to CA and related metric approaches, see Weller and Romney (1990). Greenacre (2007) provides a much more thorough introduction with few mathematical prerequisites. More advanced treatments are given by Greenacre (1984) and Gower and Hand (1996).

In some respects, CA can be thought of as an analogue to principal components for nominal variables. It is also possible to interpret CA in reciprocal averaging (Greenacre 1984, 96–102; Cox and Cox 2001, 193–200), in optimal scaling (Greenacre 1984, 102–108), and in canonical correlations (Greenacre 1984, 108–116; Gower and Hand 1996, 183–185). Scaling refers to the assignment of scores to the categories of the row and column variables. Different criteria for the assignment of scores have been proposed, generally with different solutions. If the aim is to maximize the correlation between the scored row and column, the problem can be formulated in terms of CA. The optimal scores are the coordinates on the first dimension. The coordinates on the second and subsequent dimensions maximize the correlation between row and column scores subject to orthogonality constraints. See also [MV] ca postestimation.

## A first example

## Example 1: A well-known correspondence analysis example

We illustrate CA with an example of smoking behavior by different ranks of personnel. This example is often used in the CA literature (for example, Greenacre 1984, 55; Greenacre 2007, 66), so you have probably encountered these (artificial) data before. By using these familiar data, we make it easier to relate the literature on CA to the output of the ca command.

- . use http://www.stata-press.com/data/r14/ca\_smoking
- . tabulate rank smoking

rank	none	smoking light	intensity medium	heavy	Total
senior_mngr	4	2	3	2	11
junior_mngr	4	3	7	4	18
senior_empl	25	10	12	4	51
junior_empl	18	24	33	13	88
secretary	10	6	7	2	25
Total	61	45	62	25	193

ca displays the results of a CA on two categorical variables in a multipanel format.

. ca rank smoking

espondence an 5 active rows 4 active colu	5	Number of o Pearson chi Prob > chi2 Total inert Number of d Expl. inert	2(12) = = ia = im. =	193 16.44 0.1718 0.0852 2 99.51	
Dimension	singular value	principal inertia	chi2	percent	cumul percent
dim 1 dim 2 dim 3	.2734211 .1000859 .0203365	.0747591 .0100172 .0004136	14.43 1.93 0.08	87.76 11.76 0.49	87.76 99.51 100.00
total		.0851899	16.44	100	

Statistics for row and column categories in symmetric normalization

		overall		d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
rank						
senior mngr	0.057	0.893	0.031	0.126	0.092	0.003
junior mngr	0.093	0.991	0.139	-0.495	0.526	0.084
senior empl	0.264	1.000	0.450	0.728	0.999	0.512
junior empl	0.456	1.000	0.308	-0.446	0.942	0.331
secretary	0.130	0.999	0.071	0.385	0.865	0.070
smoking						
none	0.316	1.000	0.577	0.752	0.994	0.654
light	0.233	0.984	0.083	-0.190	0.327	0.031
medium	0.321	0.983	0.148	-0.375	0.982	0.166
heavy	0.130	0.995	0.192	-0.562	0.684	0.150

	dimension_2					
Categories	coord	sqcorr	contrib			
rank						
senior mngr	0.612	0.800	0.214			
junior mngr	0.769	0.465	0.551			
senior empl	0.034	0.001	0.003			
junior empl	-0.183	0.058	0.152			
secretary	-0.249	0.133	0.081			
smoking						
none	0.096	0.006	0.029			
light	-0.446	0.657	0.463			
medium	-0.023	0.001	0.002			
heavy	0.625	0.310	0.506			

The order in which we specify the variables is mostly immaterial. The first variable (rank) is also called the row variable, and the second (smoking) is the column variable. This ordering is important only as far as the interpretation of some options and some labeling of output are concerned. For instance, the option norowpoints suppresses the table with row points, that is, the categories of rank. ca requires two integer-valued variables. The rankings of the categories and the actual values used to code categories are not important. Thus, rank may be coded 1, 2, 3, 4, 5, or 0, 1, 4, 9, 16, or -2, -1, 0, 1, 2; it does not matter. We do suggest assigning value labels to the variables to improve the interpretability of tables and plots.

Correspondence analysis seeks to offer a low-dimensional representation describing how the row and column categories contribute to the inertia in a table. ca reports Pearson's test of independence, just like tabulate with the chi2 option. Inertia is Pearson's chi-squared statistic divided by the sample size, 16.44/193 = 0.0852. Pearson's chi-squared test has significance level p = 0.1718, casting doubt on any association between rows and columns. Still, given the prominence of this example in the CA literature, we will continue.

The first panel produced by ca displays the decomposition of total inertia in orthogonal dimensions—analogous to the decomposition of the total variance in principal component analysis (see [MV] pca). The first dimension accounts for 87.76% of the inertia; the second dimension accounts for 11.76% of the inertia. Because the dimensions are orthogonal, we may add the contributions of the two dimensions and say that the two leading dimensions account for 87.76% + 11.76% = 99.52% of the total inertia. A two-dimensional representation seems in order. The remaining output is discussed later.

### How many dimensions?

#### Example 2: Specifying the number of dimensions

In the first example with the smoking data, we displayed coordinates and statistics for a twodimensional approximation of the rows and columns. This is the default. We can specify more or fewer dimensions with the option dimensions (). The maximum number is  $\min(n_r - 1, n_c - 1)$ . At this maximum, the chi-squared distances between the rows and columns are exactly represented by CA; 100% of the inertia is accounted for. This is called the saturated model; the fitted values of the CA model equal the observed correspondence table.

The minimum number of dimensions is one; the model with zero dimensions would be a model of independence of the rows and columns. With one dimension, the rows and columns of the table are identified by points on a line, with distance on the line approximating the chi-squared distance in the table, and a biplot is no longer feasible.

. ca rank smokin	g, dim(1)				
Correspondence a	nalysis		Number of o	bs =	193
-	•		Pearson chi	2(12) =	16.44
			Prob > chi2	=	0.1718
			Total inert	ia =	0.0852
5 active row	S		Number of d	im. =	1
4 active col	umns		Expl. inert	ia (%) =	87.76
	singular	principal			cumul
Dimension	value	inertia	chi2	percent	percent
dim 1	.2734211	.0747591	14.43	87.76	87.76
dim 2	.1000859	.0100172	1.93	11.76	99.51
dim 3	.0203365	.0004136	0.08	0.49	100.00
total		.0851899	16.44	100	

Statistics for row and column categories in symmetric normalization

	overall			dimension_1		
Categories	mass	quality	%inert	coord	sqcorr	contrib
rank						
senior mngr	0.057	0.092	0.031	0.126	0.092	0.003
junior mngr	0.093	0.526	0.139	-0.495	0.526	0.084
senior empl	0.264	0.999	0.450	0.728	0.999	0.512
junior empl	0.456	0.942	0.308	-0.446	0.942	0.331
secretary	0.130	0.865	0.071	0.385	0.865	0.070
smoking						
none	0.316	0.994	0.577	0.752	0.994	0.654
light	0.233	0.327	0.083	-0.190	0.327	0.031
medium	0.321	0.982	0.148	-0.375	0.982	0.166
heavy	0.130	0.684	0.192	-0.562	0.684	0.150

The first panel produced by ca does not depend on the number of dimensions extracted; thus, we will always see all singular values and the percentage of inertia explained by the associated dimensions. In the second panel, the only thing that depends on the number of dimensions is the overall quality of the approximation. The overall quality is the sum of the quality scores on the extracted dimensions and so increases with the number of extracted dimensions. The higher the quality, the better the chi-squared distances with other rows (columns) are represented by the extracted number of dimensions. In a saturated model, the overall quality is 1 for each row and column category.

So, how many dimensions should we retain? It is common for researchers to extract the minimum number of dimensions in a CA to explain at least 90% of the inertia, analogous to similar heuristic rules on the number of components in principal component analysis. We could probably also search for a scree, the number of dimensions where the singular values flatten out (see [MV] screeplot). A screeplot of the singular values can be obtained by typing

. screeplot e(Sv)
 (output omitted)

where e(Sv) is the name where ca has stored the singular values.

1

## Statistics on the points

#### Example 3: A more compact table of row and column statistics

We now turn our attention to the second panel. The overall section of the panel lists the following statistics:

- The mass of the category, that is, the proportion in the marginal distribution. The masses of all categories of a variable add up to 1.
- The quality of the approximation for a category, expressed as a number between 0 (very bad) and 1 (perfect). In a saturated model, quality is 1.
- The percentage of inertia contained in the category. Categories are divided through by the total inertia; the inertias of the categories of a variable add up to 100%.

For each of the dimensions, the panel lists the following:

- The coordinate of the category.
- The squared residuals between the profile and the categories. The sum of the squared residuals over the dimensions adds up to the quality of the approximation for the category.
- The contribution made by the categories to the dimensions. These add up to 1 over all categories of a variable.

The table with point statistics becomes pretty large, especially with more than two dimensions. ca can also list the second panel in a more compact form, saving space by multiplying all entries by 1,000; see Greenacre (2007).

. ca rank smoking, dim(2) compact Correspondence analysis Number of obs 193 Pearson chi2(12) 16.44 Prob > chi2 0.1718 Total inertia = 0.0852 5 active rows Number of dim. 2 Expl. inertia (%) = 99.51 4 active columns

	Dimension	singular value	principal inertia	chi2	percent	cumul percent
-	dim 1 dim 2 dim 3	.2734211 .1000859 .0203365	.0747591 .0100172 .0004136	00172 1.93		87.76 99.51 100.00
-	total	.020000	.0851899	16.44	100	

overall dimension 1								ension	2
Categories	mass	qualt	%inert	coord	sqcor	contr	coord	sqcor	contr
rank									
senior mngr	57	893	31	126	92	3	612	800	214
junior mngr	93	991	139	-495	526	84	769	465	551
senior empl	264	1000	450	728	999	512	34	1	3
junior empl	456	1000	308	-446	942	331	-183	58	152
secretary	130	999	71	385	865	70	-249	133	81
smoking									
none	316	1000	577	752	994	654	96	6	29
light	233	984	83	-190	327	31	-446	657	463
medium	321	983	148	-375	982	166	-23	1	2
heavy	130	995	192	-562	684	150	625	310	506

Statistics for row and column categories in symmetric norm. (x 1000)

#### 1

### Normalization and interpretation of correspondence analysis

The normalization method used in CA determines whether and how the similarity of the row categories, the similarity of the column categories, and the relationship (association) between the row and column variables can be interpreted in terms of the row and column coordinates and the origin of the plot.

How does one compare row points—provided that the normalization method allows such a comparison? Formally, the Euclidean distance between the row points approximates the chi-squared distances between the corresponding row profiles. Thus in the biplot, row categories mapped close together have similar row profiles; that is, the distributions on the column variable are similar. Row categories mapped widely apart have dissimilar row profiles. Moreover, the Euclidean distance between a row point and the origin approximates the chi-squared distance from the row profile and the row centroid, so it indicates how different a category is from the population.

An analogous interpretation applies to column points.

For the association between the row and column variables: in the CA biplot, you should not interpret the distance between a row point r and a column point c as the relationship of r and c. Instead, think in terms of the vectors origin to r (OR) and origin to c (OC). Remember that CA decomposes scaled deviations d(r,c) from independence and d(r,c) is approximated by the inner product of OR and OC. The larger the absolute value of d(r,c), the stronger the association between r and c. In geometric terms, d(r,c) can be written as the product of the length of OR, the length of OC, and the cosine of the angle between OR and OC.

What does this mean? First, consider the effects of the angle. The association in (r,c) is strongly positive if OR and OC point in roughly the same direction; the frequency of (r,c) is much higher than expected under independence, so r tends to flock together with c—if the points r and c are close together. Similarly, the association is strongly negative if OR and OC point in opposite directions. Here the frequency of (r,c) is much lower than expected under independence, so r and c are unlikely to occur simultaneously. Finally, if OR and OC are roughly orthogonal (angle =  $\pm 90$ ), the deviation from independence is small.

Second, the association of r and c increases with the lengths of OR and OC. Points far from the origin tend to have large associations. If a category is mapped close to the origin, all its associations with categories of the other variable are small: its distribution resembles the marginal distribution.

Here are the interpretations enabled by the main normalization methods as specified in the normalize() option.

Normalization	Similarity	Similarity	Association
method	row cat.	column cat.	row vs. column
symmetric	No	No	Yes
principal	Yes	Yes	No
row	Yes	No	Yes
column	No	Yes	Yes

If we say that a comparison between row categories or between column categories is not possible, we really mean that the chi-squared distance between row profiles or column profiles is actually approximated by a weighted Euclidean distance between the respective plots in which the weights depend on the inertia of the dimensions rather than on the standard Euclidean distance.

You may want to do a CA in principal normalization to study the relationship between the categories of a variable and do a CA in symmetric normalization to study the association of the row and column categories.

### Plotting the points

#### Example 4: A correspondence biplot

In our discussion of normalizations, we stated that CA offers simple geometric interpretations to the similarity of categories and the association of the variables. We may specify the option plot with ca during estimation or during replay.

dim 2

dim 3

total

.1000859

.0203365

. ca, norowpoin	t nocolpoint pl	.ot			
Correspondence analysis			Number of o Pearson chi Prob > chi2 Total inert	2(12) =	193 16.44 0.1718 0.0852
5 active ro		Number of d Expl. inert	2 99.51		
Dimension	singular value	principal inertia	chi2	percent	cumul percent
dim 1	.2734211	.0747591	14.43	87.76	87.76

.0100172

.0004136

.0851899

1.93

0.08

16.44

11.76

100

0.49

Correspondence analysis biplot
●junior_mngr  ♣ heavy ● senior_mngr
A none  Senior_empl  A none  Senior_empl
Amedium  ● junior_empl  ● secretary
-15 0 .5 1 Dimension 1 (87.8%)

The options norowpoint and nocolpoint suppress the large tables of statistics for the rows and columns. If we did not request the plot during estimation, we can still obtain it with the cabiplot postestimation command. Unlike requesting the plot at estimation time, cabiplot allows us to fine-tune the plot; see [MV] ca postestimation plots.

The horizontal dimension seems to distinguish smokers from nonsmokers, whereas the vertical dimensions can be interpreted as intensity of smoking. Because the orientations from the origin to none and from the origin to senior\_empl are so close, we conclude that senior employees tend not to smoke. Similarly, junior managers tend to be heavy smokers, and junior employees tend to be medium smokers.

# Supplementary points

A useful feature of CA is the ability to locate supplementary rows and columns in the space generated by the "active" rows and columns (see Greenacre [1984, 70-74]; Greenacre [2007, chap. 12], for an extensive discussion). Think of supplementary rows and columns as having mass 0; therefore, supplementary points do not influence the approximating space—their contribution values are zero.

1

99.51

100.00

### Example 5: Supplementary rows and columns

In our example, we want to include the national distribution of smoking intensity as a supplementary row.

ca requires that we define the supplementary row distributions as rows of a matrix. In this example, we have only one supplementary row, with the percentages of the smoking categories in a national sample. The matrix should have one row per supplementary row category and as many columns as there are active columns. We define the row name to obtain appropriately labeled output.

```
. matrix S_row = (42, 29, 20, 9)
. matrix rowname S_row = national
```

Before we show the CA analysis with the supplementary row, we also include two supplementary columns for the rank distribution of alcoholic beverage drinkers and nondrinkers. It will be interesting to see where smoking is located relative to drinking and nondrinking.

. matrix colnames S\_col = nondrink drink

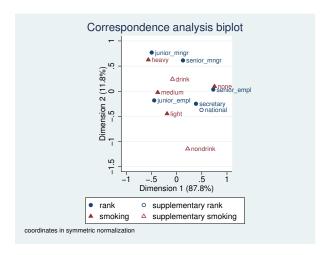
We now invoke ca, specifying the names of the matrices with supplementary rows and columns with the options rowsupp() and colsupp().

. ca rank smoking, rowsupp(S\_row) colsupp(S\_col) plot

				_		
Corr	espondence ar	nalysis		Number of o	bs =	193
	-	•		Pearson chi	2(12) =	16.44
				Prob > chi2	=	0.1718
				Total inert	ia =	0.0852
	5 active + 1	supplementary	rows	Number of d	im. =	2
	4 active + 2	supplementary	columns	Expl. inert	ia (%) =	99.51
		singular	principal			cumul
	Dimension	value	inertia	chi2	percent	percent
	dim 1	.2734211	.0747591	14.43	87.76	87.76
	dim 2	.1000859	.0100172	1.93	11.76	99.51
	dim 3	.0203365	.0004136	0.08	0.49	100.00
	total		.0851899	16.44	100	

Statistics for row and column categories in symmetric normalization  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

				,		
		overall		1	imension_	
Categories	mass	quality	%inert	coord	sqcorr	contrib
rank						
senior mngr	0.057	0.893	0.031	0.126	0.092	0.003
junior mngr	0.093	0.991	0.139	-0.495	0.526	0.084
senior empl	0.264	1.000	0.450	0.728	0.999	0.512
junior empl	0.456	1.000	0.308	-0.446	0.942	0.331
secretary	0.130	0.999	0.071	0.385	0.865	0.070
suppl_rows						
national	0.518	0.761	0.644	0.494	0.631	
smoking						
none	0.316	1.000	0.577	0.752	0.994	0.654
light	0.233	0.984	0.083	-0.190	0.327	0.031
medium	0.321	0.983	0.148	-0.375	0.982	0.166
heavy	0.130	0.995	0.192	-0.562	0.684	0.150
suppl_cols						
nondrink	0.119	0.439	0.460	0.220	0.040	
drink	0.881	0.838	0.095	-0.082	0.202	
	l d	imension_	2			
Categories	coord	sqcorr	contrib			
rank						
senior mngr	0.612	0.800	0.214			
junior mngr	0.769	0.465	0.551			
senior empl	0.034	0.001	0.003			
junior empl	-0.183	0.058	0.152			
secretary	-0.249	0.133	0.081			
suppl_rows						
national	-0.372	0.131				
smoking						
none	0.096	0.006	0.029			
light	-0.446	0.657	0.463			
medium	-0.023	0.001	0.002			
heavy	0.625	0.310	0.506			
suppl_cols						
nondrink	-1.144	0.398				
drink	0.241	0.636				
	1					



The first panel and the information about the five active rows and the four active columns have not changed—the approximating space is fully determined by the active rows and columns and is independent of the location of the supplementary rows and columns.

The table with statistics for the row and column categories now also contains entries for the supplementary rows and columns. The contrib entries for the supplementary points are blank. Supplementary points do not "contribute to" the location of the dimensions—their contribution is 0.000, but displaying blanks makes the point more clearly. All other columns for the supplementary points are informative. The inertia of supplementary points is the chi-squared distance to the respective centroid. The coordinates of supplementary points are obtained by applying the transition equations of the CA. Correlations of the supplementary profiles with the dimensions are also well defined. Finally, we may consider the quality of the two-dimensional approximation for the supplementary points. These are lower than for the active points, which will be the case in most applications—the active points exercise influence on the dimensions to improve their quality, whereas the supplementary points simply have to accept the dimensions as determined by the active points.

If we look at the biplot, the supplementary points are shown along with the active points. We may interpret the supplementary points just like the active points. Secretaries are close to the national sample in terms of smoking. Drinking alcohol is closer to the smoking categories than to nonsmoking, indicating that alcohol consumption and smoking are similar behaviors—but concluding that the *same* people smoke and drink is not possible because we do not have three-way data.

4

# Matrix input

## Example 6: Correspondence analysis of a frequency table

If we want to do a CA of a published two-way frequency table, we typically do not have immediate access to the data in the form of a dataset. We could enter the data with frequency weights.

```
. input rank smoking freq
            1
                     1
                     2
                           2
  2.
            1
            1
                     3
                          3
 (output omitted)
 19.
           5
                     3
                          7
 20.
            5
                     4
                          2
21.
      end
```

- . label define vl\_rank 1 "senior\_mngr" ...
- . label value rank vl\_rank
- . label define vl\_smoke 1 "none" ...
- . label value smoke vl\_smoke
- . ca rank smoking [fw=freq] (output omitted)

Or we may enter the data as a matrix and use camat. First, we enter the frequency matrix with proper column and row names and then list the matrix for verification.

- . matrix F =  $(4,2,3,2 \setminus 4,3,7,4 \setminus 25,10,12,4 \setminus 18,24,33,13 \setminus 10,6,7,2)$
- . matrix colnames F = none light medium heavy
- . matrix rownames F = senior\_mngr junior\_mngr senior\_empl junior\_empl secretary
- . matlist F, border

	none	light	medium	heavy
senior_mngr	4	2	3	2
junior_mngr	4	3	7	4
senior_empl	25	10	12	4
junior_empl	18	24	33	13
secretary	10	6	7	2

We can use camat on F to obtain the same results as from the raw data. We use the compact option for a more compact table.

1

```
. camat F, compact
```

. ca	mac i, compac					
Corr	espondence ar	nalysis		Number of o	obs =	193
			Pearson chi	.2(12) =	16.44	
				Prob > chi2 =		0.1718
			Total inert	ia =	0.0852	
	5 active rows	3		Number of d	lim. =	2
	4 active colu	ımns		Expl. inert	ia (%) =	99.51
		singular	principal			cumul
	Dimension	value	inertia	chi2	percent	percent
	dim 1	.2734211	.0747591	14.43	87.76	87.76
	dim 2	.1000859	.0100172	1.93	11.76	99.51
	dim 3	.0203365	.0004136	0.08	0.49	100.00
	total		.0851899	16.44	100	

Statistics for row and column categories in symmetric norm. (x 1000)

Categories	_	verall	 %inert	coord	ension sacor		coord	ension sacor	
rows						_			
senior mngr	57	893	31	126	92	3	612	800	214
junior mngr	93	991	139	-495	526	84	769	465	551
senior empl	264	1000	450	728	999	512	34	1	3
junior empl	456	1000	308	-446	942	331	-183	58	152
secretary	130	999	71	385	865	70	-249	133	81
columns									
none	316	1000	577	752	994	654	96	6	29
light	233	984	83	-190	327	31	-446	657	463
medium	321	983	148	-375	982	166	-23	1	2
heavy	130	995	192	-562	684	150	625	310	506

## Example 7: Correspondence analysis of nonfrequency data

The command camat may also be used for a CA of nonfrequency data. The data should be nonnegative, with strictly positive margins. An example are the compositional data on the distribution of government R&D funds over 11 areas in five European countries in 1989; the data are listed in Greenacre (1993, 82). The expenditures are scaled to 1,000 within country, to focus the analysis on the intranational distribution policies. Moreover, with absolute expenditures, small countries, such as The Netherlands, would have been negligible in the analysis.

We enter the data as a Stata matrix. The command matrix input (see [P] matrix define) allows us to input row entries separated by blanks, rather than by commas; rows are separated by the backward slash (\).

```
. matrix input RandD = (
    18 19 14 14
    12
       34
             4
                15
                    31 \
    44
        33
           36
                58
                    25 \
    37
        88
            67 101
    42
       20
            36
               28
                   43 \
    90 156 107 224 176 \
    28 50 59 88
                  28 \
   165 299 120 303 407 \
    48 128 147
                62 103 \
   484 127 342 70 28 \
    32 46 68 37 113)
```

total

```
. matrix colnames RandD = Britain West_Germany France Italy Netherlands
. matrix rownames RandD = earth_exploration pollution human_health
> energy agriculture industry space university
> nonoriented defense other
```

We perform a CA, suppressing the voluminous row- and column-point statistics. We want to show a biplot, and therefore we select symmetric normalization.

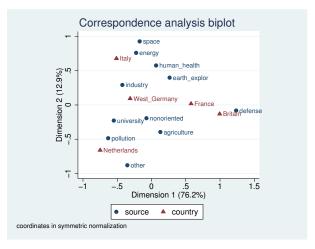
. camat RandD, dim(2) norm(symm) rowname(source) colname(country) norowpoints
> nocolpoints plot

espondence and service and ser	ws	Number of o Pearson chi Prob > chi2 Total inert Number of d Expl. inert	2(40) =	5,000 1321.55 0.0000 0.2643 2 89.08	
Dimension	singular value	principal inertia	chi2	percent	cumul percent
dim 1 dim 2 dim 3 dim 4	.448735 .1846219 .1448003 .0888532	.2013631 .0340852 .0209671 .0078949	1006.82 170.43 104.84 39.47	76.18 12.90 7.93 2.99	76.18 89.08 97.01 100.00

1321.55

100

.2643103



The two dimensions account for 89% of the inertia in this example, justifying an interpretation of the biplot. Let us focus on the position of The Netherlands. The orientation of The Netherlands from the origin is in the same direction as the orientation of pollution and university from the origin, indicating that The Netherlands spends more on academic research and on research to reduce environmental pollution than the average country. Earth exploration and human health are in the opposite direction, indicating investments much lower than average in these areas. Industry and agriculture are approximately orthogonal to the orientation of The Netherlands, indicating average investments by The Netherlands in these areas. Britain and France have big military investments, whereas Germany and Italy have more of an industrial orientation.

#### □ Technical note

The interpretation of the biplot is not fully in line with what we easily see in the row and column profiles—surprisingly, Greenacre does not seem to feel the need to comment on this. Why is this the case? The clue is in the statistics we did not show. Although the two dimensions account for 90% of the total inertia, this does not mean that all rows and columns are approximated to this extent. There are some row and column categories that are not well described in two dimensions. For instance, the quality of the source categories nonoriented, agriculture, and earth\_exploration are only 0.063, 0.545, and 0.584, respectively, indicating that these rows are poorly represented in a two-dimensional space. The quality of West\_Germany is also rather low at 0.577. Adding a third dimension improves the quality of the category nonoriented but hardly affects the other two problematic categories. This effect can be seen only from the squared correlations between the third dimension and the profiles of the row and column categories—these correlations are small for all categories but nonoriented. Thus, nonoriented does not seem to really belong with the other categories and should probably be omitted from the analysis.

#### Crossed variables

ca can include interactions between variables in the analysis; variables that contain interactions are called crossed or stacked variables, whereas the variables that make them up are the crossing or stacking variables.

#### Example 8: Correspondence analysis with crossed variables

We illustrate crossed variables with ca by using the ISSP (1993) data from [MV] mca, which explores attitudes toward science and the environment. We are interested in whether responses to item A differ with education and gender. The item asks for a response to the statement "We believe too often in science, and not enough in feelings or faith," with a 1 indicating strong agreement and a 5 indicating strong disagreement. We are interested in how education and gender influence response. We cross the variables sex and edu into one demographic variable labeled demo to explore this question.

. use http://www.stata-press.com/data/r14/issp93
(Selection from ISSP (1993))

Total

. tabulate A edu

too much science, not	1 4	education (6	categories	)	
enough feelings&faith	1	primary c	_		Total
agree strongly	7	59	29	11	119
agree	15	155	84	27	322
neither agree nor dis	7	84	65	18	204
disagree	8	68	54	26	178
disagree strongly	1	12	10	12	48
Total	38	378	242	94	871
	educat	cion (6			
too much science, not	categ	gories)			
enough feelings&faith	tertiary	tertiary	Total		
agree strongly	5	8	119		
agree	20	21	322		
neither agree nor dis	11	19	204		
disagree	8	14	178		
disagree strongly	5	8	48		

70

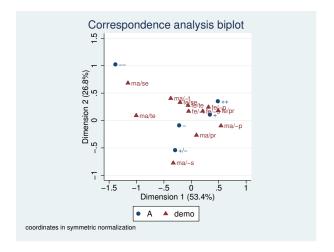
871

We notice immediately the long labels for variable A and on edu. We replace these labels with short labels that can be abbreviated, so that in our analysis we will easily be able to identify categories. We use the length(2) option to ca to ensure that labels from each of the crossing variables are restricted to two characters.

- . label define response 1 "++" 2 "+" 3 "+/-" 4 "-" 5 "--"
- . label values A response
- . label define education 1 "-pri" 2 "pri" 3 "-sec" 4 "sec" 5 "-ter" 6 "ter"
- . label values edu education
- . ca A (demo: sex edu), norowpoints nocolpoints length(2) plot norm(symmetric)

Correspondence analysis	Number of obs	=	871
	Pearson chi2(44)	=	72.52
	Prob > chi2	=	0.0043
	Total inertia	=	0.0833
5 active rows	Number of dim.	=	2
12 active columns	<pre>Expl. inertia (%)</pre>	=	80.17
singular principal			cumul

Dimension	singular value	principal inertia	chi2	percent	cumul percent
dim 1	.2108455	.0444558	38.72	53.39	53.39
dim 2	.14932	.0222965	19.42	26.78	80.17
dim 3	.1009876	.0101985	8.88	12.25	92.42
dim 4	.0794696	.0063154	5.50	7.58	100.00
total		.0832662	72.52	100	



We see clearly that the responses of the males vary more widely than those of the females. Strong agreement with item A is most closely associated with females with little education, and strong disagreement is most closely associated with males with a secondary or tertiary education. Educated males are more closely associated with a negative response than educated females are, and females with little education are more closely associated with a positive response than males with little education are.

#### Stored results

Let r be the number of rows, c be the number of columns, and f be the number of retained dimensions. ca and camat store the following in e():

```
Scalars
    e(N)
                        number of observations
    e(f)
                        number of dimensions (factors, axes); maximum of min(r-1,c-1)
                        total inertia = e(X2)/e(N)
    e(inertia)
    e(pinertia)
                        inertia explained by e(f) dimensions
    e(X2)
                        \chi^2 statistic
    e(X2\_df)
                        degrees of freedom (r-1)(c-1)
    e(X2_p)
                        p-value for e(X2)
Macros
    e(cmd)
                        ca (even for camat)
    e(cmdline)
                        command as typed
    e(Rcrossvars)
                        row crossing variable names (ca only)
    e(Ccrossvars)
                        column crossing variable names (ca only)
    e(varlist)
                        the row and column variable names (ca only)
    e(wtype)
                        weight type (ca only)
    e(wexp)
                        weight expression (ca only)
                        title in estimation output
    e(title)
    e(ca_data)
                        variables or crossed
    e(Cname)
                        name for columns
    e(Rname)
                        name for rows
    e(norm)
                        normalization method
    e(sv_unique)
                        1 if the singular values are unique, 0 otherwise
    e(properties)
                        nob noV eigen
    e(estat_cmd)
                        program used to implement estat
    e(predict)
                        program used to implement predict
    e(marginsnotok)
                        predictions disallowed by margins
Matrices
    e(Ccoding)
                        column categories (1 \times c) (ca only)
    e(Rcoding)
                        row categories (1 \times r) (ca only)
    e(GSC)
                        column statistics (c \times 3(1+f))
    e(GSR)
                        row statistics (r \times 3(1+f))
                        normalized column coordinates (c \times f)
    e(TC)
    e(TR)
                        normalized row coordinates (r \times f)
                        singular values (1 \times f)
    e(Sv)
    e(C)
                        column coordinates (c \times f)
    e(R)
                        row coordinates (r \times f)
    e(c)
                        column mass (margin) (c \times 1)
    e(r)
                        row mass (margin) (r \times 1)
                        analyzed matrix (r \times c)
    e(P)
                        supplementary column statistics
    e(GSC_supp)
    e(GSR_supp)
                        supplementary row statistics
    e(PC_supp)
                        principal coordinates supplementary column points
    e(PR_supp)
                        principal coordinates supplementary row points
    e(TC_supp)
                        normalized coordinates supplementary column points
    e(TR_supp)
                        normalized coordinates supplementary row points
Functions
    e(sample)
                        marks estimation sample (ca only)
```

#### Methods and formulas

Our presentation of simple CA follows that of Greenacre (1984, 83–125); see also Blasius and Greenacre (1994) and Rencher and Christensen (2012, 565–580). See Greenacre and Blasius (1994) for a concise presentation of CA from a computational perspective. Simple CA seeks a geometric representation of the rows and column of a (two mode) matrix with nonnegative entries in a common

low-dimensional space so that chi-squared distances between the rows and between the columns are well approximated by the Euclidean distances in the common space.

Let  ${\bf N}$  be an  $I\times J$  matrix with nonnegative entries and strictly positive margins.  ${\bf N}$  may be frequencies of a two-way cross-tabulation, but this is not assumed in most of CA. Let  $n=N_{++}$  be the overall sum of  $N_{ij}$  ("number of observations"). Define the correspondence table as the matrix  ${\bf P}$  where  $P_{ij}=N_{ij}/n$ , so the overall sum of  $P_{ij}$  is  $P_{++}=1$ . Let  ${\bf r}={\bf P}{\bf 1}$  be the row margins, also known as the row masses, with elements  $r_i>0$ . Similarly,  ${\bf c}={\bf P}'{\bf 1}$  contains the column margins, or column masses, with elements  $c_i>0$ .

CA is defined in terms of the generalized singular value decomposition (GSVD) of  $\mathbf{P} - \mathbf{rc'}$  with respect to the inner products normed by  $\mathbf{D}_r^{-1}$  and  $\mathbf{D}_c^{-1}$ , where  $\mathbf{D}_r = \operatorname{diag}(\mathbf{r})$  and  $\mathbf{D}_c = \operatorname{diag}(\mathbf{c})$ . The GSVD can be expressed in terms of the orthonormal (or standard) SVD of the standardized residuals

$$\mathbf{Z} = \mathbf{D}_r^{-\frac{1}{2}} (\mathbf{P} - \mathbf{r} \mathbf{c}') \mathbf{D}_c^{-\frac{1}{2}} \quad \text{with elements} \quad Z_{ij} = \frac{P_{ij} - r_i c_j}{\sqrt{r_i c_j}}$$

Denote by  $\mathbf{Z} = \mathbf{R} \boldsymbol{\Lambda} \mathbf{C}'$  the SVD of  $\mathbf{Z}$  with  $\mathbf{R}' \mathbf{R} = \mathbf{C}' \mathbf{C} = \mathbf{I}$  and  $\boldsymbol{\Lambda}$  a diagonal matrix with singular values in decreasing order. ca displays a warning message if  $\mathbf{Z}$  has common singular values.

The total principal inertia of the correspondence table  ${\bf P}$  is defined as  $\chi^2/n=\sum_{i,j}Z_{ij}^2$ , where  $\chi^2$  is Pearson's chi-squared statistic. We can express the inertia of  ${\bf P}$  in terms of the singular values of  ${\bf Z}$ :

$$\text{inertia} = \frac{1}{n}\chi^2 = \sum_{k=1}^{\min(I-1,J-1)} \lambda_k^2$$

The inertia accounted for by d dimensions is  $\sum_{k=1}^{d} \lambda_k^2$ . The fraction of inertia accounted for (explained) by the d dimensions is defined as

explained inertia = 
$$\frac{\sum_{k=1}^{d} \lambda_k^2}{\sum_{k=1}^{\min(I-1,J-1)} \lambda_k^2}$$

Principal row  $(\widetilde{R}_{ik})$  and principal column  $(\widetilde{C}_{jk})$  coordinates are defined as

$$\widetilde{R}_{ik} = \frac{R_{ik}\lambda_k}{\sqrt{r_i}} = (\mathbf{D}_r^{-\frac{1}{2}}\mathbf{R}\boldsymbol{\Lambda})_{ik} \qquad \widetilde{C}_{jk} = \frac{C_{jk}\lambda_k}{\sqrt{c_j}} = (\mathbf{D}_c^{-\frac{1}{2}}\mathbf{C}\boldsymbol{\Lambda})_{jk}$$

The  $\alpha$ -normalized row and column coordinates are defined as

$$R_{ik}^{(\alpha)} = \frac{R_{ik}\lambda_k^{\alpha}}{\sqrt{r_i}} \qquad C_{jk}^{(\alpha)} = \frac{C_{jk}\lambda_k^{1-\alpha}}{\sqrt{c_j}}$$

The row principal coordinates are obtained with  $\alpha = 1$ . The column principal coordinates are obtained with  $\alpha = 0$ . The symmetric coordinates are obtained with  $\alpha = 1/2$ .

Decomposition of inertia by rows  $(\operatorname{In}^{(r)})$  and by columns  $(\operatorname{In}^{(c)})$  is defined as

$$\operatorname{In}_{i}^{(r)} = \sum_{i=1}^{J} Z_{ij}^{2} \qquad \operatorname{In}_{j}^{(c)} = \sum_{i=1}^{I} Z_{ij}^{2}$$

Quality of subspace approximations for the row and column categories are defined as

$$Q_i^{(r)} = \frac{r_i}{\ln_i^{(r)}} \sum_{k=1}^d \widetilde{R}_{ik}^2 \qquad \qquad Q_j^{(c)} = \frac{c_j}{\ln_j^{(c)}} \sum_{k=1}^d \widetilde{C}_{jk}^2$$

If  $d = \min(I - 1, J - 1)$ , the quality index satisfies  $Q_i^{(r)} = Q_i^{(c)} = 1$ .

CA provides several diagnostics for a more detailed analysis of inertia: what do the categories contribute to the inertia explained by the dimensions, and what do the dimensions contribute to the inertia explained for the categories?

The relative contributions of row i  $(G_{ik}^{(r)})$  and of column j  $(G_{jk}^{(c)})$  to the inertia of principal dimension k are defined as

$$G_{ik}^{(r)} = \frac{r_i \widetilde{R}_{ik}^2}{\lambda_k^2} \qquad \qquad G_{jk}^{(c)} = \frac{c_j \widetilde{C}_{jk}^2}{\lambda_k^2}$$

$$G_{+k}^{(r)} = G_{+k}^{(c)} = 1.$$

The correlations  $H_{ik}^{(r)}$  of the ith row profile and kth principal row dimension and, analogously,  $H_{ik}^{(c)}$  for columns are

$$H_{ik}^{(r)} = \frac{r_i}{\ln_i^{(r)}} \widetilde{R}_{ik}^2 \qquad \qquad H_{jk}^{(c)} = \frac{c_j}{\ln_i^{(c)}} \widetilde{C}_{jk}^2 \label{eq:hik}$$

We now define the quantities returned by the estat subcommands after ca. The row profiles are  $\mathbf{U} = \mathbf{D}_r^{-1} \mathbf{P}$ . The chi-squared distance between rows  $i_1$  and  $i_2$  of  $\mathbf{P}$  is defined as the Mahalanobis distance between the respective row profiles  $\mathbf{U}_{i_1}$  and  $\mathbf{U}_{i_2}$  with respect to  $\mathbf{D}_c$ ,

$$(\mathbf{U}_{i_1} - \mathbf{U}_{i_2})\mathbf{D}_c^{-1}(\mathbf{U}_{i_1} - \mathbf{U}_{i_2})'$$

The column profiles and the chi-squared distances between columns are defined analogously. The chi-squared distances for the approximated correspondence table are defined analogously in terms of  $\hat{\mathbf{P}}$ .

The fitted or reconstructed values  $\hat{P}_{ij}$  are

$$\widehat{P}_{ij} = r_i c_j \left( 1 + \lambda_k^{-1} \sum_{k=1}^d \widetilde{R}_{ik} \widetilde{C}_{jk} \right)$$

## References

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### Also see

- [MV] ca postestimation Postestimation tools for ca and camat
- [MV] ca postestimation plots Postestimation plots for ca and camat
- [MV] mca Multiple and joint correspondence analysis
- [R] tabulate twoway Two-way table of frequencies
- [U] 20 Estimation and postestimation commands

## **Title**

ca postestimation — Postestimation tools for ca and camat

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

### **Postestimation commands**

The following postestimation commands are of special interest after ca and camat:

Command	Description
cabiplot	biplot of row and column points
caprojection	CA dimension projection plot
estat coordinates	display row and column coordinates
estat distances	display $\chi^2$ distances between row and column profiles
estat inertia	display inertia contributions of the individual cells
estat loadings	display correlations of profiles and axes
estat profiles	display row and column profiles
*estat summarize	estimation sample summary
estat table	display fitted correspondence table
screeplot	plot singular values

<sup>\*</sup> estat summarize is not available after camat.

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results
†predict	fitted values, row coordinates, or column coordinates

<sup>\*</sup> All estimates subcommands except table and stats are available.

<sup>†</sup> predict is not available after camat.

## predict

### **Description for predict**

predict creates a new variable containing predictions such as fitted values and row or column scores.

## Menu for predict

Statistics > Postestimation

## Syntax for predict

${\tt predict}$	[type]	newvar	[if]	[in]	[ ,	statistic ]	
-----------------	--------	--------	------	------	-----	-------------	--

statistic	Description
Main	
<u>f</u> it	fitted values; the default
<pre>rowscore(#)</pre>	row score for dimension #
<pre>colscore(#)</pre>	column score for dimension #

predict is not available after camat.

## **Options for predict**

Main

fit specifies that fitted values for the correspondence analysis model be computed. fit displays the fitted values  $p_{ij}$  according to the correspondence analysis model. fit is the default.

rowscore(#) generates the row score for dimension #, that is, the appropriate elements from the normalized row coordinates.

colscore(#) generates the column score for dimension #, that is, the appropriate elements from the normalized column coordinates.

#### estat

## **Description for estat**

estat coordinates displays the row and column coordinates.

estat distances displays the  $\chi^2$  distances between the row profiles and between the column profiles. Also, the  $\chi^2$  distances between the row and column profiles to the respective centers (marginal distributions) are displayed. Optionally, the fitted profiles rather than the observed profiles are used.

estat inertia displays the inertia  $(\chi^2/N)$  contributions of the individual cells.

estat loadings displays the correlations of the row and column profiles and the axes, comparable to the loadings of principal component analysis.

estat profiles displays the row and column profiles; the row (column) profile is the conditional distribution of the row (column) given the column (row). This is equivalent to specifying the row and column options with the tabulate command; see [R] tabulate twoway.

estat summarize displays summary information about the row and column variables over the estimation sample.

estat table displays the fitted correspondence table. Optionally, the observed "correspondence table" and the expected table under independence are displayed.

#### Menu for estat

Statistics > Postestimation

## Syntax for estat

```
Display row and column coordinates
  estat coordinates [ , norow nocolumn format(%fmt) ]
Display chi-squared distances between row and column profiles
  estat <u>di</u>stances [, norow <u>nocol</u>umn approx <u>for</u>mat(%fmt)]
Display inertia contributions of cells
  estat <u>in</u>ertia [, <u>to</u>tal <u>nosc</u>ale <u>for</u>mat(%fmt)]
Display correlations of profiles and axes
  estat loadings [, norow nocolumn format(%fmt)]
Display row and column profiles
  estat profiles [, norow nocolumn format(%fmt)]
```

Display summary information

estat  $\underline{\text{summarize}}$  [,  $\underline{\text{lab}}$ els  $\underline{\text{nohea}}$ der  $\underline{\text{noweights}}$ ]

Display fitted correspondence table

estat <u>ta</u>ble [, fit obs <u>in</u>dependence <u>nosc</u>ale <u>for</u>mat(%fmt)]

options	Description
norow	suppress display of row results
<u>nocol</u> umn	suppress display of column results
<pre>format(%fmt)</pre>	display format; default is format(%9.4f)
approx	display distances between fitted (approximated) profiles
<u>to</u> tal	add row and column margins
<u>nosc</u> ale	display $\chi^2$ contributions; default is inertias = $\chi^2/N$ (with estat inertia)
<u>lab</u> els	display variable labels
<u>nohea</u> der	suppress the header
<u>nowei</u> ghts	ignore weights
fit	display fitted values from correspondence analysis model
obs	display correspondence table ("observed table")
<u>in</u> dependence	display expected values under independence
<u>nosc</u> ale	suppress scaling of entries to 1 (with estat table)

## Options for estat

norow, an option used with estat coordinates, estat distances, and estat profiles, suppresses the display of row results.

nocolumn, an option used with estat coordinates, estat distances, and estat profiles, suppresses the display of column results.

format(%fmt), an option used with many of the subcommands of estat, specifies the display format for the matrix, for example, format(%8.3f). The default is format(%9.4f).

approx, an option used with estat distances, computes distances between the fitted profiles. The default is to compute distances between the observed profiles.

total, an option used with estat inertia, adds row and column margins to the table of inertia or  $\chi^2$   $(\chi^2/N)$  contributions.

noscale, as an option used with estat inertia, displays  $\chi^2$  contributions rather than inertia  $(=\chi^2/N)$  contributions. (See below for the description of noscale with estat table.)

labels, an option used with estat summarize, displays variable labels.

noheader, an option used with estat summarize, suppresses the header.

noweights, an option used with estat summarize, ignores the weights, if any. The default when weights are present is to perform a weighted summarize on all variables except the weight variable itself. An unweighted summarize is performed on the weight variable.

fit, an option used with estat table, displays the fitted values for the correspondence analysis model. fit is implied if obs and independence are not specified.

obs, an option used with estat table, displays the observed table with nonnegative entries (the "correspondence table").

independence, an option used with estat table, displays the expected values  $p_{ij}$  assuming independence of the rows and columns,  $p_{ij} = r_i c_j$ , where  $r_i$  is the mass of row i and  $c_i$  is the mass of column j.

noscale, as an option used with estat table, normalizes the displayed tables to the sum of the original table entries. The default is to scale the tables to overall sum 1. (See above for the description of noscale with estat inertia.)

## Remarks and examples

Remarks are presented under the following headings:

Postestimation statistics Predicting new variables

#### Postestimation statistics

After you conduct a correspondence analysis, there are several additional tables to help you understand and interpret your results. Some of these tables resemble tables produced by other Stata commands but are provided as part of the ca postestimation suite of commands for a unified presentation style.

#### Example 1: estat profiles, estat distances, estat table

We continue with the classic example of correspondence analysis, namely, the data on smoking in organizations. We extract only one dimension.

- . use http://www.stata-press.com/data/r14/ca\_smoking
- . ca rank smoking, dim(1)

total

		, , ,				
Correspondence analysis				Number of o Pearson chi Prob > chi2 Total inert	2(12) =	193 16.44 0.1718 0.0852
	5 active rows 4 active colu	=		Number of d Expl. inert	im. =	1 87.76
	Dimension	singular value	principal inertia	chi2	percent	cumul percent
•	dim 1 dim 2 dim 3	.2734211 .1000859 .0203365	.0747591 .0100172 .0004136	14.43 1.93 0.08	87.76 11.76 0.49	87.76 99.51 100.00

.0851899

16.44

100

60

		overall		d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
rank						
senior mngr	0.057	0.092	0.031	0.126	0.092	0.003
junior mngr	0.093	0.526	0.139	-0.495	0.526	0.084
senior empl	0.264	0.999	0.450	0.728	0.999	0.512
junior empl	0.456	0.942	0.308	-0.446	0.942	0.331
secretary	0.130	0.865	0.071	0.385	0.865	0.070
smoking						
none	0.316	0.994	0.577	0.752	0.994	0.654
light	0.233	0.327	0.083	-0.190	0.327	0.031
medium	0.321	0.982	0.148	-0.375	0.982	0.166
heavy	0.130	0.684	0.192	-0.562	0.684	0.150

Statistics for row and column categories in symmetric normalization

CA analyzes the similarity of row and of column categories by comparing the row profiles and the column profiles—some may prefer to talk about conditional distributions for a two-way frequency distribution, but CA is not restricted to this type of data.

### . estat profiles

Row profiles (rows normalized to 1)

	none	light	medium	heavy	mass
senior mngr	0.3636	0.1818	0.2727	0.1818	0.0570
junior mngr	0.2222	0.1667	0.3889	0.2222	0.0933
senior empl	0.4902	0.1961	0.2353	0.0784	0.2642
junior empl	0.2045	0.2727	0.3750	0.1477	0.4560
secretary	0.4000	0.2400	0.2800	0.0800	0.1295
mass	0.3161	0.2332	0.3212	0.1295	

Column profiles (columns normalized to 1)

	none	light	medium	heavy	mass
senior mngr junior mngr senior empl junior empl secretary	0.0656 0.0656 0.4098 0.2951 0.1639	0.0444 0.0667 0.2222 0.5333 0.1333	0.0484 0.1129 0.1935 0.5323 0.1129	0.0800 0.1600 0.1600 0.5200 0.0800	0.0570 0.0933 0.2642 0.4560 0.1295
mass	0.3161	0.2332	0.3212	0.1295	

The tables also include the row and column masses—marginal probabilities. Two row categories are similar to the extent that their row profiles (that is, their distribution over the columns) are the same. Similar categories could be collapsed without distorting the information in the table. In CA, similarity or dissimilarity of the row categories is expressed in terms of the  $\chi^2$  distances between the rows. These are sums of squares, weighted with the inverse of the column masses. Thus a difference is counted "heavier" (inertia!) the smaller the respective column mass. In the table, we also add the  $\chi^2$  distances of the rows to the row centroid, that is, to the marginal distribution. This allows us to easily see which row categories are similar to each other as well as which row categories are similar to the population.

. estat distances, nocolumn

Chi2 distances between the row profiles

rank	junior_~r	senior_~l	junior_~l	secretary	center
senior_mngr junior_mngr senior_empl junior_empl secretary	0.3448	0.3721 0.6812	0.3963 0.3044 0.6174	0.3145 0.5622 0.2006 0.4347	0.2166 0.3569 0.3808 0.2400 0.2162

We see that senior employees are especially dissimilar from junior managers in terms of their smoking behavior but are rather similar to secretaries. Also the senior employees are least similar to the average staff member among all staff categories.

One of the goals of CA is to come up with a low-dimensional representation of the rows and columns in a common space. One way to see the adequacy of this representation is to inspect the implied approximation for the  $\chi^2$  distances—are the similarities between the row categories and between the column categories adequately represented in lower dimensions?

. estat distances, nocolumn approx

Chi2 distances between the dim=1 approximations of the row profiles

rank	junior_~r	senior_~l	junior_~l	secretary	center
senior_mngr junior_mngr senior_empl junior_empl secretary	0.3247	0.3148 0.6396	0.2987 0.0260 0.6135	0.1353 0.4600 0.1795 0.4340	0.0658 0.2590 0.3806 0.2330 0.2011

Some of the row distances are obviously poorly approximated, whereas the quality of other approximations is hardly affected. The dissimilarity in smoking behavior between junior managers and junior employees is particularly poorly represented in one dimension. From the CA with two dimensions, the second dimension is crucial to adequately represent the senior managers and the junior managers. By itself, this does not explain where the one-dimensional approximation fails; for this, we would have to take a closer look at the representation of the smoking categories as well.

A correspondence analysis can also be seen as equivalent to fitting the model

$$P_{ij} = r_i c_j (1 + R_{i1} C_{j1} + R_{i2} C_{j2} + \cdots)$$

to the correspondence table  $\mathbf{P}$  by some sort of least squares, with parameters  $r_i$ ,  $c_j$ ,  $R_{ij}$ , and  $C_{jk}$ . We may compare the (observed) table  $\mathbf{P}$  with the fitted table  $\hat{\mathbf{P}}$  to assess goodness of fit informally. Here we extract only one dimension, and so the fitted table is

$$\widehat{P}_{ij} = r_i c_j (1 + \widehat{R}_{i1} \widehat{C}_{j1})$$

with  $\mathbf{R}$  and  $\mathbf{C}$  the coordinates in symmetric (or row principal or column principal) normalization. We display the observed and fitted tables.

. estat table, fit obs

Correspondence table (normalized to overall sum = 1)

	none	light	medium	heavy
senior_mngr junior_mngr senior_empl junior_empl	0.0207 0.0207 0.1295 0.0933 0.0518	0.0104 0.0155 0.0518 0.1244 0.0311	0.0155 0.0363 0.0622 0.1710 0.0363	0.0104 0.0207 0.0207 0.0674 0.0104
secretary	0.0516	0.0311	0.0363	0.0104

Approximation for dim = 1 (normalized to overall sum = 1)

	none	light	medium	heavy
senior_mngr	0.0197	0.0130	0.0174	0.0069
junior_mngr	0.0185	0.0238	0.0355	0.0154
senior_empl	0.1292	0.0531	0.0617	0.0202
junior_empl	0.0958	0.1153	0.1710	0.0738
secretary	0.0528	0.0280	0.0356	0.0132

Interestingly, some categories (for example, the junior employees, the nonsmokers, and the medium smokers) are very well represented in one dimension, whereas the quality of the fit of other categories is rather poor. This can, of course, also be inferred from the quality column in the ca output. We would consider the fit unsatisfactory and would refit the model with a second dimension.

1

#### □ Technical note

If the data are two-way cross-classified frequencies, as with ca, it may make sense to assume that the data are multinomial distributed, and the parameters can be estimated by maximum likelihood. The estimator has well-established properties in contrast to the estimation method commonly used in CA. One advantage is that sampling variability, for example, in terms of standard errors of the parameters, can be easily assessed. Also, the likelihood-ratio test against the saturated model may be used to select the number of dimensions to be extracted. See Van der Heijden and de Leeuw (1985).

## Predicting new variables

If you use ca to obtain the optimal scaling positions for the rows and columns, you may use predict to obtain the corresponding scores in the normalization used.

## ▶ Example 2: Predictions

First, we obtain scores for the first dimension.

- . quietly ca rank smoking, normalize(symmetric) dim(2)
- . predict r1, row(1)
- . predict c1, col(1)
- . describe r1 c1

variable name	storage type	display format	value label	variable label
r1 c1		%9.0g %9.0g		<pre>rank score(1) in symmetric norm. smoking score(1) in symmetric norm.</pre>

. correlate r1 c1 (obs=193)

	r1	c1
r1 c1	1.0000 0.2734	1.0000

The correlation of r1 and c1 is 0.2734, which equals the first singular value reported in the first panel by ca. In the same way, we may obtain scores for the second dimension.

- . predict r2, row(2)
- . predict c2, col(2)
- . correlate r1 r2 c1 c2

(obs=193)

	r1	r2	c1	c2
r1	1.0000			
r2	-0.0000	1.0000		
c1	0.2734	0.0000	1.0000	
c2	0.0000	0.1001	0.0000	1.0000

The correlation between the row and column scores r2 and c2 for the second dimension is 0.1001, which is the same as the second singular value. Moreover, the row scores for dimensions 1 and 2 are not correlated, nor are the column scores.

1

Obtaining the fitted values of the CA model is also possible,

$$\pi_{ij} = r_i c_j (1 + R_{i1} C_{i1} + R_{i2} C_{i2})$$

where R and C are the row and column scales in symmetric normalization. These may be used, say, to compute fit measures, for instance, from the Cressie-Read power family to analyze the fit of the CA model (Weesie 1997).

#### Stored results

```
estat distances stores the following in r():
Matrices
                   \chi^2 distances between the columns and between the columns and the column center
    r(Dcolumns)
                   \chi^2 distances between the rows and between the rows and the row center
estat inertia stores the following in r():
Matrices
                   matrix of (squared) inertia (or \chi^2) contributions
    r(Q)
estat loadings stores the following in r():
Matrices
    r(LC)
                   column loadings
    r(LR)
                   row loadings
estat profiles stores the following in r():
Matrices
    r(Pcolumns)
                   column profiles (columns normalized to 1)
    r(Prows)
                   row profiles (rows normalized to 1)
estat table stores the following in r():
Matrices
    r(Fit)
                   fitted (reconstructed) values
    r(Fit0)
                   fitted (reconstructed) values, assuming independence of row and column variables
    r(Obs)
                   correspondence table
```

## Methods and formulas

See Methods and formulas in [MV] ca for information.

## References

Van der Heijden, P. G. M., and J. de Leeuw. 1985. Correspondence analysis used complementary to loglinear analysis. Psychometrika 50: 429–447.

Weesie, J. 1997. sg68: Goodness-of-fit statistics for multinomial distributions. *Stata Technical Bulletin* 36: 26–28. Reprinted in *Stata Technical Bulletin Reprints*, vol. 6, pp. 183–186. College Station, TX: Stata Press.

Also see References in [MV] ca.

### Also see

```
    [MV] ca — Simple correspondence analysis
    [MV] ca postestimation plots — Postestimation plots for ca and camat
    [MV] screeplot — Scree plot
    [U] 20 Estimation and postestimation commands
```

## **Title**

ca postestimation plots — Postestimation plots for ca and camat

Postestimation commands cabiplot caprojection Remarks and examples References Also see

# **Postestimation commands**

The following postestimation commands are of special interest after ca and camat:

Command	Description
cabiplot	biplot of row and column points
caprojection	CA dimension projection plot

Description

## cabiplot

## **Description for cabiplot**

cabiplot produces a plot of the row points or column points, or a biplot of the row and column points. In this plot, the (Euclidean) distances between row (column) points approximates the  $\chi^2$  distances between the associated row (column) profiles if the CA is properly normalized. Similarly, the association between a row and column point is approximated by the inner product of vectors from the origin to the respective points (see [MV] ca).

## Menu for cabiplot

 ${\it Statistics} > {\it Multivariate analysis} > {\it Correspondence analysis} > {\it Postestimation after CA} > {\it Biplot of row and column points}$ 

## Syntax for cabiplot

ontions

cabiplot [, options]

options	Description	
Main		
dim(# #)	the two dimensions to be displayed; default is dim(2 1)	
norow	suppress row coordinates	
<u>nocol</u> umn	suppress column coordinates	
<u>xneg</u> ate	negate the data relative to the $x$ axis	
ynegate	negate the data relative to the $y$ axis	
$\underline{\mathtt{max}}\mathtt{length}(\#)$	maximum number of characters for labels; default is maxlength(12)	
<u>or</u> igin	display the origin on the plot	
<pre>originlopts(line_options)</pre>	affect rendition of origin axes	
Rows		
<pre>rowopts(row_opts)</pre>	affect rendition of rows	
Columns		
<pre>colopts(col_opts)</pre>	affect rendition of columns	
Y axis, X axis, Titles, Legend, Overa	all	
twoway_options	any options other than by() documented in [G-3] twoway_options	
row_opts and col_opts	Description	
plot_options	change look of markers (color, size, etc.) and look or position of marker labels	
<pre>suppopts(plot_options)</pre>	change look of supplementary markers and look or position of supplementary marker labels	
plot_options	Description	
marker_options	change look of markers (color, size, etc.)	
marker_label_options	add marker labels; change look or position	

#### Options for cabiplot

dim(##) identifies the dimensions to be displayed. For instance, dim(3 2) plots the third dimension (vertically) versus the second dimension (horizontally). The dimension number cannot exceed the number of extracted dimensions. The default is dim(2 1).

norow suppresses plotting of row points.

nocolumn suppresses plotting of column points.

xnegate specifies that the x-axis values are to be negated (multiplied by -1).

ynegate specifies that the y-axis values are to be negated (multiplied by -1).

maxlength(#) specifies the maximum number of characters for row and column labels; the default is maxlength(12).

origin specifies that the origin be displayed on the plot. This is equivalent to adding the options xline(0, lcolor(black) lwidth(vthin)) yline(0, lcolor(black) lwidth(vthin)) to the cabiplot command.

originlopts (line\_options) affects the rendition of the origin axes; see [G-3] line\_options.

Rows

rowopts (row\_opts) affects the rendition of the rows. The following row\_opts are allowed:

plot\_options affect the rendition of row markers, including their shape, size, color, and outline (see [G-3] marker\_options) and specify if and how the row markers are to be labeled (see [G-3] marker\_label\_options).

supports (plot\_options) affects supplementary markers and supplementary marker labels; see above for description of plot\_options.

Columns

colopts (col\_opts) affects the rendition of columns. The following col\_opts are allowed:

plot\_options affect the rendition of column markers, including their shape, size, color, and outline (see [G-3] marker\_options) and specify if and how the column markers are to be labeled (see [G-3] marker\_label\_options).

suppopts(plot\_options) affects supplementary markers and supplementary marker labels; see above for description of plot\_options.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option).

cabiplot automatically adjusts the aspect ratio on the basis of the range of the data and ensures that the axes are balanced. As an alternative, the twoway\_option aspectratio() can be used to override the default aspect ratio. cabiplot accepts the aspectratio() option as a suggestion only and will override it when necessary to produce plots with balanced axes; that is, distance on the x axis equals distance on the y axis.

twoway\_options, such as xlabel(), xscale(), ylabel(), and yscale() should be used with caution. These axis\_options are accepted but may have unintended side effects on the aspect ratio. See [G-3] twoway\_options.

### caprojection

#### **Description for caprojection**

caprojection produces a line plot of the row and column coordinates. The goal of this graph is to show the ordering of row and column categories on each principal dimension of the analysis. Each principal dimension is represented by a vertical line; markers are plotted on the lines where the row and column categories project onto the dimensions.

#### Menu for caprojection

Statistics > Multivariate analysis > Correspondence analysis > Postestimation after CA > Dimension projection plot

#### Syntax for caprojection

caprojection [, options]

options	Description
Main	
dim(numlist)	dimensions to be displayed; default is all
norow	suppress row coordinates
<u>nocol</u> umn	suppress column coordinates
<u>alt</u> ernate	alternate labels
<pre>maxlength(#)</pre>	number of characters displayed for labels; default is maxlength(12)
combine_options	affect the rendition of the combined column and row graphs
Rows	
<pre>rowopts(row_opts)</pre>	affect rendition of rows
Columns	
$\underline{\mathtt{col}}\mathtt{opts}(\mathit{col\_opts})$	affect rendition of columns
Y axis, X axis, Titles, Legend, Over	erall
twoway_options	any options other than by() documented in [G-3] twoway_options
row_opts and col_opts	Description
plot_options	change look of markers (color, size, etc.) and look or position of marker labels
<pre>suppopts(plot_options)</pre>	change look of supplementary markers and look or position of supplementary marker labels
plot_options	Description
<u> </u>	*
marker_options	change look of markers (color, size, etc.)
marker_label_options	add marker labels; change look or position

#### Options for caprojection

Main

dim(numlist) identifies the dimensions to be displayed. By default, all dimensions are displayed.

norow suppresses plotting of rows.

nocolumn suppresses plotting of columns.

alternate causes adjacent labels to alternate sides.

maxlength(#) specifies the maximum number of characters for row and column labels; the default is maxlength(12).

combine\_options affect the rendition of the combined plot; see [G-2] **graph combine**. combine\_options may not be specified with either norow or nocolumn.

Rows

rowopts (row\_opts) affects the rendition of rows. The following row\_opts are allowed:

plot\_options affect the rendition of row markers, including their shape, size, color, and outline (see [G-3] marker\_options) and specify if and how the row markers are to be labeled (see [G-3] marker\_label\_options).

supports (plot\_options) affects supplementary markers and supplementary marker labels; see above for description of plot\_options.

Columns

colopts (col\_opts) affects the rendition of columns. The following col\_opts are allowed:

plot\_options affect the rendition of column markers, including their shape, size, color, and outline (see [G-3] marker\_options) and specify if and how the column markers are to be labeled (see [G-3] marker\_label\_options).

supports(plot\_options) affects supplementary markers and supplementary marker labels; see above for description of plot\_options.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option).

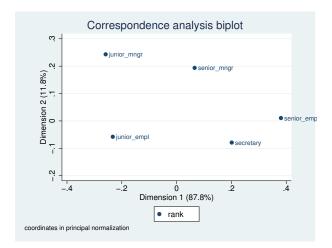
### Remarks and examples

In example 4 of [MV] ca, we showed that plots can be obtained simply by specifying the plot option during estimation (or replay). If the default plot is not exactly what you want, the cabiplot postestimation command provides control over the appearance of the plot.

### Example 1: cabiplot

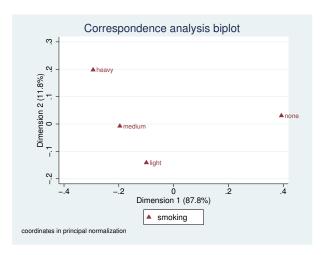
For instance, if we constructed a CA in row principal normalization, we would want to look only at the (points for the) row categories, omitting the column categories. In this normalization, the Euclidean distances between the row points approximate the  $\chi^2$  distances between the corresponding row profiles, but the Euclidean distances between the column categories are a distortion of the  $\chi^2$  distances of the column profiles. We can use cabiplot with the nocolumn option to suppress the graphing of the column points.

- . use http://www.stata-press.com/data/r14/ca\_smoking
- . quietly ca rank smoking, norm(principal)
- . cabiplot, nocolumn legend(on label(1 rank))



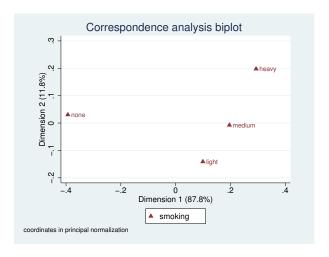
The default graph would not have provided a legend, so we included legend(on label(1 rank)) to produce one. We see that secretaries have smoking behavior that is rather similar to that of senior employees but rather dissimilar to that of the junior managers, with the other two ranks taking intermediate positions. Because we actually specified the principal normalization, we may also interpret the distances between the smoking categories as approximations to  $\chi^2$  distances.

. cabiplot, norow legend(on label(1 smoking))



You may not like the orientation of the dimensions. For instance, in this plot, the smokers are on the left and the nonsmokers are on the right. It is more natural to locate the nonsmokers on the left and the smokers on the right so that smoking increases from left to right. This is accomplished with the xnegate option.

. cabiplot, xnegate norow legend(on label(1 smoking))



#### □ Technical note

To see that negating is possible, think in terms of the fitted values

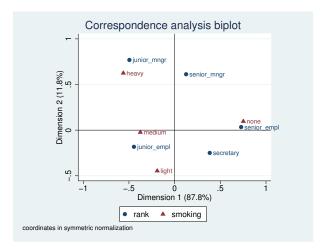
$$\hat{P}_{ij} = r_i c_j (1 + \hat{R}_{i1} \hat{C}_{j1} + \hat{R}_{i2} \hat{C}_{j2} + \cdots)$$

If the sign of the first column of  $\mathbf{R}$  and  $\mathbf{C}$  is changed at the same time, the fitted values are not affected. This is true for all CA statistics, and it holds true for other columns of  $\mathbf{R}$  and  $\mathbf{C}$  as well.

### Example 2: cabiplot with symmetric normalization

Using the symmetric normalization allows us to display a biplot where row categories may be compared with column categories. We execute ca again, with the normalize(symmetric) option, but suppress the output. This normalization somewhat distorts the interpretation of the distances between row points (or column points) as approximations to  $\chi^2$  distances. Thus the similarity of the staff categories (or smoking categories) cannot be adequately assessed. However, this plot allows us to study the association between smoking and rank.

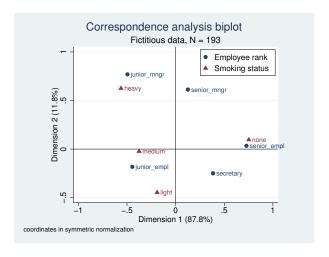
- . quietly ca rank smoking, normalize(symmetric) dim(2)
- . cabiplot, origin



With this symmetric normalization, we do not interpret the distances between categories of smoking and rank. Rather, we have to think in terms of vectors from the origin. The inner product of vectors approximates the residuals from a model of independence of the rows and columns. The inner product depends on the lengths of the vectors and the (cosine of the) angle between the vectors. If the vectors point in the same direction, the residuals are positive—these row and column categories tend to occur together. In our example, we see that senior employees tend to be nonsmokers. If the vectors point in opposite directions, the residuals are negative—these row and column categories tend to be exclusive. In our example, senior managers tend not to be light smokers. Finally, if the vectors are orthogonal (±90 degrees), the residuals tend to be small; that is, the observed frequencies correspond to what we expect under independence. For instance, junior managers have an average rate of light smoking.

Using various graph options, we can enhance the look of the plot.

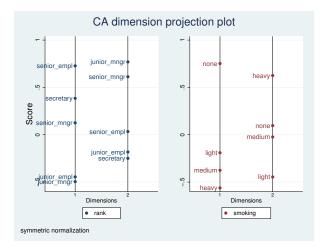
- . cabiplot, origin subtitle("Fictitious data, N = 193")
- > legend(pos(2) ring(0) col(1) lab(1 Employee rank) lab(2 Smoking status))



### ▶ Example 3: caprojection

caprojection produces a projection plot of the row and column coordinates after ca or camat and is especially useful if we think of CA as optimal scaling of the categories of the variables to maximize the correlations between the row and column variables. We continue where we left off with our previous example.

. caprojection



This example has relatively few categories, so we could visualize the orderings of the rows and columns from the previous biplots. However, CA is often used with larger problems, and in those cases, a projection plot is a useful presentation device.

#### References

See References in [MV] ca.

#### Also see

[MV] ca — Simple correspondence analysis

[MV] ca postestimation — Postestimation tools for ca and camat

[MV] screeplot — Scree plot

1

#### **Title**

**candisc** — Canonical linear discriminant analysis

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

### Description

candisc performs canonical linear discriminant analysis (LDA). What is computed is the same as with [MV] discrim lda. The difference is in what is presented. See [MV] discrim for other discrimination commands.

#### **Quick start**

Canonical linear discriminant analysis of v1, v2, v3, and v4 for groups defined by catvar candisc v1 v2 v3 v4, group(catvar)

As above, but use prior probabilities proportional to group size candisc v1 v2 v3 v4, group(catvar) priors(proportional)

Present the leave-one-out classification table in addition to standard output candisc v1 v2 v3 v4, group(catvar) lootable

As above, but suppress the resubstitution classification table candisc v1 v2 v3 v4, group(catvar) lootable notable

#### Menu

Statistics > Multivariate analysis > Discriminant analysis > Canonical linear discriminant analysis

### **Syntax**

candisc varlist [if] [in] [weight], group(groupvar) [options]

options	Description
Model	
*group(groupvar)	variable specifying the groups
priors(priors)	group prior probabilities
$\overline{\underline{\text{tie}}}$ s(ties)	how ties in classification are to be handled
Reporting	
<u>not</u> able	suppress resubstitution classification table
<u>loo</u> table	display leave-one-out classification table
<u>nost</u> ats	suppress display of canonical statistics
<u>noco</u> ef	suppress display of standardized canonical discriminant function coefficients
<u>nostr</u> uct	suppress display of canonical structure matrix
<u>nom</u> eans	suppress display of group means on canonical variables
priors	Description
equal	equal prior probabilities; the default
 proportional	group-size-proportional prior probabilities
<u> </u>	row or column vector containing the group prior probabilities
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities
ties	Description
missing	ties in group classification produce missing values; the default
random	ties in group classification are broken randomly
first	ties in group classification are set to the first tied group

<sup>\*</sup>group() is required.

statsby and xi are allowed; see [U] 11.1.10 Prefix commands.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

### **Options**

group(groupvar) is required and specifies the name of the grouping variable. groupvar must be a numeric variable.

priors (priors) specifies the prior probabilities for group membership. The following priors are

priors (equal) specifies equal prior probabilities. This is the default.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors (matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties (ties) specifies how ties in group classification will be handled. The following ties are allowed:

ties (missing) specifies that ties in group classification produce missing values. This is the default.

ties(random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

Reporting

notable suppresses the computation and display of the resubstitution classification table.

lootable displays the leave-one-out classification table.

nostats suppresses the display of the table of canonical statistics.

nocoef suppresses the display of the standardized canonical discriminant function coefficients.

nostruct suppresses the display of the canonical structure matrix.

nomeans suppresses the display of group means on canonical variables.

### Remarks and examples

See [MV] discrim for background on discriminant analysis (classification) and see [MV] discrim lda for more information on linear discriminant analysis. What candisc displays by default with

. candisc x y z, group(group)

you can also obtain with the following sequence of discrim commands and estat postestimation commands.

- . discrim x y z, group(group) notable
- . estat canontest
- . estat loadings
- . estat structure
- . estat grmeans, canonical
- . estat classtable

The candisc command will appeal to those performing descriptive LDA.

### Example 1

Example 2 of [MV] discrim knn introduces a head-measurement dataset from Rencher and Christensen (2012, 291) that has six discriminating variables and three groups. The three groups are high school football players, college football players, and nonplayers. The data were collected as a preliminary step in determining the relationship between helmet design and neck injuries.

Descriptive discriminant analysis allows us to explore the relationship in this dataset between head measurements and the separability of the three groups.

. use http://www.stata-press.com/data/r14/head (Table 8.3 Head measurements, Rencher and Christensen (2012))

. candisc wdim circum fbeye eyehd earhd jaw, group(group)

Canonical linear discriminant analysis

Fcn	Canon. Corr.	Eigen- value	Vari Prop.	ance Cumul.	Like- lihood Ratio	F	df1	df2	Prob>F	
		1.91776 .115931								

Ho: this and smaller canon. corr. are zero;

e = exact F

Standardized canonical discriminant function coefficients

	function1	function2
wdim	.6206412	.9205834
circum	0064715	0009114
fbeye	0047581	021145
eyehd	7188123	.5997882
earhd	3965116	3018196
jaw	5077218	9368745

#### Canonical structure

	function1	function2
wdim	.1482946	.3766581
circum	2714134	.1305383
fbeye	1405813	061071
eyehd	824502	.5363578
earhd	5177312	.1146999
jaw	2119042	3895934

Group means on canonical variables

group	function1	function2
high school college	-1.910378 1.16399	0592794 3771343
nonplayer	.7463888	.4364137

Resubstitution classification summary

Key
Number Percent

True group	Classified high school	college	nonplayer	Total
high school	26	1	3	30
	86.67	3.33	10.00	100.00
college	1	20	9	30
	3.33	66.67	30.00	100.00
nonplayer	2	8	20	30
	6.67	26.67	66.67	100.00
Total	29	29	32	90
	32.22	32.22	35.56	100.00
Priors	0.3333	0.3333	0.3333	

As seen in the canonical correlation table, the first linear discriminant function accounts for almost 95% of the variance. The standardized discriminant function coefficients (loadings) indicate that two of the variables, circum (head circumference) and fbeye (front-to-back measurement at eye level), have little discriminating ability for these three groups. The first discriminant function is contrasting wdim (head width at widest dimension) to a combination of eyehd (eye-to-top-of-head measurement), earhd (ear-to-top-of-head measurement), and jaw (jaw width).

The canonical structure coefficients, which measure the correlation between the discriminating variables and the discriminant function, are also shown. There is controversy on whether the standardized loadings or the structure coefficients should be used for interpretation; see Rencher and Christensen (2012, 301) and Huberty (1994, 262–264).

The group means on the canonical variables are shown, giving some indication of how the groups are separated. The means on the first function show the high school group separated farthest from the other two groups.

The resubstitution classification table, also known as a confusion matrix, indicates how many observations from each group are classified correctly or misclassified into the other groups. The college and nonplayer groups appear to have more misclassifications between them, indicating that these two groups are harder to separate.

All the postestimation tools of discrim lda are available after candisc; see [MV] discrim lda postestimation. For example, estat grsummarize can produce discriminating-variable summaries for each of our three groups.

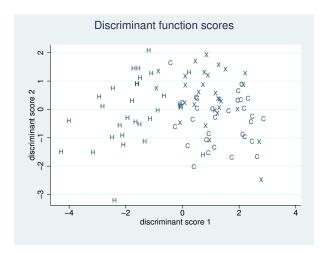
. estat grsummarize Estimation sample candisc Summarized by group

Mean	group high school	college	nonplayer	Total
wdim	15.2	15.42	15.58	15.4
circum	58.937	57.37967	57.77	58.02889
fbeye	20.10833	19.80333	19.81	19.90722
eyehd	13.08333	10.08	10.94667	11.37
earhd	14.73333	13.45333	13.69667	13.96111
jaw	12.26667	11.94333	11.80333	12.00444
N	30	30	30	90

A score plot graphs observation scores from the first two discriminant functions; see [MV] scoreplot. After candisc, scoreplot automatically labels the points with the value labels assigned to the groups. The value labels for our three groups are long—the resulting graph is too crowded.

To overcome this, we create a new label language (see [D] label language), define one letter labels for the groups, assign this label to our group variable, and then call scoreplot. We then reset the label language back to the default containing the longer, more descriptive value labels.

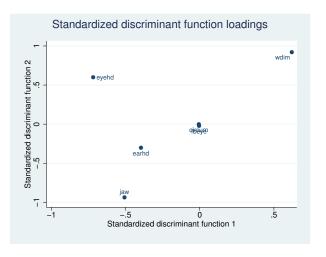
- . label language short, new (language short now current language)
- . label define fball 1 "H" 2 "C" 3 "X"
- . label values group fball
- . scoreplot, msymbol(i) aspect(.625)
- . label language default



The score plot illustrates the separation due to the first and second canonical linear discriminant functions. As expected from our examination of the earlier descriptive output, the high school group (labeled H) is reasonably well separated from the college (labeled C) and nonplayer (labeled X) groups. There is some separation in the second dimension between the college and nonplayer groups, but with substantial overlap.

A loading plot provides a graphical way of looking at the standardized discriminant function coefficients (loadings) that we previously examined in tabular form.

#### . loadingplot



circum and fbeye are near the origin, indicating that they provide almost no discriminating ability in comparison to the other discriminating variables. The relative locations of the remaining variables indicate their contribution to the discriminant functions.

#### Stored results

candisc stores the same items in e() as [MV] discrim Ida with the exception that e(subcmd) is not set and the following e() results are different:

```
Macros
   e(cmd)
                 candisc
                 Canonical linear discriminant analysis
   e(title)
```

#### Methods and formulas

See Methods and formulas in [MV] discrim lda for information.

#### References

```
Huberty, C. J. 1994. Applied Discriminant Analysis. New York: Wiley.
Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.
```

#### Also see

[MV] discrim lda — Linear discriminant analysis

#### **Title**

#### canon — Canonical correlations

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

Acknowledgment References Also see

### **Description**

canon estimates canonical correlations and provides the coefficients for calculating the appropriate linear combinations corresponding to those correlations.

canon typed without arguments redisplays previous estimation results.

#### **Quick start**

Canonical correlations between 2 sets of variables

canon (x1 x2 x3 x4) (y1 y2 y3 y4)

As above, but display y1-y4 first and then x1-x4

canon (y1 y2 y3 y4) (x1 x2 x3 x4)

As above, and display linear combinations for only the first 2 canonical correlations canon (y1 y2 y3 y4) (x1 x2 x3 x4), first(2)

As above, and display the linear combinations for only the second canonical correlation canon (y1 y2 y3 y4) (x1 x2 x3 x4), 1c(2)

With different numbers of variables in each set

canon (y1 y2 y3) (x1 x2 x3 x4 x5)

#### Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Canonical correlations

### **Syntax**

canon  $(varlist_1)$   $(varlist_2)$  [if] [in] [weight] [, options]

options	Description
Model	
lc(#)	calculate the linear combinations for canonical correlation #
<pre>first(#)</pre>	calculate the linear combinations for the first # canonical correlations
$\underline{\mathtt{nocon}}\mathtt{stant}$	do not subtract means when calculating correlations
Reporting	
<u>stdc</u> oef	output matrices of standardized coefficients
<u>stde</u> rr	display raw coefficients and conditionally estimated standard errors
$\underline{l}$ evel(#)	set confidence level; default is level(95)
test(numlist)	display significance tests for the specified canonical correlations
<u>notest</u> s	do not display tests
<pre>format(%fmt)</pre>	numerical format for coefficient matrices; default is format(%8.4f)

by and statsby are allowed; see [U] 11.1.10 Prefix commands.

aweights and fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

### **Options**

Model

1c(#) specifies that linear combinations for canonical correlation # be calculated. By default, all are calculated.

first(#) specifies that linear combinations for the first # canonical correlations be calculated. By default, all are calculated.

noconstant specifies that means not be subtracted when calculating correlations.

Reporting

- stdcoef specifies that the first part of the output contain the standard coefficients of the canonical correlations in matrix form. The default is to present the raw coefficients of the canonical correlations in matrix form.
- stderr specifies that the first part of the output contains the raw coefficients of the canonical correlations, the conditionally estimated standard errors, and the conditionally estimated confidence intervals in the standard estimation table. The default is to present the raw coefficients of the canonical correlations in matrix form.
- level(#) specifies the confidence level, as a percentage, for confidence intervals of the coefficients.
  The default is level(95) or as set by set level; see [U] 20.7 Specifying the width of confidence intervals. These "confidence intervals" are the result of an approximate calculation; see the technical note later in this entry.
- test(numlist) specifies that significance tests of the canonical correlations in the numlist be displayed. Because of the nature of significance testing, if there are three canonical correlations, test(1) will test the significance of all three correlations, test(2) will test the significance of canonical correlations 2 and 3, and test(3) will test the significance of the third canonical correlation alone.

notests specifies that significance tests of the canonical correlation not be displayed.

format(%fmt) specifies the display format for numbers in coefficient matrices; see [D] format. format(%8.4f) is the default. format() may not be specified with stderr.

### Remarks and examples

Canonical correlations attempt to describe the relationships between two sets of variables. Given two sets of variables,  $\mathbf{X} = (x_1, x_2, \dots, x_K)$  and  $\mathbf{Y} = (y_1, y_2, \dots, y_L)$ , the goal is to find linear combinations of  $\mathbf{X}$  and  $\mathbf{Y}$  so that the correlation between the linear combinations is as high as possible. That is, letting  $\hat{x}_1$  and  $\hat{y}_1$  be the linear combinations,

$$\widehat{x}_1 = \beta_{11} x_1 + \beta_{12} x_2 + \dots + \beta_{1K} x_K$$

$$\widehat{y}_1 = \gamma_{11} y_1 + \gamma_{12} y_2 + \dots + \gamma_{1L} y_L$$

you wish to find the maximum correlation between  $\hat{x}_1$  and  $\hat{y}_1$  as functions of the  $\beta$ 's and the  $\gamma$ 's. The second canonical correlation coefficient is defined as the ordinary correlation between

$$\begin{split} \widehat{x}_2 &= \beta_{21}x_1 + \beta_{22}x_2 + \dots + \beta_{2K}x_K \quad \text{and} \\ \widehat{y}_2 &= \gamma_{21}y_1 + \gamma_{22}y_2 + \dots + \gamma_{2L}y_L \end{split}$$

This correlation is maximized subject to the constraints that  $\widehat{x}_1$  and  $\widehat{x}_2$ , along with  $\widehat{y}_1$  and  $\widehat{y}_2$ , are orthogonal and that  $\widehat{x}_1$  and  $\widehat{y}_2$ , along with  $\widehat{x}_2$  and  $\widehat{y}_1$ , are also orthogonal. The third and further correlations are defined similarly. There are  $m = \min(K, L)$  such correlations.

Canonical correlation analysis originated with the work of Hotelling (1935, 1936). For an introduction, see Rencher and Christensen (2012, chap. 11), Johnson and Wichern (2007), or Afifi, May, and Clark (2012).

### Example 1

Consider two scientists trying to describe how "big" a car is. The first scientist takes physical measurements—the length, weight, headroom, and trunk space—whereas the second takes mechanical measurements—the engine displacement, mileage rating, gear ratio, and turning circle. Can they agree on a conceptual framework?

. use http://www.stata-press.com/data/r14/auto
(1978 Automobile Data)

. canon (length weight headroom trunk) (displ mpg gear\_ratio turn)

Canonical correlation analysis

Number of obs = 74

Raw coefficients for the first variable set

	1	2	3	4
length weight headroom trunk	0.0095 0.0010 0.0351 -0.0023	0.1441 -0.0037 -0.3701 -0.0343	0.0329 -0.0010 1.5361 -0.2135	0.0212 0.0007 -0.0440 -0.3253

Raw coefficients for the second variable set

	1	2	3	4
displacement mpg gear_ratio turn	0.0054 -0.0461 0.0330 0.0794	-0.0125 -0.0413 1.0280 0.3113	0.0191 0.0683 3.6596 0.0033	-0.0005 0.2478 -1.0311 0.2240
curn	0.0794	0.3113	0.0033	0.2240

Canonical correlations: 0.9476 0.3400 0.0634 0.0447

Tests of significance of all canonical correlations Statistic df1 df2 F Prob>F Wilks' lambda 16 202.271 0.0000 a.0897314 15.1900 Pillai's trace 1.01956 16 276 5.9009 0.0000 a0.0000 a Lawley-Hotelling trace 8.93344 16 258 36.0129 Roy's largest root 8.79667 4 69 151.7426 0.0000 u

e = exact, a = approximate, u = upper bound on F

By default, canon presents the raw coefficients of the canonical correlations in matrix form, reports the canonical correlations, and finally reports the tests of significance of all canonical correlations. The two views on car size are closely related: the best linear combination of the physical measurements is correlated at almost 0.95 with the best linear combination of the mechanical measurements. All the tests are significant.

To see the standardized coefficients instead of the raw coefficients, we can use the stdcoef option on replay, which gives the standardized coefficients in matrix form. We specify the notests option to suppress the display of tests this time.

. canon, stdcoef notests

Canonical correlation analysis

Number of obs =

74

Standardized coefficients for the first variable set

	1	2	3	4
length weight headroom trunk	0.2110 0.7898 0.0297 -0.0098	3.2095 -2.8469 -0.3131 -0.1466	0.7334 -0.7448 1.2995 -0.9134	0.4714 0.5308 -0.0373 -1.3914

Standardized coefficients for the second variable set

	1	2	3	4
displacement mpg gear_ratio turn	0.4932	-1.1525	1.7568	-0.0493
	-0.2670	-0.2388	0.3954	1.4337
	0.0150	0.4691	1.6698	-0.4705
	0.3493	1.3694	0.0145	0.9857

Canonical correlations:

0.9476 0.3400 0.0634 0.0447

#### □ Technical note

canon, with the stderr option, reports standard errors for the coefficients in the linear combinations; most other software does not. You should view these standard errors as lower bounds for the true standard errors. It is based on the assumption that the coefficients for one set of measurements are correct for calculating the coefficients and standard errors of the other relationship on the basis of a linear regression.

After canon, if you predict a canonical variate and regress it on the other variable set, the variance you get from the regression will be the variance you get from canon multiplied by the square of the corresponding canonical correlation.

#### Stored results

canon stores the following in e():

```
Scalars
                           number of observations
    e(N)
                           residual degrees of freedom
    e(df_r)
    e(df)
                           degrees of freedom
                           numerator degrees of freedom for significance tests
    e(df1)
    e(df2)
                           denominator degrees of freedom for significance tests
    e(n_lc)
                           the linear combination calculated
    e(n_cc)
                           number of canonical correlations calculated
    e(rank)
                           rank of e(V)
Macros
    e(cmd)
                           canon
    e(cmdline)
                           command as typed
    e(wtype)
                           weight type
                           weight expression
    e(wexp)
    e(properties)
    e(estat_cmd)
                           program used to implement estat
    e(predict)
                           program used to implement predict
    e(marginsnotok)
                           predictions disallowed by margins
Matrices
    e(b)
                           coefficient vector
                           statistics for canonical correlation #
    e(stat_#)
                           statistics for overall model
    e(stat_m)
    e(canload11)
                           canonical loadings for varlist1
    e(canload22)
                           canonical loadings for varlist2
    e(canload12)
                           correlation between varlist1 and the canonical variates from varlist2
    e(canload21)
                           correlation between varlist2 and the canonical variates from varlist1
    e(rawcoef_var1)
                           raw coefficients for varlist1
    e(rawcoef_var2)
                           raw coefficients for varlist2
    e(stdcoef_var1)
                           standardized coefficients for varlist1
    e(stdcoef_var2)
                           standardized coefficients for varlist2
    e(ccorr)
                           canonical correlation coefficients
                           correlation matrix for varlist1
    e(corr_var1)
    e(corr_var2)
                           correlation matrix for varlist2
    e(corr_mixed)
                           correlation matrix between varlist1 and varlist2
                           variance-covariance matrix of the estimators
    e(V)
Functions
    e(sample)
                           marks estimation sample
```

## Methods and formulas

Let the covariance matrix between the two sets of variables be

$$\begin{pmatrix} \mathbf{S}_{\mathbf{y}\mathbf{y}} & \mathbf{S}_{\mathbf{y}\mathbf{x}} \\ \mathbf{S}_{\mathbf{x}\mathbf{y}} & \mathbf{S}_{\mathbf{x}\mathbf{x}} \end{pmatrix}$$

Here y indicates the first variable set and x indicates the second variable set.

The squared canonical correlations are the eigenvalues of  $V = S_{yy}^{-1}S_{yx}S_{xx}^{-1}S_{xy}$  or  $W = S_{xx}^{-1}S_{xy}S_{yy}^{-1}S_{yx}$  (either will work), which are both nonsymmetric matrices (Rencher 1998, 312–317; Rencher and Christensen 2012, 385–389). Let the eigenvalues of V (and W) be called  $r_k$ , the eigenvectors of V be called  $r_k$ , and the eigenvectors of V be called  $r_k$ . These eigenvectors are the raw coefficients for calculating the canonical variates, which are the linear combinations for the two sets of variables with maximal correlation. The eigenvalue equation for V is

$$\mathbf{S}_{\mathbf{v}\mathbf{v}}^{-1}\mathbf{S}_{\mathbf{y}\mathbf{x}}\mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1}\mathbf{S}_{\mathbf{x}\mathbf{y}}\mathbf{a}_k - r_k^2\mathbf{a}_k = 0$$

Premultiplying by  $S_{xx}^{-1}S_{xy}$ , we see that

$$(\mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1}\mathbf{S}_{\mathbf{x}\mathbf{y}}\mathbf{S}_{\mathbf{y}\mathbf{y}}^{-1}\mathbf{S}_{\mathbf{y}\mathbf{x}})(\mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1}\mathbf{S}_{\mathbf{x}\mathbf{y}}\mathbf{a}_k) - r_k^2\mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1}\mathbf{S}_{\mathbf{x}\mathbf{y}}\mathbf{a}_k = 0$$

so the  $\mathbf{b}_k$  are proportional to  $\mathbf{S}_{\mathbf{x}\mathbf{y}}^{-1}\mathbf{S}_{\mathbf{x}\mathbf{y}}\mathbf{a}_k$ . Eigenvectors are determined up to a scale factor, and we choose the eigenvectors to give canonical variates with variance one. The canonical variates with correlation  $r_k$  are given by

$$\mathbf{u}_k = \mathbf{a}_k \mathbf{x}$$
 and  $\mathbf{v}_k = \mathbf{b}_k \mathbf{y}$ 

In fact

$$\mathbf{b}_k = \frac{1}{r_k} \mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1} \mathbf{S}_{\mathbf{x}\mathbf{y}} \mathbf{a}_k$$

To calculate lower bounds for the standard errors in this form, assume that the eigenvectors  $\mathbf{a}_k$  are fixed. The formula relating  $\mathbf{a}_k$  and  $\mathbf{b}_k$  is given above. The coefficients given by  $\mathbf{b}_k$  have covariance matrix

$$\frac{1-r_k^2}{r_k^2(n-k-1)}\mathbf{S}_{\mathbf{x}\mathbf{x}}^{-1}$$

Here n is the number of observations and k is the number of variables in the set x.

Likewise, we can let the correlation matrix between the two sets of variables be

$$\begin{pmatrix} \mathbf{R_{yy}} & \mathbf{R_{yx}} \\ \mathbf{R_{xy}} & \mathbf{R_{xx}} \end{pmatrix}$$

That is,  $\mathbf{R}_{yy}$  is the correlation matrix of the first set of variables with themselves,  $\mathbf{R}_{xx}$  is the correlation matrix of the second set of variables with themselves, and  $\mathbf{R}_{yx}$  (and  $\mathbf{R}_{xy}$ ) contains the cross-correlations.

Using correlation matrices, the squared canonical correlations are the eigenvalues of  $\widetilde{\mathbf{V}} = \mathbf{R}_{\mathbf{yy}}^{-1}\mathbf{R}_{\mathbf{yx}}\mathbf{R}_{\mathbf{xx}}^{-1}\mathbf{R}_{\mathbf{xy}}$  or  $\widetilde{\mathbf{W}} = \mathbf{R}_{\mathbf{xx}}^{-1}\mathbf{R}_{\mathbf{xy}}\mathbf{R}_{\mathbf{yy}}^{-1}\mathbf{R}_{\mathbf{yx}}$  (Rencher 1998, 318–319; Rencher and Christensen 2012, 389). The corresponding eigenvectors are the standardized coefficients for determining the canonical variates from the centered and standardized original variables (mean 0 and variance 1). Eigenvectors are determined only up to a scale factor; we choose the scale to give the canonical variates in standardized (variance 1) form.

If the eigenvalues are  $r_1, r_2, \ldots, r_m$  where m is the number of canonical correlations, we test the hypothesis that there is no (linear) relationship between the two variable sets. This is equivalent to the statement that none of the correlations  $r_1, r_2, \ldots, r_m$  is significant.

Wilks's (1932) lambda statistic is

$$\Lambda_1 = \prod_{i=1}^m (1 - r_i^2)$$

and is a likelihood-ratio statistic. This statistic is distributed as the Wilks  $\Lambda$ -distribution. Rejection of the null hypothesis is for small values of  $\Lambda_1$ .

Pillai's (1955) trace for canonical correlations is

$$V^{(m)} = \sum_{i=1}^{m} r_i^2$$

and the Lawley-Hotelling trace (Lawley 1938 and Hotelling 1951) is

$$U^{(m)} = \sum_{i=1}^{m} \frac{r_i^2}{1 - r_i^2}$$

Roy's (1939) largest root is given by

$$\theta = r_1^2$$

Rencher and Christensen (2012, 391–395) has tables providing critical values for these statistics and discussion on significance testing for canonical correlations.

Canonical loadings, the correlation between a variable set and its corresponding canonical variate set, are calculated by canon and used in [MV] canon postestimation.

For a note about Harold Hotelling, see [MV] hotelling.

### **Acknowledgment**

Significance testing of canonical correlations is based on the cancor package originally written by Philip B. Ender of UCLA Academic Technology Services.

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#### Also see

- [MV] canon postestimation Postestimation tools for canon
- [MV] **factor** Factor analysis
- [MV] mvreg Multivariate regression
- [MV] pca Principal component analysis
- [R] correlate Correlations (covariances) of variables or coefficients
- [R] **pcorr** Partial and semipartial correlation coefficients
- [R] regress Linear regression
- [U] 20 Estimation and postestimation commands

### **Title**

### canon postestimation — Postestimation tools for canon

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

### **Postestimation commands**

The following postestimation commands are of special interest after canon:

Command	Description
estat correlations	show correlation matrices
estat loadings	show loading matrices
estat rotate	rotate raw coefficients, standard coefficients, or loading matrices
estat rotatecompare	compare rotated and unrotated coefficients or loadings
screeplot	plot canonical correlations

The following standard postestimation commands are also available:

Command	Description
estat summarize	summary statistics for the estimation sample
estat vce	variance-covariance matrix of the estimators (VCE)
estimates	cataloging estimation results
lincom	point estimates, standard errors, testing, and inference for linear combinations of coefficients
nlcom	point estimates, standard errors, testing, and inference for nonlinear combinations of coefficients
predict	predictions, residuals, influence statistics, and other diagnostic measures
predictnl	point estimates, standard errors, testing, and inference for generalized predictions
test	Wald tests of simple and composite linear hypotheses
testnl	Wald tests of nonlinear hypotheses

# predict

# Description for predict

predict creates a new variable containing predictions such as linear combinations and their standard errors.

#### Menu for predict

Statistics > Postestimation

#### Syntax for predict

predict	[type] newvar [if] [in], statistic* [ $\underline{c}$ orrelation(#)]
statistic*	Description
Main	
u	calculate linear combination of varlist <sub>1</sub>
v	calculate linear combination of varlist2
stdu	calculate standard error of the linear combination of $varlist_1$
stdv	calculate standard error of the linear combination of varlist <sub>2</sub>

<sup>\*</sup> There is no default statistic; you must specify one statistic from the list.

These statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample.

### **Options for predict**

Main

u and v calculate the linear combinations of *varlist*<sub>1</sub> and *varlist*<sub>2</sub>, respectively. For the first canonical correlation, u and v are the linear combinations having maximal correlation. For the second canonical correlation, specified in predict with the correlation(2) option, u and v have maximal correlation subject to the constraints that u is orthogonal to the u from the first canonical correlation, and v is orthogonal to the v from the first canonical correlation. The third and higher correlations are defined similarly. Canonical correlations may be chosen either with the lc() option to canon or by specifying the correlation() option to predict.

stdu and stdv calculate the standard errors of the respective linear combinations.

correlation(#) specifies the canonical correlation for which the requested statistic is to be computed. The default is correlation(1). If the lc() option to canon was used to calculate a particular canonical correlation, then only this canonical correlation is in the estimation results. You can obtain estimates for it either by specifying correlation(1) or by omitting the correlation() option.

#### estat

### **Description for estat**

estat correlations displays the correlation matrices calculated by canon for  $varlist_1$  and  $varlist_2$  and between the two lists.

estat loadings displays the canonical loadings computed by canon.

estat rotate performs orthogonal varimax rotation of the raw coefficients, standard coefficients, or canonical loadings. Rotation is calculated on the canonical loadings regardless of which coefficients or loadings are actually rotated.

estat rotatecompare displays the rotated and unrotated coefficients or loadings and the most recently rotated coefficients or loadings. This command may be used only if estat rotate has been performed first.

#### Menu for estat

Statistics > Postestimation

#### Syntax for estat

```
Display the correlation matrices

estat correlations [, format(%fmt)]

Display the canonical loadings

estat loadings [, format(%fmt)]

Perform orthogonal varimax rotation

estat rotate [, rawcoefs stdcoefs loadings format(%fmt)]

Display the rotated and unrotated coefficients or loadings
```

estat rotatecompare [, format(%fmt)]

### **Option for estat**

format (% fmt) specifies the display format for numbers in matrices; see [D] format. format (% 8.4f) is the default.

rawcoefs, an option for estat rotate, requests the rotation of raw coefficients. It is the default. stdcoefs, an option for estat rotate, requests the rotation of standardized coefficients.

loadings, an option for estat rotate, requests the rotation of the canonical loadings.

### Remarks and examples

In addition to the coefficients presented by canon in computing canonical correlations, several other matrices may be of interest.

#### Example 1: Predictions

Recall from canon the example of two scientists trying to describe how "big" a car is. One took physical measurements—the length, weight, headroom, and trunk space—whereas the second took mechanical measurements—engine displacement, mileage rating, gear ratio, and turning radius. We discovered that these two views are closely related, with the best linear combination of the two types of measurements, the largest canonical correlation, at 0.9476. We can prove that the first canonical correlation is correct by calculating the two linear combinations and then calculating the ordinary correlation.

```
. use http://www.stata-press.com/data/r14/auto
(1978 Automobile Data)
```

- . quietly canon (length weight headroom trunk) (displ mpg gear\_ratio turn)
- . predict physical, u corr(1)
- . predict mechanical, v corr(1)
- . correlate mechanical physical (obs=74)

	mechan~l	physical
mechanical	1.0000	
physical	0.9476	1.0000

. drop mechanical physical

### Example 2: Canonical loadings

Researchers are often interested in the canonical loadings, the correlations between the original variable lists and their canonical variates. The canonical loadings are used to interpret the canonical variates. However, as shown in the technical note later in this entry, Rencher (1988; 1992; 1998, sec. 8.6.3) and Rencher and Christensen (2012, 397) have shown that there is no information in these correlations about how one variable list contributes jointly to canonical correlation with the other. Loadings are still often discussed, and estat loadings reports these as well as the cross-loadings or correlations between varlist<sub>1</sub> and the canonical variates for varlist<sub>2</sub> and the correlations between varlist<sub>2</sub> and the canonical variates for varlist<sub>1</sub>. The loadings and cross-loadings are all computed by canon.

#### . estat loadings

Canonical loadings for variable list 1

	1	2	3	4
length	0.9664	0.2481	0.0361	-0.0566
weight	0.9972	-0.0606	-0.0367	0.0235
headroom	0.5140	-0.1295	0.7134	-0.4583
trunk	0.6941	0.0644	-0.0209	-0.7167

#### Canonical loadings for variable list 2

	1	2	3	4
displacement	0.9404	-0.3091	0.1050	0.0947
mpg	-0.8569	-0.1213	0.1741	0.4697
gear_ratio	-0.7945	0.3511	0.4474	-0.2129
turn	0.9142	0.3286	-0.0345	0.2345

Correlation between variable list 1 and canonical variates from list 2

	1	2	3	4
length	0.9158	0.0844	0.0023	-0.0025
weight	0.9449	-0.0206	-0.0023	0.0011
headroom	0.4871	-0.0440	0.0452	-0.0205
trunk	0.6577	0.0219	-0.0013	-0.0320

Correlation between variable list 2 and canonical variates from list 1

	1	2	3	4
displacement	0.8912	-0.1051	0.0067	0.0042
mpg	-0.8120	-0.0413	0.0110	0.0210
gear_ratio	-0.7529	0.1194	0.0284	-0.0095
turn	0.8663	0.1117	-0.0022	0.0105

<sup>.</sup> mat load2 = r(canload22)

#### Example 3: Predictions and correlation matrices

In example 2, we saved the loading matrix for  $varlist_2$ , containing the mechanical variables, and we wish to verify that it is correct. We predict the canonical variates for  $varlist_2$  and then find the canonical correlations between the canonical variates and the original mechanical variables as a means of getting the correlation matrices, which we then display using estat correlations. The mixed correlation matrix is the same as the loading matrix that we saved.

- . predict mechanical1, v corr(1)
- . predict mechanical2, v corr(2)
- . predict mechanical3, v corr(3)
- . predict mechanical4, v corr(4)
- . quietly canon (mechanical1-mechanical4) (displ mpg gear\_ratio turn)
- . estat correlation

Correlations for variable list 1

	mechan~1	mechan~2	mechan~3	mechan~4
mechanical1 mechanical2 mechanical3 mechanical4	1.0000 -0.0000 -0.0000 -0.0000	1.0000 0.0000 -0.0000	1.0000	1.0000

#### Correlations for variable list 2

	displa~t	mpg	gear_r~o	turn
displacement mpg gear_ratio turn	1.0000 -0.7056 -0.8289 0.7768	1.0000 0.6162 -0.7192	1.0000 -0.6763	1.0000

#### Correlations between variable lists 1 and 2

	mechan~1	mechan~2	mechan~3	mechan~4
displacement	0.9404	-0.3091	0.1050	0.0947
mpg	-0.8569	-0.1213	0.1741	0.4697
gear_ratio	-0.7945	0.3511	0.4474	-0.2129
turn	0.9142	0.3286	-0.0345	0.2345

#### . matlist load2, format(%8.4f) border(bottom)

	1	2	3	4
displacement	0.9404	-0.3091	0.1050	0.0947
mpg	-0.8569	-0.1213	0.1741	0.4697
gear_ratio	-0.7945	0.3511	0.4474	-0.2129
turn	0.9142	0.3286	-0.0345	0.2345

#### 4

#### Example 4: Rotated canonical loadings

Here we observe the results of rotation of the canonical loadings, via the Kaiser varimax method outlined in Cliff and Krus (1976). This observation is often done for interpretation of the results; however, rotation destroys several fundamental properties of canonical correlation.

- . quietly canon (length weight headroom trunk) (displ mpg gear\_ratio turn)
- . estat rotate, loadings

Criterion varimax Rotation class orthogonal none

Normalization

#### Rotated canonical loadings

	1	2	3	4
length	0.3796	0.7603	0.4579	0.2613
weight	0.6540	0.5991	0.3764	0.2677
headroom	0.0390	0.1442	0.3225	0.9347
trunk	0.1787	0.2052	0.8918	0.3614
displacement	0.7638	0.4424	0.2049	0.4230
mpg	-0.3543	-0.4244	-0.8109	-0.1918
gear_ratio	-0.9156	-0.3060	-0.2292	0.1248
turn	0.3966	0.8846	0.2310	0.0832

#### Rotation matrix

	1	2	3	4
1 2 3 4	0.5960 -0.6821 -0.3213 0.2761	0.6359 0.6593 0.1113 0.3856	0.3948 0.1663 -0.3400 -0.8372	0.2908 -0.2692 0.8768 -0.2724

. estat rotatecompare

Rotated canonical loadings — orthogonal varimax

	1	2	3	4
length	0.3796	0.7603	0.4579	0.2613
weight	0.6540	0.5991	0.3764	0.2677
headroom	0.0390	0.1442	0.3225	0.9347
trunk	0.1787	0.2052	0.8918	0.3614
displacement	0.7638	0.4424	0.2049	0.4230
mpg	-0.3543	-0.4244	-0.8109	-0.1918
gear_ratio	-0.9156	-0.3060	-0.2292	0.1248
turn	0.3966	0.8846	0.2310	0.0832

#### Unrotated canonical loadings

	1	2	3	4
length	0.9664	0.2481	0.0361	-0.0566
weight	0.9972	-0.0606	-0.0367	0.0235
headroom	0.5140	-0.1295	0.7134	-0.4583
trunk	0.6941	0.0644	-0.0209	-0.7167
displacement	0.9404	-0.3091	0.1050	0.0947
mpg	-0.8569	-0.1213	0.1741	0.4697
gear_ratio	-0.7945	0.3511	0.4474	-0.2129
turn	0.9142	0.3286	-0.0345	0.2345

#### □ Technical note

estat loadings reports the canonical loadings or correlations between a *varlist* and its corresponding canonical variates. It is widely claimed that the loadings provide a more valid interpretation of the canonical variates. Rencher (1988; 1992; 1998, sec. 8.6.3) and Rencher and Christensen (2012, 397) has shown that a weighted sum of the correlations between an  $x_j \in varlist_1$  and the canonical variates from  $varlist_1$  is equal to the squared multiple correlation between  $x_j$  and the variables in  $varlist_2$ . The correlations do not give new information on the importance of a given variable in the context of the others. Rencher and Christensen (2012, 397) notes, "The researcher who uses these correlations for interpretation is unknowingly reducing the multivariate setting to a univariate one."

#### Stored results

estat correlations stores the following in r():

rotation matrix

```
r(corr_var1)
                        correlations for varlist1
    r(corr_var2)
                        correlations for varlist<sub>2</sub>
    r(corr_mixed)
                        correlations between varlist_1 and varlist_2
estat loadings stores the following in r():
Matrices
    r(canload11)
                        canonical loadings for varlist1
    r(canload22)
                        canonical loadings for varlist2
    r(canload21)
                        correlations between varlist2 and the canonical variates for varlist1
    r(canload12)
                        correlations between varlist_1 and the canonical variates for varlist_2
estat rotate stores the following in r():
Macros
    r(coefficients) coefficients rotated
    r(class)
                        rotation classification
    r(criterion)
                        rotation criterion
Matrices
    r(AT)
                        rotated coefficient matrix
```

### Methods and formulas

r(T)

Cliff and Krus (1976) state that they use the Kaiser varimax method with normalization for rotation. The loading matrix, the correlation matrix between the original variables and their canonical variates, is already normalized. Consequently, normalization is not required, nor is it offered as an option.

Rotation after canonical correlation is a subject fraught with controversy. Although some researchers wish to rotate coefficients and loadings for greater interpretability, and Cliff and Krus (1976) have shown that some properties of canonical correlations are preserved by orthogonal rotation, rotation does destroy some of the fundamental properties of canonical correlation. Rencher (1992), Rencher and Christensen (2012), and Thompson (1996) contribute on the topic. Rencher speaks starkly against rotation. Thompson explains why rotation is desired as well as why it is at odds with the principles of canonical correlation analysis.

The researcher is encouraged to consider carefully his or her goals in canonical correlation analysis and these references when evaluating whether rotation is an appropriate tool to use.

Harris (2001) gives an amusing critique on the misuse of canonical loadings in the interpretation of canonical correlation analysis results. As mentioned, Rencher (1988; 1992; 1998, sec. 8.6.3) and Rencher and Christensen (2012, 397) critique the use of canonical loadings.

#### References

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#### Also see

[MV] **canon** — Canonical correlations

[MV] rotatemat — Orthogonal and oblique rotations of a Stata matrix

[MV] screeplot — Scree plot

[U] 20 Estimation and postestimation commands

#### Title

**cluster** — Introduction to cluster-analysis commands

Description Syntax Remarks and examples References Also see

### **Description**

Stata's cluster-analysis routines provide several hierarchical and partition clustering methods, postclustering summarization methods, and cluster-management tools. This entry presents an overview of cluster analysis, the cluster and clustermat commands (also see [MV] clustermat), as well as Stata's cluster-analysis management tools. The hierarchical clustering methods may be applied to the data by using the cluster command or to a user-supplied dissimilarity matrix by using the clustermat command.

The cluster command has the following subcommands, which are detailed in their respective manual entries.

#### Partition-clustering methods for observations

kmeans	[MV] cluster k	kmeans and	kmedians	Kmeans cluster analysis
kmedians	[MV] cluster k	kmeans and	kmedians	Kmedians cluster analysis

#### Hierarchical clustering methods for observations

singlelinkage	[MV] cluster linkage	Single-linkage cluster analysis
averagelinkage	[MV] cluster linkage	Average-linkage cluster analysis
${\tt completelinkage}$	[MV] cluster linkage	Complete-linkage cluster analysis
waveragelinkage	[MV] cluster linkage	Weighted-average linkage cluster analysis
medianlinkage	[MV] cluster linkage	Median-linkage cluster analysis
centroidlinkage	[MV] cluster linkage	Centroid-linkage cluster analysis
wardslinkage	[MV] cluster linkage	Ward's linkage cluster analysis

#### Postclustering commands

stop	[MV] cluster stop	Cluster-analysis stopping rules
dendrogram	[MV] cluster dendrogram	Dendrograms for hierarchical cluster analysis
generate	[MV] cluster generate	Generate summary or grouping variables from a cluster analysis

#### Us

		variables from a cluster analysis
ser utilities		
notes	[MV] cluster notes	Place notes in cluster analysis
dir	[MV] cluster utility	Directory list of cluster analyses
list	[MV] cluster utility	List cluster analyses
drop	[MV] cluster utility	Drop cluster analyses
use	[MV] cluster utility	Mark cluster analysis as most recent one
rename	[MV] cluster utility	Rename cluster analyses
renamevar	[MV] cluster utility	Rename cluster-analysis variables

#### **Programmer utilities**

	[MV] cluster programming subroutines	Add cluster-analysis routines
query	[MV] cluster programming utilities	Obtain cluster-analysis attributes
set	[MV] cluster programming utilities	Set cluster-analysis attributes
delete	[MV] cluster programming utilities	Delete cluster-analysis attributes
parsedistance	[MV] cluster programming utilities	Parse (dis)similarity measure names
measures	[MV] cluster programming utilities	Compute (dis)similarity measures

The clustermat command has the following subcommands, which are detailed along with the related cluster command manual entries. Also see [MV] clustermat.

#### Hierarchical clustering methods for matrices

[MV] measure\_option

singlelinkage	[MV] cluster linkage	Single-linkage cluster analysis
averagelinkage	[MV] cluster linkage	Average-linkage cluster analysis
completelinkage	[MV] cluster linkage	Complete-linkage cluster analysis
waveragelinkage	[MV] cluster linkage	Weighted-average linkage cluster analysis
medianlinkage	[MV] cluster linkage	Median-linkage cluster analysis
centroidlinkage	[MV] cluster linkage	Centroid-linkage cluster analysis
wardslinkage	[MV] cluster linkage	Ward's linkage cluster analysis

Also, the clustermat stop postclustering command has syntax similar to that of the cluster stop command; see [MV] cluster stop. For the remaining postclustering commands and user utilities, you may specify either cluster or clustermat—it does not matter which.

If you are new to Stata's cluster-analysis commands, we recommend that you first read this entry and then read the following:

Option for similarity and dissimilarity measures

[MV] clustermat	Cluster analysis of a dissimilarity matrix
[MV] cluster kmeans and kmedians	Kmeans and kmedians cluster analysis
[MV] cluster linkage	Hierarchical cluster analysis
[MV] cluster dendrogram	Dendrograms for hierarchical cluster analysis
[MV] cluster stop	Cluster-analysis stopping rules
[MV] cluster generate	Generate summary or grouping variables from a
	cluster analysis

### **Syntax**

```
Cluster analysis of data

cluster subcommand ...

Cluster analysis of a dissimilarity matrix

clustermat subcommand ...
```

### Remarks and examples

Remarks are presented under the following headings:

Introduction to cluster analysis Stata's cluster-analysis system Data transformations and variable selection Similarity and dissimilarity measures Partition cluster-analysis methods Hierarchical cluster-analysis methods Agglomerative methods Lance and Williams's recurrence formula Dissimilarity transformations and the Lance and Williams formula Warning concerning similarity or dissimilarity choice Synonyms Reversals Hierarchical cluster analysis applied to a dissimilarity matrix User-supplied dissimilarities Clustering variables instead of observations Postclustering commands Cluster-management tools

### Introduction to cluster analysis

Cluster analysis attempts to determine the natural groupings (or clusters) of observations. Sometimes this process is called "classification", but this term is used by others to mean discriminant analysis, which is related but is not the same; see [MV] **discrim**. To avoid confusion, we will use "cluster analysis" or "clustering" when referring to finding groups in data. Defining cluster analysis is difficult (maybe impossible). Kaufman and Rousseeuw (1990) start their book by saying, "Cluster analysis is the art of finding groups in data." Everitt et al. (2011, 7) use the terms "cluster", "group", and "class" and say, concerning a formal definition for these terms, "In fact it turns out that such formal definition is not only difficult but may even be misplaced."

Everitt et al. (2011) and Gordon (1999) provide examples of the use of cluster analysis, such as in refining or redefining diagnostic categories in psychiatry, detecting similarities in artifacts by archaeologists to study the spatial distribution of artifact types, discovering hierarchical relationships in taxonomy, and identifying sets of similar cities so that one city from each class can be sampled in a market research task. Also, the activity now called "data mining" relies extensively on cluster-analysis methods.

We view cluster analysis as an exploratory data-analysis technique. According to Everitt, "Many cluster-analysis techniques have taken their place alongside other exploratory data-analysis techniques as tools of the applied statistician. The term exploratory is important here because it explains the largely absent 'p-value', ubiquitous in many other areas of statistics. . . . Clustering methods are intended largely for generating rather than testing hypotheses" (1993, 10).

Although some have said that there are as many cluster-analysis methods as there are people performing cluster analysis. This is a gross understatement! There exist infinitely more ways to perform a cluster analysis than people who perform them.

There are several general types of cluster-analysis methods, each having many specific methods. Also, most cluster-analysis methods allow a variety of distance measures for determining the similarity or dissimilarity between observations. Some of the measures do not meet the requirements to be called a distance metric, so we use the more general term "dissimilarity measure" in place of distance. Similarity measures may be used in place of dissimilarity measures. There are an infinite number of similarity and dissimilarity measures. For instance, there are an infinite number of Minkowski distance metrics, with the familiar Euclidean, absolute-value, and maximum-value distances being special cases.

In addition to cluster method and dissimilarity measure choice, if you are performing a cluster analysis, you might decide to perform data transformations and/or variable selection before clustering. Then you might need to determine how many clusters there really are in the data, which you can do using stopping rules. There is a surprisingly large number of stopping rules mentioned in the literature. For example, Milligan and Cooper (1985) compare 30 different stopping rules.

Looking at all of these choices, you can see why there are more cluster-analysis methods than people performing cluster analysis.

#### Stata's cluster-analysis system

Stata's cluster and clustermat commands were designed to allow you to keep track of the various cluster analyses performed on your data. The main clustering subcommands—singlelinkage, averagelinkage, completelinkage, waveragelinkage, medianlinkage, centroidlinkage, wardslinkage (see [MV] cluster linkage), kmeans, and kmedians (see [MV] cluster kmeans and kmedians)—create named Stata cluster objects that keep track of the variables these methods create and hold other identifying information for the cluster analysis. These cluster objects become part of your dataset. They are saved with your data when your data are saved and are retrieved when you again use your dataset; see [D] save and [D] use.

Post-cluster-analysis subcommands are available with the cluster and clustermat commands so that you can examine the created clusters. Cluster-management tools are provided that allow you to add information to the cluster objects and to manipulate them as needed. The main clustering subcommands, postclustering subcommands, and cluster-management tools are discussed in the following sections.

Stata's clustering methods fall into two general types: partition and hierarchical. These two types are discussed below. There exist other types, such as fuzzy partition (where observations can belong to more than one group). Stata's cluster command is designed so that programmers can extend it by adding more methods; see [MV] cluster programming subroutines and [MV] cluster programming utilities for details.

#### □ Technical note

If you are familiar with Stata's large array of estimation commands, be careful to distinguish between cluster analysis (the cluster command) and the vce(cluster clustvar) option (see [R] vce\_option) allowed with many estimation commands. Cluster analysis finds groups in data. The vce(cluster clustvar) option allowed with various estimation commands indicates that the observations are independent across the groups defined by the option but are not necessarily independent within those groups. A grouping variable produced by the cluster command will seldom satisfy the assumption behind the use of the vce(cluster clustvar) option.

Stata's cluster command has no built-in data transformations, but because Stata has full data management and statistical capabilities, you can use other Stata commands to transform your data before calling the cluster command. Standardizing the variables is sometimes important to keep a variable with high variability from dominating the cluster analysis. In other cases, standardizing variables hides the true groupings present in the data. The decision to standardize or perform other data transformations depends on the type of data and the nature of the groups.

Data transformations (such as standardization of variables) and the variables selected for use in clustering can also greatly affect the groupings that are discovered. These and other cluster-analysis data issues are covered in Milligan and Cooper (1988) and Schaffer and Green (1996) and in many of the cluster-analysis texts, including Anderberg (1973); Gordon (1999); Everitt et al. (2011); and Späth (1980).

#### Similarity and dissimilarity measures

Several similarity and dissimilarity measures have been implemented for Stata's clustering commands for both continuous and binary variables. For information, see [MV] *measure\_option*.

#### Partition cluster-analysis methods

Partition methods break the observations into a distinct number of nonoverlapping groups. Stata has implemented two partition methods, kmeans and kmedians.

One of the more commonly used partition clustering methods is called kmeans cluster analysis. In kmeans clustering, the user specifies the number of clusters, k, to create using an iterative process. Each observation is assigned to the group whose mean is closest, and then based on that categorization, new group means are determined. These steps continue until no observations change groups. The algorithm begins with k seed values, which act as the k group means. There are many ways to specify the beginning seed values.

A variation of kmeans clustering is kmedians clustering. The same process is followed in kmedians as in kmeans, except that medians, instead of means, are computed to represent the group centers at each step. See [MV] cluster kmeans and kmedians for the details of the cluster kmeans and cluster kmedians commands.

These partition-clustering methods will generally be quicker and will allow larger datasets than the hierarchical clustering methods outlined next. However, if you wish to examine clustering to various numbers of clusters, you will need to execute cluster many times with the partition methods. Clustering to various numbers of groups by using a partition method typically does not produce clusters that are hierarchically related. If this relationship is important for your application, consider using one of the hierarchical methods.

### Hierarchical cluster-analysis methods

Hierarchical clustering creates hierarchically related sets of clusters. Hierarchical clustering methods are generally of two types: agglomerative or divisive.

Agglomerative hierarchical clustering methods begin with each observation's being considered as a separate group (N groups each of size 1). The closest two groups are combined (N-1 groups, one of size 2 and the rest of size 1), and this process continues until all observations belong to the same group. This process creates a hierarchy of clusters.

In addition to choosing the similarity or dissimilarity measure to use in comparing 2 observations, you can choose what to compare between groups that contain more than 1 observation. The method used to compare groups is called a linkage method. Stata's cluster and clustermat commands provide several hierarchical agglomerative linkage methods, which are discussed in the next section.

Unlike hierarchical agglomerative clustering, divisive hierarchical clustering begins with all observations belonging to one group. This group is then split in some fashion to create two groups. One of these two groups is then split to create three groups; one of these three is then split to create four groups, and so on, until all observations are in their own separate group. Stata currently has no divisive hierarchical clustering commands. There are relatively few mentioned in the literature, and they tend to be particularly time consuming to compute.

To appreciate the underlying computational complexity of both agglomerative and divisive hierarchical clustering, consider the following information paraphrased from Kaufman and Rousseeuw (1990). The first step of an agglomerative algorithm considers N(N-1)/2 possible fusions of observations to find the closest pair. This number grows quadratically with N. For divisive hierarchical clustering, the first step would be to find the best split into two nonempty subsets, and if all possibilities were considered, it would amount to  $2^{(N-1)}-1$  comparisons. This number grows exponentially with N.

### Agglomerative methods

Stata's cluster and clustermat commands provide the following hierarchical agglomerative linkage methods: single, complete, average, Ward's method, centroid, median, and weighted average. There are others mentioned in the literature, but these are the best-known methods.

Single-linkage clustering computes the similarity or dissimilarity between two groups as the similarity or dissimilarity between the closest pair of observations between the two groups. Complete-linkage clustering, on the other hand, uses the farthest pair of observations between the two groups to determine the similarity or dissimilarity of the two groups. Average-linkage clustering uses the average similarity or dissimilarity of observations between the groups as the measure between the two groups. Ward's method joins the two groups that result in the minimum increase in the error sum of squares. The other linkage methods provide alternatives to these basic linkage methods.

The cluster singlelinkage and clustermat singlelinkage commands implement single-linkage hierarchical agglomerative clustering; see [MV] cluster linkage for details. Single-linkage clustering suffers (or benefits, depending on your point of view) from what is called chaining. Because the closest points between two groups determine the next merger, long, thin clusters can result. If this chaining feature is not what you desire, consider using one of the other methods, such as complete linkage or average linkage. Because of special properties that can be computationally exploited, single-linkage clustering is faster and uses less memory than the other linkage methods.

Complete-linkage hierarchical agglomerative clustering is implemented by the cluster completelinkage and clustermat completelinkage commands; see [MV] cluster linkage for details. Complete-linkage clustering is at the other extreme from single-linkage clustering. Complete linkage produces spatially compact clusters, so it is not the best method for recovering elongated cluster structures. Several sources, including Kaufman and Rousseeuw (1990), discuss the chaining of single linkage and the clumping of complete linkage.

Kaufman and Rousseeuw (1990) indicate that average linkage works well for many situations and is reasonably robust. The cluster averagelinkage and clustermat averagelinkage commands provide average-linkage clustering; see [MV] cluster linkage.

Ward (1963) presented a general hierarchical clustering approach where groups were joined to maximize an objective function. He used an error-sum-of-squares objective function to illustrate. Ward's method of clustering became synonymous with using the error-sum-of-squares criteria. Kaufman and

Rousseeuw (1990) indicate that Ward's method does well with groups that are multivariate normal and spherical but does not do as well if the groups are of different sizes or have unequal numbers of observations. The cluster wardslinkage and clustermat wardslinkage commands provide Ward's linkage clustering; see [MV] cluster linkage.

At each step of the clustering, centroid linkage merges the groups whose means are closest. The centroid of a group is the componentwise mean and can be interpreted as the center of gravity for the group. Centroid linkage differs from average linkage in that centroid linkage is concerned with the distance between the means of the groups, whereas average linkage looks at the average distance between the points of the two groups. The cluster centroidlinkage and clustermat centroidlinkage commands provide centroid-linkage clustering; see [MV] cluster linkage.

Weighted-average linkage and median linkage are variations on average linkage and centroid linkage, respectively. In both cases, the difference is in how groups of unequal size are treated when merged. In average linkage and centroid linkage, the number of elements of each group is factored into the computation, giving correspondingly larger influence to the larger group. These two methods are called unweighted because each observation carries the same weight. In weighted-average linkage and median linkage, the two groups are given equal weighting in determining the combined group, regardless of the number of observations in each group. These two methods are said to be weighted because observations from groups with few observations carry more weight than observations from groups with many observations. The cluster waveragelinkage and clustermat waveragelinkage commands provide weighted-average linkage clustering. The cluster medianlinkage and clustermat medianlinkage commands provide median linkage clustering; see [MV] cluster linkage.

#### Lance and Williams's recurrence formula

Lance and Williams (1967) developed a recurrence formula that defines, as special cases, most of the well-known hierarchical clustering methods, including all the hierarchical clustering methods found in Stata. Anderberg (1973); Jain and Dubes (1988); Kaufman and Rousseeuw (1990); Gordon (1999); Everitt et al. (2011); and Rencher and Christensen (2012) discuss the Lance–Williams formula and how most popular hierarchical clustering methods are contained within it.

From the notation of Everitt et al. (2011, 78), the Lance-Williams recurrence formula is

$$d_{k(ij)} = \alpha_i d_{ki} + \alpha_j d_{kj} + \beta d_{ij} + \gamma |d_{ki} - d_{kj}|$$

where  $d_{ij}$  is the distance (or dissimilarity) between cluster i and cluster j;  $d_{k(ij)}$  is the distance (or dissimilarity) between cluster k and the new cluster formed by joining clusters i and j; and  $\alpha_i$ ,  $\alpha_j$ ,  $\beta$ , and  $\gamma$  are parameters that are set based on the particular hierarchical cluster-analysis method.

The recurrence formula allows, at each new level of the hierarchical clustering, the dissimilarity between the newly formed group and the rest of the groups to be computed from the dissimilarities of the current grouping. This approach can result in a large computational savings compared with recomputing at each step in the hierarchy from the observation-level data. This feature of the recurrence formula allows clustermat to operate on a similarity or dissimilarity matrix instead of the data.

The following table shows the values of  $\alpha_i$ ,  $\alpha_j$ ,  $\beta$ , and  $\gamma$  for the hierarchical clustering methods implemented in Stata.  $n_i$ ,  $n_j$ , and  $n_k$  are the number of observations in group i, j, and k, respectively.

Clustering linkage method	$lpha_i$	$lpha_j$	β	$\gamma$
Single	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$
Complete	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$
Average	$\frac{n_i}{n_i + n_j}$	$\frac{n_j}{n_i + n_j}$	0	0
Weighted average	$\frac{1}{2}$	$\frac{1}{2}$	0	0
Centroid	$\frac{n_i}{n_i + n_j}$	$\frac{n_j}{n_i + n_j}$	$-\alpha_i \alpha_j$	0
Median	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{4}$	0
Ward's	$\frac{n_i + n_k}{n_i + n_j + n_k}$	$\frac{n_j + n_k}{n_i + n_j + n_k}$	$\frac{-n_k}{n_i + n_j + n_k}$	0

For information on the use of various similarity and dissimilarity measures in hierarchical clustering, see the next two sections.

#### Dissimilarity transformations and the Lance and Williams formula

The Lance-Williams formula, which is used as the basis for computing hierarchical clustering in Stata, is designed for use with dissimilarity measures. Before performing hierarchical clustering, Stata transforms similarity measures, both continuous and binary, to dissimilarities. After cluster analysis, Stata transforms the fusion values (heights at which the various groups join in the hierarchy) back to similarities.

Stata's cluster command uses

$$dissimilarity = 1 - similarity$$

to transform from a similarity to a dissimilarity measure and back again; see Kaufman and Rousseeuw (1990, 21). Stata's similarity measures range from either 0 to 1 or -1 to 1. The resulting dissimilarities range from 1 down to 0 and from 2 down to 0, respectively.

For continuous data, Stata provides both the L2 and L2squared dissimilarity measures, as well as both the L(#) and Lpower(#) dissimilarity measures. Why have both an L2 and L2squared dissimilarity measure, and why have both an L(#) and Lpower(#) dissimilarity measure?

For single- and complete-linkage hierarchical clustering (and for kmeans and kmedians partition clustering), there is no need for the additional L2squared and Lpower(#) dissimilarities. The same cluster solution is obtained when using L2 and L2squared (or L(#) and Lpower(#)), except that the resulting heights in the dendrogram are raised to a power.

However, for the other hierarchical clustering methods, there is a difference. For some of these other hierarchical clustering methods, the natural default for dissimilarity measure is L2squared. For instance, the traditional Ward's (1963) method is obtained by using the L2squared dissimilarity option.

### Warning concerning similarity or dissimilarity choice

With hierarchical centroid, median, Ward's, and weighted-average linkage clustering, Lance and Williams (1967); Anderberg (1973); Jain and Dubes (1988); Kaufman and Rousseeuw (1990); Everitt et al. (2011); and Gordon (1999) give various levels of warnings about using many of the similarity and dissimilarity measures ranging from saying that you should never use anything other than the default squared Euclidean distance (or Euclidean distance) to saying that the results may lack a useful interpretation.

Example 2 of [MV] **cluster linkage** illustrates part of the basis for this warning. The simple matching coefficient is used on binary data. The range of the fusion values for the resulting hierarchy is not between 1 and 0, as you would expect for the matching coefficient. The conclusions from the cluster analysis, however, agree well with the results obtained in other ways.

Stata does not restrict your choice of similarity or dissimilarity. If you are not familiar with these hierarchical clustering methods, use the default dissimilarity measure.

#### **Synonyms**

Cluster-analysis methods have been developed by researchers in many different disciplines. Because researchers did not always know what was happening in other fields, many synonyms for the different hierarchical cluster-analysis methods exist.

Blashfield and Aldenderfer (1978) provide a table of equivalent terms. Jain and Dubes (1988) and Day and Edelsbrunner (1984) also mention some of the synonyms and use various acronyms. Here is a list of synonyms:

#### Single linkage

Nearest-neighbor method Minimum method Hierarchical analysis Space-contracting method Elementary linkage analysis Connectedness method

#### Complete linkage

Furthest-neighbor method Maximum method Compact method Space-distorting method Space-dilating method Rank-order typal analysis Diameter analysis

#### Average linkage

Arithmetic-average clustering
Unweighted pair-group method using
arithmetic averages
UPGMA
Unweighted clustering
Group-average method
Unweighted group mean
Unweighted pair-group method

#### Weighted-average linkage

Weighted pair-group method using arithmetic averages WPGMA Weighted group-average method

#### Centroid linkage

Unweighted centroid method Unweighted pair-group centroid method UPGMC

Nearest-centroid sorting

Weighted group method

#### Median linkage

Gower's method Weighted centroid method Weighted pair-group centroid method WPGMC Weighted pair method

#### Ward's method

Minimum-variance method Error-sum-of-squares method Hierarchical grouping to minimize tr(W) HGROUP

#### Reversals

Unlike the other hierarchical methods implemented in Stata, centroid linkage and median linkage (see [MV] cluster linkage) can (and often do) produce reversals or crossovers; see Anderberg (1973), Jain and Dubes (1988), Gordon (1999), and Rencher and Christensen (2012). Normally, the dissimilarity or clustering criterion increases monotonically as the agglomerative hierarchical clustering progresses from many to few clusters. (For similarity measures, it monotonically decreases.) The dissimilarity value at which k+1 clusters form will be larger than the value at which k clusters form. When the dissimilarity does not increase monotonically through the levels of the hierarchy, it is said to have reversals or crossovers.

The word *crossover*, in this context, comes from the appearance of the resulting dendrogram (see [MV] **cluster dendrogram**). In a hierarchical clustering without reversals, the dendrogram branches extend in one direction (increasing dissimilarity measure). With reversals, some of the branches reverse and go in the opposite direction, causing the resulting dendrogram to be drawn with crossing lines (crossovers).

When reversals happen, Stata still produces correct results. You can still generate grouping variables (see [MV] cluster generate) and compute stopping rules (see [MV] cluster stop). However, the cluster dendrogram command will not draw a dendrogram with reversals; see [MV] cluster dendrogram. In all but the simplest cases, dendrograms with reversals are almost impossible to interpret visually.

### Hierarchical cluster analysis applied to a dissimilarity matrix

What if you want to perform a cluster analysis using a similarity or dissimilarity measure that Stata does not provide? What if you want to cluster variables instead of observations? The clustermat command gives you the flexibility to do either; see [MV] clustermat.

### User-supplied dissimilarities

There are situations where the dissimilarity between objects is evaluated subjectively (perhaps on a scale from 1 to 10 by a rater). These dissimilarities may be entered in a matrix and passed to the clustermat command to perform hierarchical clustering. Likewise, if Stata does not offer the dissimilarity measure you desire, you may compute the dissimilarities yourself and place them in a matrix and then use clustermat to perform the cluster analysis. [MV] clustermat illustrates both of these situations.

### Clustering variables instead of observations

Sometimes you want to cluster variables rather than observations, so you can use the cluster command. One approach to clustering variables in Stata is to use xpose (see [D] xpose) to transpose the variables and observations and then to use cluster. Another approach is to use the matrix dissimilarity command with the variables option (see [MV] matrix dissimilarity) to produce a dissimilarity matrix for the variables. This matrix is then passed to clustermat to obtain the hierarchical clustering. See [MV] clustermat.

## Postclustering commands

Stata's cluster stop and clustermat stop commands are used to determine the number of clusters. Two stopping rules are provided, the Caliński and Harabasz (1974) pseudo-F index and the Duda, Hart, and Stork (2001, sec. 10.10) Je(2)/Je(1) index with associated pseudo-T-squared. You can easily add stopping rules to the cluster stop command; see [MV] cluster stop for details.

The cluster dendrogram command presents the dendrogram (cluster tree) after a hierarchical cluster analysis; see [MV] **cluster dendrogram**. Options allow you to view the top portion of the tree or the portion of the tree associated with a group. These options are important with larger datasets because the full dendrogram cannot be presented.

The cluster generate command produces grouping variables after hierarchical clustering; see [MV] cluster generate. These variables can then be used in other Stata commands, such as those that tabulate, summarize, and provide graphs. For instance, you might use cluster generate to create a grouping variable. You then might use the pca command (see [MV] pca) to obtain the first two principal components of the data. You could follow that with a graph (see Stata Graphics Reference Manual) to plot the principal components, using the grouping variable from the cluster generate command to control the point labeling of the graph. This method would allow you to get one type of view into the clustering behavior of your data.

### Cluster-management tools

You may add notes to your cluster analysis with the cluster notes command; see [MV] cluster notes. This command also allows you to view and delete notes attached to the cluster analysis.

The cluster dir and cluster list commands allow you to list the cluster objects and attributes currently defined for your dataset. cluster drop lets you remove a cluster object. See [MV] cluster utility for details.

Cluster objects are referred to by name. If no name is provided, many of the cluster commands will, by default, use the cluster object from the most recently performed cluster analysis. The cluster use command tells Stata which cluster object to use. You can change the name attached to a cluster object with the cluster rename command and the variables associated with a cluster analysis with the cluster renamevar command. See [MV] cluster utility for details.

You can exercise fine control over the attributes that are stored with a cluster object; see [MV] cluster programming utilities.

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### Also see

- [MV] **clustermat** Introduction to clustermat commands
- [MV] cluster programming subroutines Add cluster-analysis routines
- [MV] cluster programming utilities Cluster-analysis programming utilities
- [MV] **discrim** Discriminant analysis

#### **Title**

**clustermat** — Introduction to clustermat commands

Description Syntax Remarks and examples References Also see

# **Description**

clustermat performs hierarchical cluster analysis on the dissimilarity matrix *matname*. clustermat is part of the cluster suite of commands; see [MV] cluster. All Stata hierarchical clustering methods are allowed with clustermat. The partition-clustering methods (kmeans and kmedians) are not allowed because they require the data.

See [MV] cluster for a listing of all the cluster and clustermat commands. The cluster dendrogram command (see [MV] cluster dendrogram) will display the resulting dendrogram, the clustermat stop command (see [MV] cluster stop) will help in determining the number of groups, and the cluster generate command (see [MV] cluster generate) will produce grouping variables. Other useful cluster subcommands include notes, dir, list, drop, use, rename, and renamevar; see [MV] cluster notes and [MV] cluster utility.

## **Syntax**

clustermat linkage matname ...

linkage	Description
singlelinkage averagelinkage completelinkage	single-linkage cluster analysis average-linkage cluster analysis complete-linkage cluster analysis
waveragelinkage medianlinkage	weighted-average linkage cluster analysis median-linkage cluster analysis
<u>cent</u> roidlinkage <u>ward</u> slinkage	centroid-linkage cluster analysis Ward's linkage cluster analysis

See [MV] cluster linkage.

clustermat stop has similar syntax to that of cluster stop; see [MV] cluster stop. For the remaining postclustering subcommands and user utilities, you may specify either cluster or clustermat—it does not matter which.

# Remarks and examples

If you are clustering observations by using one of the similarity or dissimilarity measures provided by Stata, the cluster command is what you need. If, however, you already have a dissimilarity matrix or can produce one for a dissimilarity measure that Stata does not provide, or if you want to cluster variables instead of observations, the clustermat command is what you need.

#### Example 1

Table 6 of Kaufman and Rousseeuw (1990) provides a subjective dissimilarity matrix among 11 sciences. Fourteen postgraduate economics students from different parts of the world gave subjective dissimilarities among these 11 sciences on a scale from 0 (identical) to 10 (very different). The final dissimilarity matrix was obtained by averaging the results from the students.

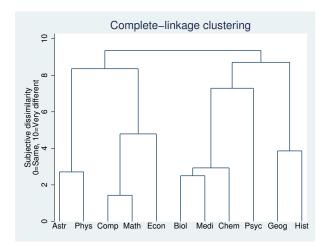
We begin by creating a label variable and a shorter version of the label variable corresponding to the 11 sciences. Then we create a row vector containing the lower triangle of the dissimilarity matrix.

```
. input str13 science
           science
  1. Astronomy
  2. Biology
  3. Chemistry
  4. Computer sci.
  5. Economics
  6. Geography
  7. History
  8. Mathematics
  9. Medicine
 10. Physics
 11. Psychology
. generate str4 shortsci = substr(science,1,4)
. matrix input D = (
> 0.00
> 7.86 0.00
> 6.50 2.93 0.00
> 5.00 6.86 6.50 0.00
> 8.00 8.14 8.21 4.79 0.00
> 4.29 7.00 7.64 7.71 5.93 0.00
> 8.07 8.14 8.71 8.57 5.86 3.86 0.00
> 3.64 7.14 4.43 1.43 3.57 7.07 9.07 0.00
> 8.21 2.50 2.93 6.36 8.43 7.86 8.43 6.29 0.00
> 2.71 5.21 4.57 4.21 8.36 7.29 8.64 2.21 5.07 0.00
> 9.36 5.57 7.29 7.21 6.86 8.29 7.64 8.71 3.79 8.64 0.00 )
```

There are several ways that we could have stored the dissimilarity information in a matrix. To avoid entering both the upper and lower triangle of the matrix, we entered the dissimilarities as a row vector containing the lower triangular entries of the dissimilarity matrix, including the diagonal of zeros (although there are options that would allow us to omit the diagonal of zeros). We typed matrix input  $D = \ldots$  instead of matrix  $D = \ldots$  so that we could omit the commas between entries; see [P] matrix define.

We now perform a complete-linkage cluster analysis on these dissimilarities. The name() option names the cluster analysis. We will name it complink. The shape(lower) option is what signals that the dissimilarity matrix is stored as a row vector containing the lower triangle of the dissimilarity matrix, including the diagonal of zeros. The add option indicates that the resulting cluster information should be added to the existing dataset. Here the existing dataset consists of the science label variable and the shortened version shortsci. See [MV] cluster linkage for details concerning these options. The short labels are passed to cluster dendrogram so that we can see which subjects were most closely related when viewing the dendrogram; see [MV] cluster dendrogram.

- . clustermat completelinkage D, shape(lower) add name(complink)
- . cluster dendrogram complink, labels(shortsci)
- > title(Complete-linkage clustering)
- > ytitle("Subjective dissimilarity" "0=Same, 10=Very different")



From the dendrogram, we see that mathematics and computer science were deemed most similar and that the economists most closely related their field of study to those two disciplines.

1

## Example 2

Stata does not provide the Bray and Curtis (1957) dissimilarity measure first described by Odum (1950). Using the same notation as that found in [MV] measure\_option, we find that the Bray-Curtis dissimilarity between observations i and j is

$$\frac{\sum_{a=1}^{p} |x_{ia} - x_{ja}|}{\sum_{a=1}^{p} (x_{ia} + x_{ja})}$$

Stata does not provide this measure because of the many cases where the measure is undefined (because of dividing by zero). However, when the data are positive the Bray-Curtis dissimilarity is well behaved.

Even though Stata does not automatically provide this measure, it is easy to obtain it and then use it with clustermat to perform hierarchical clustering. The numerator of the Bray-Curtis dissimilarity measure is the L1 (absolute value) distance. We use the matrix dissimilarity command (see [MV] matrix dissimilarity) to obtain the L1 dissimilarity matrix and then divide the elements of that matrix by the appropriate values to obtain the Bray-Curtis dissimilarity.

Fisher (1936) presented data, originally from Anderson (1935), on three species of iris. Measurements of the length and width of the sepal and petal were obtained for 50 samples of each of the three iris species. We obtained the data from Morrison (2005). Here we demonstrate average-linkage clustering of these 150 observations.

```
. use http://www.stata-press.com/data/r14/iris, clear
(Iris data)
```

. summarize seplen sepwid petlen petwid

Variable	Obs	Mean	Std. Dev.	Min	Max
seplen	150	5.843333	.8280661	4.3	7.9
sepwid	150	3.057333	.4358663	2	4.4
petlen	150	3.758	1.765298	1	6.9
petwid	150	1.199333	.7622377	.1	2.5

- . matrix dissimilarity irisD = seplen sepwid petlen petwid, L1
- . egen rtot = rowtotal(seplen sepwid petlen petwid)

```
forvalues a = 1/150 {
2.    forvalues b = 1/150 {
3.         mat irisD['a', 'b'] = irisD['a', 'b']/(rtot['a']+rtot['b'])
4.    }
5. }
```

. matlist irisD[1..5,1..5]

		obs1	obs2	obs3	obs4	obs5
obs	s1	0				
obs	s2	.035533	0			
obs	s3	.0408163	.026455	0		
obs	s4	.0510204	.026455	.0212766	0	
obs	s5	.0098039	.035533	.0408163	.0510204	0

The egen rowtotal() function provided the row totals used in the denominator of the Bray-Curtis dissimilarity measure; see [D] egen. We listed the dissimilarities between the first 5 observations.

We now compute the average-linkage cluster analysis on these 150 observations (see [MV] cluster linkage) and examine the Caliński–Harabasz pseudo-F index and the Duda–Hart Je(2)/Je(1) index (cluster stopping rules; see [MV] cluster stop) to try to determine the number of clusters.

- . clustermat averagelink irisD, name(iris) add
- . clustermat stop, variables(seplen sepwid petlen petwid)

Number of clusters	Calinski/ Harabasz pseudo-F
2	502.82
3	299.96
4	201.58
5	332.89
6	288.61
7	244.61
8	252.39
9	223.28
10	268.47
11	241.51
12	232.61
13	233.46
14	255.84
15	273.96

. clustermat stop, variables(seplen sepwid petlen petwid) rule(duda)

Number of clusters	Duda, Je(2)/Je(1)	/Hart pseudo T-squared
1	0.2274	502.82
2	0.8509	17.18
3	0.8951	5.63
4	0.4472	116.22
5	0.6248	28.23
6	0.9579	2.55
7	0.5438	28.52
8	0.8843	5.10
9	0.5854	40.37
10	0.0000	.
11	0.8434	6.68
12	0.4981	37.28
13	0.5526	25.91
14	0.6342	16.15
15	0.6503	3.23

The stopping rules are not conclusive here. From the Duda-Hart pseudo-T-squared (small values) you might best conclude that there are three, six, or eight natural clusters. The Caliński and Harabasz pseudo-F (large values) indicates that there might be two, three, or five groups.

With the iris data, we know the three species. Let's compare the average-linkage hierarchical cluster solutions with the actual species. The cluster generate command (see [MV] cluster generate) will generate grouping variables for our hierarchical cluster analysis.

- . cluster generate g = groups(2/6)
- . tabulate g2 iris

	Iris species				
g2	setosa	versicolo	virginica	Total	
1 2	50 0	0 50	0 50	50 100	
Total	50	50	50	150	

. tabulate g3 iris

g3		Iris specie versicolo		Total
1 2 3	50 0 0	0 46 4	0 50 0	50 96 4
Total	50	50	50	150

. tabulate g4 iris

	Iris species				
g4	setosa	versicolo	virginica	Total	
1	49	0	0	49	
2	1	0	0	1	
3	0	46	50	96	
4	0	4	0	4	
Total	50	50	50	150	

tabulate	ø5	iris

		Iris specie	s	
g5	setosa	versicolo	virginica	Total
1	49	0	0	49
2	1	0	0	1
3	0	45	15	60
4	0	1	35	36
5	0	4	0	4
Total	50	50	50	150

#### . tabulate g6 iris

	Iris species				
g6	setosa	versicolo	virginica	Total	
1	41	0	0	41	
2	8	0	0	8	
3	1	0	0	1	
4	0	45	15	60	
5	0	1	35	36	
6	0	4	0	4	
Total	50	50	50	150	

The two-group cluster solution splits Iris setosa from Iris versicolor and Iris virginica. The threeand four-group cluster solutions appear to split off some outlying observations from the two main groups. The five-group solution finally splits most of Iris virginica from the Iris versicolor but leaves some overlap.

Though this is not shown here, cluster solutions that better match the known species can be found by using dissimilarity measures other than Bray-Curtis.

## 4

# ▶ Example 3

The cluster command clusters observations. If you want to cluster variables, you have two choices. You can use xpose (see [D] xpose) to transpose the variables and observations, or you can use matrix dissimilarity with the variables option (see [MV] matrix dissimilarity) and then use clustermat.

In example 2 of [MV] cluster kmeans and kmedians, we introduce the women's club data. Thirty women were asked 35 yes-no questions. In [MV] cluster kmeans and kmedians, our interest was in clustering the 30 women for placement at luncheon tables. Here our interest is in understanding the relationship among the 35 variables. Which questions produced similar response patterns from the 30 women?

- . use http://www.stata-press.com/data/r14/wclub, clear
- . describe

Contains data from http://www.stata-press.com/data/r14/wclub.dta

obs: 30 vars: 35 size: 1,050

1 May 2014 16:56

variable name	storage type	display format	value label	variable label
bike	byte	%8.0g		enjoy bicycle riding Y/N
bowl	byte	%8.0g		enjoy bowling Y/N
swim	byte	%8.0g		enjoy swimming Y/N
jog	byte	%8.0g		enjoy jogging Y/N
hock	byte	%8.0g		enjoy watching hockey Y/N
foot	byte	%8.0g		enjoy watching football Y/N
base	byte	%8.0g		enjoy baseball Y/N
bask	byte	%8.0g		enjoy basketball Y/N
arob	byte	%8.0g		participate in aerobics Y/N
fshg	byte	%8.0g		enjoy fishing Y/N
dart	byte	%8.0g		enjoy playing darts Y/N
clas	byte	%8.0g		enjoy classical music $Y/N$
cntr	byte	%8.0g		enjoy country music Y/N
jazz	byte	%8.0g		enjoy jazz music Y/N
rock	byte	%8.0g		enjoy rock and roll music $Y/N$
west	byte	%8.0g		enjoy reading western novels $Y/N$
romc	byte	%8.0g		enjoy reading romance novels Y/N
scif	byte	%8.0g		enjoy reading sci. fiction $Y/N$
biog	byte	%8.0g		enjoy reading biographies $Y/N$
fict	byte	%8.0g		enjoy reading fiction $Y/N$
hist	byte	%8.0g		enjoy reading history Y/N
cook	byte	%8.0g		enjoy cooking Y/N
shop	byte	%8.0g		enjoy shopping Y/N
soap	byte	%8.0g		enjoy watching soap operas Y/N
sew	byte	%8.0g		enjoy sewing $Y/N$
crft	byte	%8.0g		enjoy craft activities $Y/N$
auto	byte	%8.0g		enjoy automobile mechanics $Y/N$
pokr	byte	%8.0g		enjoy playing poker Y/N
brdg	byte	%8.0g		enjoy playing bridge Y/N
kids	byte	%8.0g		have children Y/N
hors	byte	%8.0g		have a horse Y/N
cat	byte	%8.0g		have a cat Y/N
dog	byte	%8.0g		have a dog $Y/N$
bird	byte	%8.0g		have a bird $Y/N$
fish	byte	%8.0g		have a fish Y/N

Sorted by:

The matrix dissimilarity command allows us to compute the Jaccard similarity measure (the Jaccard option), comparing variables (the variables option) instead of observations, saving one minus the Jaccard measure (the dissim(oneminus) option) as a dissimilarity matrix.

- . matrix dissimilarity clubD = , variables Jaccard dissim(oneminus)
- . matlist clubD[1..5,1..5]

	bike	bowl	swim	jog	hock
bike	0				
bowl	.7333333	0			
swim	.5625	.625	0		
jog	.6	.8235294	.5882353	0	
hock	.8461538	.6	.8	.8571429	0

We pass the clubD matrix to clustermat and ask for a single-linkage cluster analysis. We need to specify the clear option to replace the 30 observations currently in memory with the 35 observations containing the cluster results. Using the labelvar() option, we also ask for a label variable, question, to be created from the clubD matrix row names. To see the resulting cluster analysis, we call cluster dendrogram; see [MV] cluster dendrogram.

- . clustermat singlelink clubD, name(club) clear labelvar(question) number of observations (\_N) was 0, now 35
- . describe

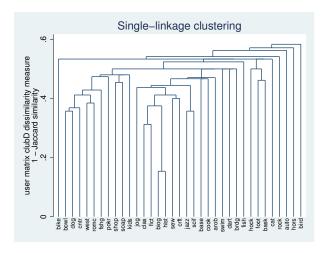
Contains	data	
obs:		35
vars:		4
size:		490

variable name	storage type	display format	value label	variable label	
<pre>club_id club_ord club_hgt question</pre>	byte byte double str4	%8.0g %8.0g %10.0g %9s			

#### Sorted by:

Note: Dataset has changed since last saved.

ytitle(1 - Jaccard similarity, suffix)



From these 30 women, we see that the biog (enjoy reading biographies) and hist (enjoy reading history) questions were most closely related. auto (enjoy automobile mechanics), hors (have a horse), and bird (have a bird) seem to be the least related to the other variables. These three variables, in turn, merge last into the supergroup containing the remaining variables.

### References

Anderson, E. 1935. The irises of the Gaspe Peninsula. Bulletin of the American Iris Society 59: 2-5.

Bray, R. J., and J. T. Curtis. 1957. An ordination of the upland forest communities of southern Wisconsin. Ecological Monographs 27: 325–349.

Fisher, R. A. 1936. The use of multiple measurements in taxonomic problems. Annals of Eugenics 7: 179-188.

Kaufman, L., and P. J. Rousseeuw. 1990. Finding Groups in Data: An Introduction to Cluster Analysis. New York: Wiley.

Morrison, D. F. 2005. Multivariate Statistical Methods. 4th ed. Belmont, CA: Duxbury.

Odum, E. P. 1950. Bird populations of the Highlands (North Carolina) plateau in relation to plant succession and avian invasion. *Ecology* 31: 587–605.

### Also see

[MV] **cluster programming subroutines** — Add cluster-analysis routines

[MV] cluster programming utilities — Cluster-analysis programming utilities

[MV] **cluster** — Introduction to cluster-analysis commands

### **Title**

cluster dendrogram — Dendrograms for hierarchical cluster analysis

Description Quick start Menu Syntax
Options Remarks and examples Reference Also see

# **Description**

cluster dendrogram produces dendrograms (also called cluster trees) for a hierarchical clustering. See [MV] cluster for a discussion of cluster analysis, hierarchical clustering, and the available cluster commands.

Dendrograms graphically present the information concerning which observations are grouped together at various levels of (dis)similarity. At the bottom of the dendrogram, each observation is considered its own cluster. Vertical lines extend up for each observation, and at various (dis)similarity values, these lines are connected to the lines from other observations with a horizontal line. The observations continue to combine until, at the top of the dendrogram, all observations are grouped together.

The height of the vertical lines and the range of the (dis)similarity axis give visual clues about the strength of the clustering. Long vertical lines indicate more distinct separation between the groups. Long vertical lines at the top of the dendrogram indicate that the groups represented by those lines are well separated from one another. Shorter lines indicate groups that are not as distinct.

#### **Quick start**

```
Dendrogram of most recent cluster analysis cluster dendrogram
```

Same as above

cluster tree

As above, but orient horizontally instead of vertically

cluster tree, horizontal

Dendrogram of cluster analysis named myclus

cluster tree myclus

As above, and apply leaf labels from variable mylabels instead of observation numbers cluster tree myclus, labels(mylabels)

As above, but rotate leaf labels 90 degrees and reduce text size by half

```
cluster tree myclus, labels(mylabels) ///
    xlabel(, angle(90) labsize(*.5))
```

Show top 20 branches and associated frequencies from most recent cluster analysis cluster tree, cutnumber(20) showcount

### Menu

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Dendrograms

# **Syntax**

cluster <u>dend</u> rogram [cl	$name \ ] \ [if] \ [in] \ [, options]$
option	Description
Main	
quick	do not center parent branches
<u>la</u> bels( <i>varname</i> )	name of variable containing leaf labels
<pre>cutnumber(#)</pre>	display top # branches only
<pre>cutvalue(#)</pre>	display branches above # (dis)similarity measure only
<u>showc</u> ount	display number of observations for each branch
<pre>countprefix(string)</pre>	prefix the branch count with string; default is "n="
<pre>countsuffix(string)</pre>	suffix the branch count with string; default is empty string
<u>counti</u> nline	put branch count in line with branch label
<u>vert</u> ical	orient dendrogram vertically (default)
<u>hor</u> izontal	orient dendrogram horizontally
Plot	
line_options	affect rendition of the plotted lines
Add plots	
<pre>addplot(plot)</pre>	add other plots to the dendrogram
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by () documented in [G-3] twoway_options

Note: cluster tree is a synonym for cluster dendrogram.

In addition to the restrictions imposed by if and in, the observations are automatically restricted to those that were used in the cluster analysis.

# **Options**

Main

quick switches to a different style of dendrogram in which the vertical lines go straight up from the observations instead of the default action of being recentered after each merge of observations in the dendrogram hierarchy. Some people prefer this representation, and it is quicker to render.

labels(varname) specifies that varname be used in place of observation numbers for labeling the observations at the bottom of the dendrogram.

cutnumber(#) displays only the top # branches of the dendrogram. With large dendrograms, the
lower levels of the tree can become too crowded. With cutnumber(), you can limit your view
to the upper portion of the dendrogram. Also see the cutvalue() option.

cutvalue(#) displays only those branches of the dendrogram that are above the # (dis)similarity measure. With large dendrograms, the lower levels of the tree can become too crowded. With cutvalue(), you can limit your view to the upper portion of the dendrogram. Also see the cutnumber() option.

- showcount requests that the number of observations associated with each branch be displayed below the branches. showcount is most useful with cutnumber() and cutvalue() because, otherwise, the number of observations for each branch is one. When this option is specified, a label for each branch is constructed by using a prefix string, the branch count, and a suffix string.
- countprefix(string) specifies the prefix string for the branch count label. The default is countprefix(n=). This option implies the use of the showcount option.
- countsuffix(string) specifies the suffix string for the branch count label. The default is an empty string. This option implies the use of the showcount option.
- countinline requests that the branch count be put in line with the corresponding branch label. The branch count is placed below the branch label by default. This option implies the use of the showcount option.
- vertical and horizontal specify whether the x and y coordinates are to be swapped before plotting—vertical (the default) does not swap the coordinates, whereas horizontal does.

Plot
line_options affect the rendition of the lines; see [G-3] line_options.
Add plots
addplot(plot) allows adding more graph twoway plots to the graph; see [G-3] addplot_option.
Y axis, X axis, Titles, Legend, Overall
twoway ontions are any of the options documented in [G-3] twoway ontions, excluding by (). These

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option).

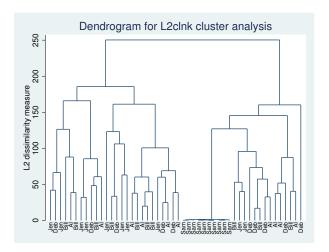
# Remarks and examples

Examples of the cluster dendrogram command can be found in [MV] cluster linkage, [MV] clustermat, [MV] cluster stop, and [MV] cluster generate. Here we illustrate some of the additional options available with cluster dendrogram.

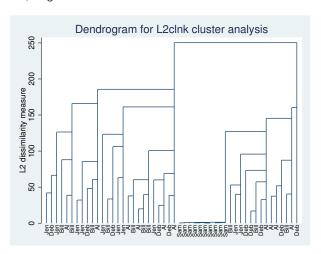
### Example 1

Example 1 of [MV] **cluster linkage** introduces a dataset with 50 observations on four variables. Here we show the dendrogram for a complete-linkage analysis:

- . use http://www.stata-press.com/data/r14/labtech
- . cluster completelinkage x1 x2 x3 x4, name(L2clnk)
- . cluster dendrogram L2clnk, labels(labtech) xlabel(, angle(90) labsize(\*.75))



The same dendrogram can be rendered in a slightly different format by using the quick option:

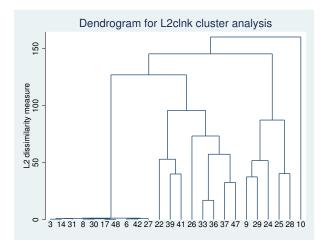


Some people prefer this style of dendrogram. As the name implies, this style of dendrogram is quicker to render.

You can use the if and in conditions to restrict the dendrogram to the observations for one subgroup. This task is usually accomplished with the cluster generate command, which creates a grouping variable; see [MV] cluster generate.

Here we show the third of three groups in the dendrogram by first generating the grouping variable for three groups and then using if in the command for cluster dendrogram to restrict it to the third of those three groups.

- . cluster generate g3 = group(3)
- . cluster tree if g3==3

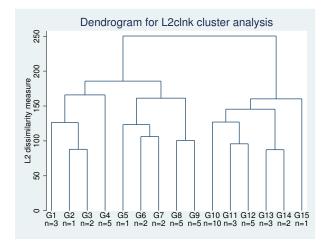


Because we find it easier to type, we used the synonym tree instead of dendrogram. We did not specify the cluster name, allowing it to default to the most recently performed cluster analysis. We also omitted the labels() and xlabel() options, which brings us back to the default action of showing, horizontally, the observation numbers.

This example has only 50 observations. When there are many observations, the dendrogram can become too crowded. You will need to limit which part of the dendrogram you display. One way to view only part of the dendrogram is to use if and in to limit to one particular group, as we did above.

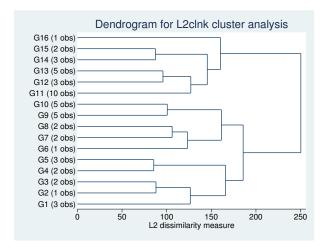
The other way to limit your view of the dendrogram is to specify that you wish to view only the top portion of the tree. The cutnumber() and cutvalue() options allow you to do this:

. cluster tree, cutn(15) showcount



We limited our view to the top 15 branches of the dendrogram with cutn(15). By default, the 15 branches were labeled G1-G15. The showcount option provided, below these branch labels, the number of observations in each of the 15 groups.

The cutvalue() option provides another way to limit the view to the top branches of the dendrogram. With this option, you specify the similarity or dissimilarity value at which to trim the tree.



This time, we limited the dendrogram to those branches with dissimilarity greater than 75.3 by using the cutvalue(75.3) option. There were 16 branches (groups) that met that restriction. We used the countprefix() and countsuffix() options to display the number of observations in each branch as "(# obs)" instead of "n=#". The countinline option puts the branch counts in line with

4

the branch labels. We specified the horizontal option and the angle(0) suboption of ylabel() to get a horizontal dendrogram with horizontal branch labels.

#### □ Technical note

Programmers can control the graphical procedure executed when cluster dendrogram is called. This ability will be helpful to programmers adding new hierarchical clustering methods that require a different dendrogram algorithm. See [MV] cluster programming subroutines for details.

### Reference

Falcaro, M., and A. Pickles. 2010. riskplot: A graphical aid to investigate the effect of multiple categorical risk factors. Stata Journal 10: 61–68.

### Also see

[MV] **cluster** — Introduction to cluster-analysis commands

[MV] **clustermat** — Introduction to clustermat commands

#### Title

**cluster generate** — Generate summary or grouping variables from a cluster analysis

Description Quick start Menu Syntax Options
Remarks and examples Also see

# **Description**

cluster generate creates summary or grouping variables from a hierarchical cluster analysis; the result depends on the function. A single variable may be created containing a group number based on the requested number of groups or cutting the dendrogram at a specified (dis)similarity value. A set of new variables may be created if a range of group sizes is specified.

Users can add more cluster generate functions; see [MV] cluster programming subroutines.

## **Quick start**

```
Generate grouping variable g5 with 5 groups from the most recent cluster analysis cluster generate g5 = groups(5)
```

```
As above, 4 grouping variables (g4, g5, g6, and g7) with 4, 5, 6, and 7 groups cluster generate g = groups(4/7)
```

```
As above, but use the cluster analysis named myclus cluster generate g = groups(4/7), name(myclus)
```

Generate grouping variable mygroups from the most recent cluster analysis by cutting the dendrogram at dissimilarity value 38

```
cluster generate mygroups = cut(38)
```

#### Menu

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Summary variables from cluster analysis

# **Syntax**

Generate grouping variables for specified numbers of clusters

```
cluster generate { newvar | stub } = groups(numlist) [, options]
```

Generate grouping variable by cutting the dendrogram

```
cluster generate newvar = cut(\#) [, \underline{n}ame(clname)]
```

Description
name of cluster analysis to use in producing new variables
produce error message for ties; default
ignore requests that result in ties
produce results for largest number of groups smaller than your request
produce results for smallest number of groups larger than your request

# **Options**

name(clname) specifies the name of the cluster analysis to use in producing the new variables. The default is the name of the cluster analysis last performed, which can be reset by using the cluster use command; see [MV] cluster utility.

ties(error | skip | fewer | more) indicates what to do with the groups() function for ties. A hierarchical cluster analysis has ties when multiple groups are generated at a particular (dis)similarity value. For example, you might have the case where you can uniquely create two, three, and four groups, but the next possible grouping produces eight groups because of ties.

ties(error), the default, produces an error message and does not generate the requested variables.

ties(skip) specifies that the offending requests be ignored. No error message is produced, and only the requests that produce unique groupings will be honored. With multiple values specified in the groups() function, ties(skip) allows the processing of those that produce unique groupings and ignores the rest.

ties(fewer) produces the results for the largest number of groups less than or equal to your request. In the example above with groups(6) and using ties(fewer), you would get the same result that you would by using groups(4).

ties(more) produces the results for the smallest number of groups greater than or equal to your request. In the example above with groups(6) and using ties(more), you would get the same result that you would by using groups(8).

## Remarks and examples

cluster generate provides two built-in functions: groups() and cut(). Examples of how to use the groups () function can be found in [MV] cluster dendrogram, [MV] cluster linkage, and [MV] cluster stop. More examples of the groups() and cut() functions of cluster generate are provided here.

The groups (numlist) function generates grouping variables, giving the grouping for the specified numbers of clusters from a hierarchical cluster analysis. If one number is given, newvar is produced with group numbers going from 1 to the number of clusters requested. If more than one number is specified, a new variable is generated for each number by using the provided stub name appended with the number.

The cut (#) function generates a grouping variable corresponding to cutting the dendrogram (see [MV] cluster dendrogram) of a hierarchical cluster analysis at the specified (dis)similarity value.

You may find it easier to understand these functions by looking at a dendrogram from a hierarchical cluster analysis. The cluster dendrogram command produces dendrograms (cluster trees) from a hierarchical cluster analysis; see [MV] cluster dendrogram.

### Example 1

Example 1 of [MV] cluster linkage examines a dataset with 50 observations with four variables. Here we use complete-linkage clustering and use the groups() function of cluster generate to produce a grouping variable, splitting the data into two groups.

- . use http://www.stata-press.com/data/r14/labtech
- . cluster completelinkage x1 x2 x3 x4, name(L2clnk)
- . cluster dendrogram L2clnk, xlabel(, angle(90) labsize(\*.75)) (graph omitted)
- . cluster generate g2 = group(2), name(L2clnk)
- . codebook g2

g2 (unlabeled)

numeric (byte)

range: [1,2]units: missing .: 0/50 unique values:

tabulation: Freq. Value 26 1 24 2

. by g2, sort: summarize	: X*
--------------------------	------

-> g2 = 1					
Variable	Obs	Mean	Std. Dev.	Min	Max
x1	26	91.5	37.29432	17.4	143
x2	26	74.58077	41.19319	4.8	142.1
x3	26	101.0077	36.95704	16.3	147.9
x4	26	71.77308	43.04107	6.6	146.1
-> g2 = 2					
Variable	Obs	Mean	Std. Dev.	Min	Max
x1	24	18.8	23.21742	0	77
x2	24	30.05833	37.66979	0	143.6
x3	24	18.54583	21.68215	.2	69.7
x4	24	41.89167	43.62025	.1	130.9

The group() function of cluster generate created a grouping variable named g2, with ones indicating the 26 observations that belong to the left main branch of the dendrogram and twos indicating the 24 observations that belong to the right main branch of the dendrogram. The summary of the x variables used in the cluster analysis for each group shows that the second group is characterized by lower values.

We could have obtained the same grouping variable by using the cut() function of cluster generate.

- . cluster generate g2cut = cut(200)
- . table g2 g2cut

g2	g2cut 1 2
1	26
2	24

We did not need to specify the name() option because this was the latest cluster analysis performed, which is the default. The table output shows that we obtained the same result with cut(200) as with group(2) for this example.

How many groups are produced if we cut the tree at the value 105.2?

- . cluster generate z = cut(105.2)
- . codebook z, tabulate(20)

z (unlabeled)

type: numeric (byte)

range: [1,11] units: 1 unique values: 11 missing .: 0/50

unique values: 11 missing tabulation: Freq. Value

3 1
3 2
5 3
1 4
2 5
2 6
10 7
10 8
8 9
5 10
1 11

The codebook command (see [D] codebook) shows that the result of cutting the dendrogram at the value 105.2 produced 11 groups ranging in size from 1 to 10 observations.

The group() function of cluster generate may be used to create multiple grouping variables with one call. Here we create the grouping variables for groups of size 3-12:

- . cluster generate gp = gr(3/12)
- . summarize gp\*

Variable	0bs	Mean	Std. Dev.	Min	Max
gp3	50	2.26	.8033095	1	3
gp4	50	3.14	1.030356	1	4
gp5	50	3.82	1.438395	1	5
gp6	50	3.84	1.461897	1	6
gp7	50	3.96	1.603058	1	7
gp8	50	4.24	1.911939	1	8
gp9	50	5.18	2.027263	1	9
gp10	50	5.94	2.385415	1	10
gp11	50	6.66	2.781939	1	11
gp12	50	7.24	3.197959	1	12

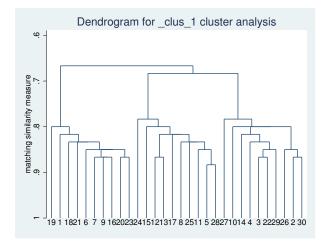
Here we used abbreviations for generate and group(). The group() function takes a numlist; see [U] 11.1.8 numlist. We specified 3/12, indicating the numbers 3-12. gp, the stub name we provide, is appended with the number as the variable name for each group variable produced.

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## Example 2

Example 2 of [MV] cluster linkage shows the following dendrogram from the single-linkage clustering of 30 observations on 60 variables. In that example, we used the group() function of cluster generate to produce a grouping variable for three groups. What happens when we try to obtain four groups from this clustering?

- . use http://www.stata-press.com/data/r14/homework, clear
- . cluster singlelinkage a1-a60, measure(matching) cluster name: \_clus\_1
- . cluster tree



```
. cluster generate g4 = group(4)
cannot create 4 groups because of ties
r(198);
```

Stata complains that it cannot create four groups from this cluster analysis.

The ties() option gives us control over this situation. We just need to decide whether we want more groups or fewer groups than we asked for when faced with ties. We demonstrate both ways.

- . cluster generate more4 = gr(4), ties(more)
- . cluster generate less4 = gr(4), ties(fewer)
- . summarize more4 less4

Variable	Obs	Mean	Std. Dev.	Min	Max
more4	30	2.933333	1.638614	1	5
less4	30		.8304548	1	3

For this cluster analysis, ties(more) with group(4) produces five groups, whereas ties(fewer) with group(4) produces three groups.

The ties(skip) option is convenient when we want to produce a range of grouping variables.

- . cluster generate group = gr(4/20), ties(skip)
- . summarize group\*

Variable	Obs	Mean	Std. Dev.	Min	Max
group5	30	2.933333	1.638614	1	5
group9	30	4.866667	2.622625	1	9
group13	30	7.066667	3.92106	1	13
group18	30	9.933333	5.419844	1	18

With this cluster analysis, the only unique groupings available are 5, 9, 13, and 18 within the range 4-20.

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## Also see

- [D] **egen** Extensions to generate
- [D] generate Create or change contents of variable
- [MV] cluster Introduction to cluster-analysis commands
- [MV] **clustermat** Introduction to clustermat commands

### **Title**

cluster kmeans and kmedians — Kmeans and kmedians cluster analysis

Description
Options
Also see

Quick start Remarks and examples Menu Methods and formulas Syntax Reference

# **Description**

cluster kmeans and cluster kmedians perform kmeans and kmedians partition cluster analysis, respectively. See [MV] **cluster** for a general discussion of cluster analysis and a description of the other cluster commands.

### **Quick start**

Kmeans cluster analysis using Euclidean distance of v1, v2, v3, and v4 to create 5 groups cluster kmeans v1 v2 v3 v4, k(5)

As above, and name the cluster analysis myclus cluster kmeans v1 v2 v3 v4, k(5) name(myclus)

Kmedians cluster analysis to create 7 groups using Canberra distance of v1, v2, and v3 cluster kmedians v1 v2 v3, k(7) measure(Canberra)

#### Menu

#### cluster kmeans

 ${\it Statistics} > {\it Multivariate analysis} > {\it Cluster analysis} > {\it Cluster data} > {\it Kmeans}$ 

#### cluster kmedians

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Kmedians

## **Syntax**

Kmeans cluster analysis

cluster  $\underline{k}$ means [varlist] [if] [in], k(#) [options]

Kmedians cluster analysis

cluster  $\underline{kmed}$ ians [varlist] [if] [in], k(#) [options]

option	Description
Main	
* k(#)	perform cluster analysis resulting in # groups
<pre>measure(measure)</pre>	similarity or dissimilarity measure; default is L2 (Euclidean)
$\underline{\mathtt{n}}\mathtt{ame}(\mathit{clname})$	name of resulting cluster analysis
Options	
<pre>start(start_option)</pre>	obtain k initial group centers by using start_option
$\underline{\underline{\mathtt{keep}}}\mathtt{centers}$	append the $k$ final group means or medians to the data
Advanced	
<pre>generate(groupvar)</pre>	name of grouping variable
<u>iter</u> ate(#)	maximum number of iterations; default is iterate(10000)

<sup>\*</sup>k(#) is required.

## **Options**

Main

k(#) is required and indicates that # groups are to be formed by the cluster analysis.

measure(*measure*) specifies the similarity or dissimilarity measure. The default is measure(L2), Euclidean distance. This option is not case sensitive. See [MV] *measure\_option* for detailed descriptions of the supported measures.

name(clname) specifies the name to attach to the resulting cluster analysis. If name() is not specified, Stata finds an available cluster name, displays it for your reference, and attaches the name to your cluster analysis.

Options

 $start(start\_option)$  indicates how the k initial group centers are to be obtained. The available  $start\_options$  are

<u>kr</u>andom [(seed#)], the default, specifies that k unique observations be chosen at random, from among those to be clustered, as starting centers for the k groups. Optionally, a random-number seed may be specified to cause the command set seed seed# (see [R] set seed) to be applied before the k random observations are chosen.

<u>firstk</u>, <u>exclude</u>] specifies that the first k observations from among those to be clustered be used as the starting centers for the k groups. With the exclude option, these first k observations are not included among the observations to be clustered.

- $\underline{\mathtt{lastk}}$ [,  $\underline{\mathtt{exclude}}$ ] specifies that the last k observations from among those to be clustered be used as the starting centers for the k groups. With the  $\underline{\mathtt{exclude}}$  option, these last k observations are not included among the observations to be clustered.
- $\underline{\underline{r}}$  and om[(seed#)] specifies that k random initial group centers be generated. The values are randomly chosen from a uniform distribution over the range of the data. Optionally, a random-number seed may be specified to cause the command  $\underline{\underline{s}}$   $\underline{\underline{s}}$   $\underline{\underline{s}}$   $\underline{\underline{s}}$   $\underline{\underline{e}}$   $\underline{\underline{e}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{\underline{e}}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{e}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{e}$   $\underline{e}$   $\underline{\underline{e}$   $\underline{e}$   $\underline{e}$
- $\underline{\underline{prandom}}[(seed\#)]$  specifies that k partitions be formed randomly among the observations to be clustered. The group means or medians from the k groups defined by this partitioning are to be used as the starting group centers. Optionally, a random-number seed may be specified to cause the command  $\underline{set}$   $\underline{seed}$  (see  $\underline{[R]}$   $\underline{set}$   $\underline{seed}$ ) to be applied before the k partitions are chosen.
- everykth specifies that k partitions be formed by assigning observations  $1, 1+k, 1+2k, \ldots$  to the first group; assigning observations  $2, 2+k, 2+2k, \ldots$  to the second group; and so on, to form k groups. The group means or medians from these k groups are to be used as the starting group centers.
- <u>segments</u> specifies that k nearly equal partitions be formed from the data. Approximately the first N/k observations are assigned to the first group, the second N/k observations are assigned to the second group, and so on. The group means or medians from these k groups are to be used as the starting group centers.
- group(varname) provides an initial grouping variable, varname, that defines k groups among the observations to be clustered. The group means or medians from these k groups are to be used as the starting group centers.

keepcenters specifies that the group means or medians from the k groups that are produced be appended to the data.

Advanced ]

generate(groupvar) provides the name of the grouping variable to be created by cluster kmeans or cluster kmedians. By default, this will be the name specified in name().

iterate(#) specifies the maximum number of iterations to allow in the kmeans or kmedians clustering algorithm. The default is iterate(10000).

# Remarks and examples

Two examples are presented, one using cluster kmeans with continuous data and the other using cluster kmeans and cluster kmedians with binary data. Both commands work similarly with the different types of data.

## Example 1

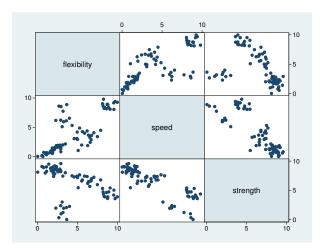
You have measured the flexibility, speed, and strength of the 80 students in your physical education class. You want to split the class into four groups, based on their physical attributes, so that they can receive the mix of flexibility, strength, and speed training that will best help them improve.

Here is a summary of the data and a matrix graph showing the data:

- . use http://www.stata-press.com/data/r14/physed
- . summarize flex speed strength

Variable	Obs	Mean	Std. Dev.	Min	Max
flexibility speed strength	80	4.402625	2.788541	.03	9.97
	80	3.875875	3.121665	.03	9.79
	80	6.439875	2.449293	.05	9.57

. graph matrix flex speed strength



As you expected, based on what you saw the first day of class, the data indicate a wide range of levels of performance for the students. The graph seems to indicate that there are some distinct groups, which leads you to believe that your plan will work well.

You decide to perform a cluster analysis to create four groups, one for each of your class assistants. You have had good experience with kmeans clustering in the past and generally like the behavior of the absolute-value distance.

You do not really care what starting values are used in the cluster analysis, but you do want to be able to reproduce the same results if you ever decide to rerun your analysis. You decide to use the  $\mathtt{krandom}()$  option to pick k of the observations at random as the initial group centers. You supply a random-number seed for reproducibility. You also add the  $\mathtt{keepcenters}$  option so that the means of the four groups will be added to the bottom of your dataset.

. table g4abs

Freq.	g4abs
15 20 10 35	1 2 3 4

. list flex speed strength in 81/L, abbrev(12)

	flexibility	speed	strength
81.	8.852	8.743333	4.358
82.	5.9465	3.4485	6.8325
83.	3.157	6.988	1.641
84.	1.969429	1.144857	8.478857

- . drop in 81/L
- (4 observations deleted)
- . tabstat flex speed strength, by(g4abs) stat(min mean max)

Summary statistics: min, mean, max

by categories of: g4abs

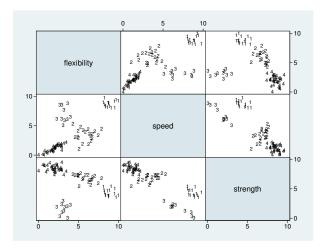
g4abs	flexib~y speed		strength
1	8.12	8.05	3.61
	8.852	8.743333	4.358
	9.97	9.79	5.42
2	4.32	1.05	5.46
	5.9465	3.4485	6.8325
	7.89	5.32	7.66
3	2.29	5.11	.05
	3.157	6.988	1.641
	3.99	8.87	3.02
4	.03 1.969429 3.48	.03 1.144857 2.17	
Total	.03	.03	.05
	4.402625	3.875875	6.439875
	9.97	9.79	9.57

After looking at the last 4 observations (which are the group means because you specified keepcenters), you decide that what you really wanted to see was the minimum and maximum values and the mean for the four groups. You remove the last 4 observations and then use the tabstat command to view the desired statistics.

Group 1, with 15 students, is already doing well in flexibility and speed but will need extra strength training. Group 2, with 20 students, needs to emphasize speed training but could use some improvement in the other categories as well. Group 3, the smallest, with 10 students, needs help with flexibility and strength. Group 4, the largest, with 35 students, has serious problems with both flexibility and speed, though they did well in the strength category.

Because you like looking at graphs, you decide to view the matrix graph again but with group numbers used as plotting symbols.

. graph matrix flex speed strength, m(i) mlabel(g4abs) mlabpos(0)



The groups, as shown in the graph, do appear reasonably distinct. However, you had hoped to have groups that were about the same size. You are curious what clustering to three or five groups would produce. For no good reason, you decide to use the first k observations as initial group centers for clustering to three groups and random numbers within the range of the data for clustering to five groups.

- . cluster k flex speed strength, k(3) name(g3abs) start(firstk) measure(abs)
- . cluster k flex speed strength, k(5) name(g5abs) start(random(33576))
- > measure(abs)
- . table g3abs g4abs, col

g3abs	1	2	g4abs 3	4	Total
1 2 3	15	18 2	10	35	10 53 17

. table g5abs g4abs, col

g5abs	1	2	g4abs 3	4	Total
1 2	15	9			15 9
3			10		10
4		11			11
5				35	35

With three groups, the unequal-group-size problem gets worse. With five groups, you still have one group with 35 observations, which is much larger than all other groups. Four groups seem like the best option for this class. You will try to help the assistant assigned to group 4 in dealing with the larger group.

You might want to investigate the results of using different random seeds in the command used to generate the 4 groups earlier in this example. Because these data do not have clearly defined,

1

well-separated clusters, there is a good chance that clusters based on different starting values will be different.

## Example 2

You have just started a women's club. Thirty women from throughout the community have sent in their requests to join. You have them fill out a questionnaire with 35 yes—no questions relating to sports, music, reading, and hobbies. A description of the 35 variables is found in example 3 of [MV] clustermat.

In planning the first meeting of the club, you want to assign seats at the five lunch tables on the basis of shared interests among the women. You really want people placed together who share the same positive interests, not who share dislikes. From all the available binary similarity measures, you decide to use the Jaccard coefficient as the binary similarity measure because it does not include jointly zero comparisons in its formula; see [MV] *measure\_option*. The Jaccard coefficient is also easy to understand.

You decide to examine the groupings produced by kmeans and kmedians clustering.

```
. use http://www.stata-press.com/data/r14/wclub, clear
```

- . cluster kmeans bike-fish, k(5) measure(Jaccard) st(firstk) name(gr5)
- . cluster kmed bike-fish, k(5) measure(Jaccard) st(firstk) name(kmedian5)

start: firstk
range: 1 0

You used the first k observations as starting centers for both kmeans and kmedians—the st(firstk) option.

What size groups did each method produce, and how closely did the results agree?

. table gr5 kmedian5, row col

	kmedian5					
gr5	1	2	3	4	5	Total
1	7					7
2	1	6				7
3			5			5
4				5		5
5	1		1		4	6
Total	9	6	6	5	4	30

There is reasonably strong agreement between the results from cluster kmeans and cluster kmedians. Because the tables can seat only eight comfortably, the grouping produced by cluster kmeans will be used because the group sizes range from five to seven, whereas the groups from cluster kmedians range from four to nine.

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### Methods and formulas

Kmeans cluster analysis and its variant, kmedians cluster analysis, are discussed in most clusteranalysis books; see *References* in [MV] **cluster**. [MV] **cluster** also provides a general discussion of cluster analysis, including kmeans and kmedians clustering, and discusses the available cluster subcommands.

Kmeans and kmedians clustering are iterative procedures that partition the data into k groups or clusters. The procedure begins with k initial group centers. Observations are assigned to the group with the closest center. The mean or median of the observations assigned to each of the groups is computed, and the process is repeated. These steps continue until all observations remain in the same group from the previous iteration.

To avoid endless loops, an observation will be reassigned to a different group only if it is closer to the other group center. For a tied distance between an observation and two or more group centers, the observation is assigned to its current group if that is one of the closest and to the lowest numbered group otherwise.

The start() option provides many ways to specify the beginning group centers. These include methods that specify the actual starting centers, as well as methods that specify initial partitions of the data from which the beginning centers are computed.

Some kmeans clustering algorithms recompute the group centers after each reassignment of an observation. Other algorithms, including Stata's cluster kmeans and cluster kmedians commands, recompute the group centers only after a complete pass through the data. A disadvantage of this method is that orphaned group centers—one that has no observations that are closest to it—can occur. The advantage of recomputing means only at the end of each pass through the data is that the sort order of the data does not potentially change your result.

Stata deals with orphaned centers by finding the observations that are farthest from the centers and using them as new group centers. The observations are then reassigned to the closest groups, including these new centers.

Continuous or binary data are allowed with cluster kmeans and cluster kmedians. The mean of a group of binary observations for a variable is the proportion of ones for that group of observations and variable. The median of a group of binary observations for a variable is almost always either zero or one. However, if there are an equal number of zeros and ones for a group, the median is 0.5. The binary similarity measures can accommodate the comparison of a binary observation to a proportion. See [MV] *measure\_option* for details on this subject and for the formulas for all the available (dis)similarity measures.

### Reference

Makles, A. 2012. Stata tip 110: How to get the optimal k-means cluster solution. Stata Journal 12: 347-351.

## Also see

```
[MV] cluster notes — Place notes in cluster analysis
```

[MV] **cluster stop** — Cluster-analysis stopping rules

[MV] cluster utility — List, rename, use, and drop cluster analyses

[MV] **cluster** — Introduction to cluster-analysis commands

[MV] **clustermat** — Introduction to clustermat commands

### Title

cluster linkage — Hierarchical cluster analysis

Description Quick start
Menu Syntax

Remarks and examples Methods and formulas

Also see

# **Description**

cluster and clustermat, with a specified linkage method, perform hierarchical agglomerative cluster analysis. The following common linkage methods are available: single, complete, average, Ward's method, centroid, median, and weighted average.

### **Quick start**

Cluster analysis of data

Single-linkage cluster analysis using Euclidean distance of v1, v2, v3, and v4 cluster singlelinkage v1 v2 v3 v4

Same as above

cluster single v1 v2 v3 v4

As above, and name the cluster analysis singclus cluster single v1 v2 v3 v4, name(singclus)

Complete-linkage cluster analysis using absolute-value distance of v1, v2, and v3 cluster completelinkage v1 v2 v3, measure(absolute)

Same as above

cluster complete v1 v2 v3, measure(L1)

Cluster analysis of dissimilarity matrix

Replace current data with solution from single-linkage cluster analysis on matrix D clustermat single D, clear

As above, and name the cluster analysis Dclus clustermat single D, clear name(Dclus)

Add solution from average-linkage cluster analysis on matrix D to the existing data clustermat averagelinkage D, add

## Menu

### cluster singlelinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Single linkage

### cluster averagelinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Average linkage

### cluster completelinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Complete linkage

### cluster waveragelinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Weighted-average linkage

### cluster medianlinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Median linkage

### cluster centroidlinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Centroid linkage

### cluster wardslinkage

Statistics > Multivariate analysis > Cluster analysis > Cluster data > Ward's linkage

# **Syntax**

```
Cluster analysis of data
```

```
cluster \mathit{linkage}\ \left[\mathit{varlist}\right]\ \left[\mathit{if}\right]\ \left[\mathit{in}\right]\ \left[\mathit{,\ cluster\_options}\right]
```

Cluster analysis of a dissimilarity matrix

clustermat  $linkage \ matname \ [if] \ [in] \ [, clustermat\_options]$ 

linkage	Description
<u>s</u> inglelinkage	single-linkage cluster analysis
<u>a</u> veragelinkage	average-linkage cluster analysis
<u>c</u> ompletelinkage	complete-linkage cluster analysis
<u>wav</u> eragelinkage	weighted-average linkage cluster analysis
<u>med</u> ianlinkage	median-linkage cluster analysis
$\underline{\mathtt{cen}}\mathtt{troidlinkage}$	centroid-linkage cluster analysis
wardslinkage	Ward's linkage cluster analysis
cluster_options	Description
Main	
<pre>measure(measure)</pre>	similarity or dissimilarity measure
$\underline{\mathtt{n}}\mathtt{ame}(\mathit{clname})$	name of resulting cluster analysis
Advanced	
generate(stub)	prefix for generated variables; default prefix is <i>clname</i>
clustermat_options	Description
Main	
$\underline{\mathtt{sh}}\mathtt{ape}(\mathit{shape})$	shape (storage method) of matname
add	add cluster information to data currently in memory
clear	replace data in memory with cluster information
<pre>labelvar(varname)</pre>	place dissimilarity matrix row names in varname
$\underline{\mathtt{n}}$ ame ( $clname$ )	name of resulting cluster analysis
Advanced	
force	perform clustering after fixing matname problems
$\underline{\mathtt{gen}}\mathtt{erate}(\mathit{stub})$	prefix for generated variables; default prefix is clname

### 144 cluster linkage — Hierarchical cluster analysis

shape	matname is stored as a
<u>f</u> ull	square symmetric matrix; the default
$\underline{\mathtt{l}}\mathtt{ower}$	vector of rowwise lower triangle (with diagonal)
<u>ll</u> ower	vector of rowwise strict lower triangle (no diagonal)
<u>u</u> pper	vector of rowwise upper triangle (with diagonal)
<u>uu</u> pper	vector of rowwise strict upper triangle (no diagonal)

# Options for cluster linkage commands

Main

measure (measure) specifies the similarity or dissimilarity measure. The default for averagelinkage, completelinkage, singlelinkage, and waveragelinkage is L2 (synonym <u>Euclidean</u>). The default for centroidlinkage, medianlinkage, and wardslinkage is L2squared. This option is not case sensitive. See [MV] measure\_option for a discussion of these measures.

Several authors advise using the L2squared *measure* exclusively with centroid, median, and Ward's linkage. See *Dissimilarity transformations and the Lance and Williams formula* and *Warning concerning similarity or dissimilarity choice* in [MV] **cluster** for details.

name(clname) specifies the name to attach to the resulting cluster analysis. If name() is not specified, Stata finds an available cluster name, displays it for your reference, and attaches the name to your cluster analysis.

Advanced

generate(stub) provides a prefix for the variable names created by cluster linkage. By default, the variable name prefix will be the name specified in name(). Three variables with the suffixes \_id, \_ord, and \_hgt are created and attached to the cluster-analysis results. Users generally will not need to access these variables directly.

Centroid linkage and median linkage can produce reversals or crossovers; see [MV] **cluster** for details. When reversals happen, cluster centroidlinkage and cluster medianlinkage also create a fourth variable with the suffix \_pht. This is a pseudoheight variable that is used by some postclustering commands to properly interpret the \_hgt variable.

# Options for clustermat linkage commands

Main

shape(shape) specifies the storage mode of *matname*, the matrix of dissimilarities. shape(full) is the default. The following shapes are allowed:

full specifies that *matname* is an  $n \times n$  symmetric matrix.

lower specifies that *matname* is a row or column vector of length n(n+1)/2, with the rowwise lower triangle of the dissimilarity matrix including the diagonal of zeros.

$$D_{11} D_{21} D_{22} D_{31} D_{32} D_{33} \dots D_{n1} D_{n2} \dots D_{nn}$$

llower specifies that *matname* is a row or column vector of length n(n-1)/2, with the rowwise lower triangle of the dissimilarity matrix excluding the diagonal.

$$D_{21} D_{31} D_{32} D_{41} D_{42} D_{43} \dots D_{n1} D_{n2} \dots D_{n,n-1}$$

upper specifies that matname is a row or column vector of length n(n+1)/2, with the rowwise upper triangle of the dissimilarity matrix including the diagonal of zeros.

$$D_{11} D_{12} \dots D_{1n} D_{22} D_{23} \dots D_{2n} D_{33} D_{34} \dots D_{3n} \dots D_{nn}$$

uupper specifies that *matname* is a row or column vector of length n(n-1)/2, with the rowwise upper triangle of the dissimilarity matrix excluding the diagonal.

$$D_{12} D_{13} \dots D_{1n} D_{23} D_{24} \dots D_{2n} D_{34} D_{35} \dots D_{3n} \dots D_{n-1,n}$$

- add specifies that clustermat's results be added to the dataset currently in memory. The number of observations (selected observations based on the if and in qualifiers) must equal the number of rows and columns of matname. Either clear or add is required if a dataset is currently in memory.
- clear drops all the variables and cluster solutions in the current dataset in memory (even if that dataset has changed since the data were last saved) before generating clustermat's results. Either clear or add is required if a dataset is currently in memory.
- labelvar(varname) specifies the name of a new variable to be created containing the row names of matrix matname.
- name (clname) specifies the name to attach to the resulting cluster analysis. If name() is not specified, Stata finds an available cluster name, displays it for your reference, and attaches the name to your cluster analysis.

Advanced

- force allows computations to continue when *matname* is nonsymmetric or has nonzeros on the diagonal. By default, clustermat will complain and exit when it encounters these conditions. force specifies that clustermat operate on the symmetric matrix (matname \* matname')/2, with any nonzero diagonal entries treated as if they were zero.
- generate(stub) provides a prefix for the variable names created by clustermat. By default, the variable name prefix is the name specified in name(). Three variables are created and attached to the cluster-analysis results with the suffixes \_id, \_ord, and \_hgt. Users generally will not need to access these variables directly.

Centroid linkage and median linkage can produce reversals or crossovers; see [MV] cluster for details. When reversals happen, clustermat centroidlinkage and clustermat medianlinkage also create a fourth variable with the suffix \_pht. This is a pseudoheight variable that is used by some of the postclustering commands to properly interpret the \_hgt variable.

## **Remarks and examples**

cluster and clustermat, with a specified linkage method, perform hierarchical agglomerative cluster analysis. The following command linkage methods are available: single, complete, average, Ward's method, centroid, median, and weighted average. These methods are described in *Agglomerative methods* of [MV] cluster. Other methods are mentioned in the literature, but these are the best-known methods.

The clustermat *linkage* commands perform hierarchical agglomerative cluster analysis on the dissimilarity matrix *matname*. See [MV] **clustermat** for a general discussion of cluster analysis of dissimilarity matrices and a description of the other clustermat commands. A general discussion of agglomerative cluster analysis is provided in *Hierarchical cluster-analysis methods* of [MV] **cluster**.

After a cluster *linkage* or clustermat *linkage* command, the cluster dendrogram command (see [MV] cluster dendrogram) displays the resulting dendrogram, the cluster stop or clustermat stop command (see [MV] cluster stop) helps determine the number of groups, and the cluster generate command (see [MV] cluster generate) produces grouping variables.

## Example 1

As the senior data analyst for a small biotechnology firm, you are given a dataset with four chemical laboratory measurements on 50 different samples of a particular plant gathered from the rain forest. The head of the expedition that gathered the samples thinks, based on information from the natives, that an extract from the plant might reduce the negative side effects associated with your company's best-selling nutritional supplement.

While the company chemists and botanists continue exploring the possible uses of the plant and plan future experiments, the head of product development asks you to look at the preliminary data and to report anything that might be helpful to the researchers.

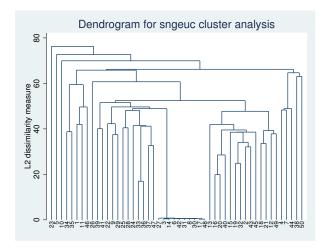
Although all 50 plants are supposed to be of the same type, you decide to perform a cluster analysis to see if there are subgroups or anomalies among them. You arbitrarily decide to use single-linkage clustering with the default Euclidean distance.

```
. use http://www.stata-press.com/data/r14/labtech
. cluster singlelinkage x1 x2 x3 x4, name(sngeuc)
. cluster list sngeuc
sngeuc (type: hierarchical, method: single, dissimilarity: L2)
    vars: sngeuc_id (id variable)
        sngeuc_ord (order variable)
        sngeuc_hgt (height variable)
    other: cmd: cluster singlelinkage x1 x2 x3 x4, name(sngeuc)
        varlist: x1 x2 x3 x4
    range: 0 .
```

The cluster singlelinkage command generated some variables and created a cluster object with the name sngeuc, which you supplied as an argument. cluster list provides details about the cluster object; see [MV] cluster utility.

What you really want to see is the dendrogram for this cluster analysis; see [MV] cluster dendrogram.

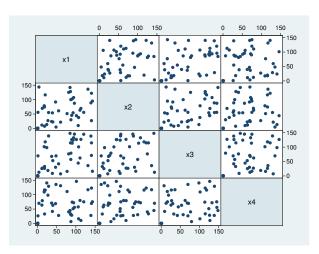
. cluster dendrogram sngeuc, xlabel(, angle(90) labsize(\*.75))



From your experience looking at dendrograms, two things jump out at you about this cluster analysis. The first is the observations showing up in the middle of the dendrogram that are all close to each other (short vertical bars) and are far from any other observations (the long vertical bar connecting them to the rest of the dendrogram). Next you notice that if you ignore those 10 observations, the rest of the dendrogram does not indicate strong clustering, as shown by the relatively short vertical bars in the upper portion of the dendrogram.

You start to look for clues why these 10 observations are so peculiar. Looking at scatterplots is usually helpful, so you examine the matrix of scatterplots.

. graph matrix x1 x2 x3 x4

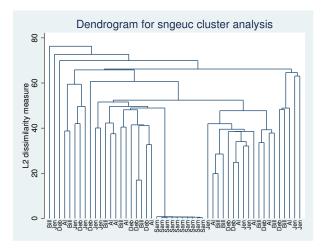


Unfortunately, these scatterplots do not indicate what might be going on.

Suddenly, from your past experience with the laboratory technicians, you have an idea of what to check next. Because of past data mishaps, the company started the policy of placing within each dataset a variable giving the name of the technician who produced the measurement. You decide

to view the dendrogram, using the technician's name as the label instead of the default observation number.

. cluster dendrogram sngeuc, labels(labtech) xlabel(, angle(90) labsize(\*.75))



Your suspicions are confirmed. Sam, one of the laboratory technicians, has messed up again. You list the data and see that all his observations are between zero and one, whereas the other four technicians' data range up to about 150, as expected. It looks like Sam forgot, once again, to calibrate his sensor before analyzing his samples. You decide to save a note of your findings with this cluster analysis (see [MV] cluster notes for the details) and to send the data back to the laboratory to be fixed.

1

### Example 2

The sociology professor of your graduate-level class gives, as homework, a dataset containing 30 observations on 60 binary variables, with the assignment to tell him something about the 30 subjects represented by the observations. You think that this assignment is too vague, but because your grade depends on it, you get to work trying to figure something out.

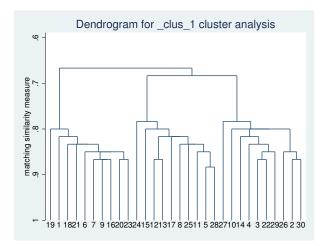
Among the analyses you try is the following cluster analysis. You decide to use single-linkage clustering with the simple matching binary coefficient because it is easy to understand. Just for fun, though it makes no difference to you, you specify the generate() option to force the generated variables to have zstub as a prefix. You let Stata pick a name for your cluster analysis by not specifying the name() option.

```
. use http://www.stata-press.com/data/r14/homework, clear
. cluster s a1-a60, measure(matching) gen(zstub)
cluster name: _clus_1
. cluster list
_clus_1 (type: hierarchical, method: single, similarity: matching)
    vars: zstub_id (id variable)
        zstub_ord (order variable)
        zstub_hgt (height variable)
    other: cmd: cluster singlelinkage a1-a60, measure(matching) gen(zstub)
    varlist: a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13 a14 a15 a16 a17
        a18 a19 a20 a21 a22 a23 a24 a25 a26 a27 a28 a29 a30 a31 a32
        a33 a34 a35 a36 a37 a38 a39 a40 a41 a42 a43 a44 a45 a46 a47
        a48 a49 a50 a51 a52 a53 a54 a55 a56 a57 a58 a59 a60
        range: 1 0
```

Stata selected \_clus\_1 as the cluster name and created the variables zstub\_id, zstub\_ord, and zstub\_hgt.

You display the dendrogram by using the cluster tree command, which is a synonym for cluster dendrogram. Because Stata uses the most recently performed cluster analysis by default, you do not need to type the name.

. cluster tree



The dendrogram seems to indicate the presence of three groups among the 30 observations. You decide that this is probably the structure your teacher wanted you to find, and you begin to write up your report. You want to examine the three groups further, so you use the cluster generate command (see [MV] cluster generate) to create a grouping variable to make the task easier. You examine various summary statistics and tables for the three groups and finish your report.

After the assignment is turned in, your professor gives you the same dataset with the addition of one more variable, truegrp, which indicates the groupings he thinks are in the data. You do a cross-tabulation of the truegrp and grp3, your grouping variable, to see if you are going to get a good grade on the assignment.

- . cluster generate grp3 = group(3)
- . table grp3 truegrp

	truegrp		
grp3	1	2	3
1		10	
2 3			10
3	10		

Other than the numbers arbitrarily assigned to the three groups, both you and your professor agree. You rest easier that night knowing that you may survive one more semester.

In addition to examining single-linkage clustering of these data, you decide to see what median-linkage clustering shows. As with the single-linkage clustering, you pick the simple matching binary coefficient to measure the similarity between groups. The name() option is used to attach the name medlink to the cluster analysis. cluster list displays the details; see [MV] cluster utility.

```
. cluster median a1-a60, measure(match) name(medlink)
. cluster list medlink
medlink (type: hierarchical, method: median, similarity: matching)
      vars: medlink_id (id variable)
            medlink_ord (order variable)
            medlink_hgt (real_height variable)
            medlink_pht (pseudo_height variable)
     other: cmd: cluster medianlinkage a1-a60, measure(match) name(medlink)
            varlist: a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13 a14 a15 a16 a17
                 a18 a19 a20 a21 a22 a23 a24 a25 a26 a27 a28 a29 a30 a31 a32
                 a33 a34 a35 a36 a37 a38 a39 a40 a41 a42 a43 a44 a45 a46 a47
                 a48 a49 a50 a51 a52 a53 a54 a55 a56 a57 a58 a59 a60
            range: 1 0
```

You attempt to use the cluster dendrogram command to display the dendrogram, but because this particular cluster analysis produced reversals, cluster dendrogram refuses to produce the dendrogram. You realize that with reversals, the resulting dendrogram would not be easy to interpret anyway.

You use the cluster generate command (see [MV] cluster generate) to create a three-group grouping variable, based on your median-linkage clustering, to compare with truegrp.

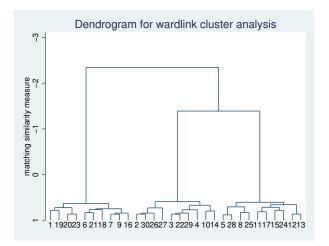
- . cluster generate medgrp3 = group(3)
- . table medgrp3 truegrp

medgrp3	truegrp 1 2		3
1 2 3	10	10	10

Because you were unable to view a dendrogram by using median-linkage clustering, you turn to Ward's linkage clustering method.

```
. cluster ward a1-a60, measure(match) name(wardlink)
. cluster list wardlink
wardlink (type: hierarchical, method: wards, similarity: matching)
      vars: wardlink_id (id variable)
           wardlink_ord (order variable)
           wardlink_hgt (height variable)
    other: cmd: cluster wardslinkage a1-a60, measure(match) name(wardlink)
            varlist: a1 a2 a3 a4 a5 a6 a7 a8 a9 a10 a11 a12 a13 a14 a15 a16 a17
                 a18 a19 a20 a21 a22 a23 a24 a25 a26 a27 a28 a29 a30 a31 a32
                 a33 a34 a35 a36 a37 a38 a39 a40 a41 a42 a43 a44 a45 a46 a47
                a48 a49 a50 a51 a52 a53 a54 a55 a56 a57 a58 a59 a60
            range: 1 0
```

#### . cluster tree wardlink



As with single-linkage clustering, the dendrogram from Ward's linkage clustering seems to indicate the presence of three groups among the 30 observations. However, notice the y-axis range for the resulting dendrogram. How can the matching similarity coefficient range from 1 to less than -2? By definition, the matching coefficient is bounded between 1 and 0. This is an artifact of the way Ward's linkage clustering is defined, and it underscores the warning mentioned in the discussion of the choice of measure. Also see Dissimilarity transformations and the Lance and Williams formula and Warning concerning similarity or dissimilarity choice in [MV] cluster for more details.

A cross-tabulation of truegrp and wardgrp3, a three-group grouping variable from this cluster analysis, is shown next.

- . cluster generate wardgrp3 = group(3)
- . table wardgrp3 truegrp

wardgrp3	t: 1	ruegrp 2	3
1 2 3	10	10	10

Other than the numbers arbitrarily assigned to the three groups, your teacher's conclusions and the results from the Ward's linkage clustering agree. So, despite the warning against using something other than squared Euclidean distance with Ward's linkage, you were still able to obtain a reasonable cluster-analysis solution with the matching similarity coefficient.

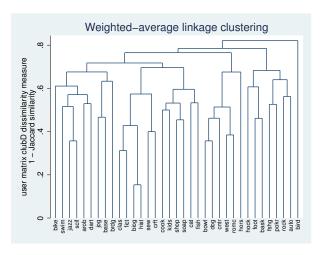
4

## ▶ Example 3

The wclub dataset contains answers from 30 women to 35 yes—no questions. The variables are described in example 3 of [MV] **clustermat**. We are interested in seeing how weighted-average linkage clustering will cluster the 35 variables (instead of the observations).

We use the matrix dissimilarity command to produce a dissimilarity matrix equal to one minus the Jaccard similarity; see [MV] matrix dissimilarity.

- . use http://www.stata-press.com/data/r14/wclub, clear
- . matrix dissimilarity clubD = , variables Jaccard dissim(oneminus)
- . clustermat waverage clubD, name(clubwav) clear labelvar(question) number of observations (\_N) was 0, now 35
- . cluster dendrogram clubwav, labels(question)
- > xlabel(, angle(90) labsize(\*.75)) title(Weighted-average linkage clustering)
- > ytitle(1 Jaccard similarity, suffix)



From these 30 women, we see that the biog (enjoy reading biographies) and hist (enjoy reading history) questions were most closely related. bird (have a bird) seems to be the least related to the other variables. It merges last into the supergroup containing the remaining variables.

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### □ Technical note

cluster commands require a significant amount of memory and execution time. With many observations, the execution time may be significant.

## Methods and formulas

[MV] cluster discusses and compares the hierarchical clustering methods.

Conceptually, hierarchical agglomerative linkage clustering proceeds as follows. The N observations start out as N separate groups, each of size one. The two closest observations are merged into one group, producing N-1 total groups. The closest two groups are then merged so that there are N-2 total groups. This process continues until all the observations are merged into one large group, producing a hierarchy of groupings from one group to N groups. The difference between the various hierarchical-linkage methods depends on how they define "closest" when comparing groups.

For single-linkage clustering, the closest two groups are determined by the closest observations between the two groups.

In complete linkage, the closest two groups are determined by the farthest observations between the two groups.

For average-linkage clustering, the closest two groups are determined by the average (dis)similarity between the observations of the two groups.

The Lance-Williams formula provides the basis for extending the well-known Ward's method of clustering into the general hierarchical-linkage framework that allows a choice of (dis)similarity measures.

Centroid linkage merges the groups whose means are closest.

Weighted-average linkage clustering is similar to average-linkage clustering, except that it gives each group of observations equal weight. Average linkage gives each observation equal weight.

Median linkage is a variation on centroid linkage in that it treats groups of unequal size differently. Centroid linkage gives each observation equal weight. Median linkage, however, gives each group of observations equal weight, meaning that with unequal group sizes, the observations in the smaller group will have more weight than the observations in the larger group.

The linkage clustering algorithm produces two variables that together act as a pointer representation of a dendrogram. To this, Stata adds a third variable used to restore the sort order, as needed, so that the two variables of the pointer representation remain valid. The first variable of the pointer representation gives the order of the observations. The second variable has one less element and gives the height in the dendrogram at which the adjacent observations in the order variable join.

When reversals happen, a fourth variable, called a pseudoheight, is produced and is used by postclustering commands with the height variable to properly interpret the ordering of the hierarchy.

See [MV] measure\_option for the details and formulas of the available measures, which include (dis)similarity measures for continuous and binary data.

Joe H. Ward, Jr. (1926-2011) was born in Austin, Texas, and obtained degrees in mathematics and educational psychology from the University of Texas. He worked as a personnel research psychologist for the U.S. Air Force Human Resources Laboratory, applying educational psychology, statistics, and computers to a wide variety of procedures, most notably the widely used clustering method named for him. In retirement, he mentored and supported high school students in computers, statistics, science fairs, and basketball.

### Also see

```
[MV] cluster dendrogram — Dendrograms for hierarchical cluster analysis
```

[MV] cluster generate — Generate summary or grouping variables from a cluster analysis

[MV] **cluster notes** — Place notes in cluster analysis

[MV] **cluster stop** — Cluster-analysis stopping rules

[MV] cluster utility — List, rename, use, and drop cluster analyses

[MV] **cluster** — Introduction to cluster-analysis commands

[MV] **clustermat** — Introduction to clustermat commands

### Title

**cluster notes** — Place notes in cluster analysis

Description Menu Syntax Remarks and examples Also see

# **Description**

cluster notes is a set of commands to manage notes for a previously run cluster analysis. You can attach notes that become part of the data and are saved when the data are saved and retrieved when the data are used. cluster notes may also be used to list notes for all defined cluster analyses or for specific cluster analyses names.

cluster notes drop allows you to drop cluster notes.

## Menu

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Cluster analysis notes

## **Syntax**

```
Add a note to a cluster analysis
```

cluster notes clname : text

List all cluster notes

cluster notes

List cluster notes associated with specified cluster analyses

cluster notes clnamelist

Drop cluster notes

cluster notes drop clname [in numlist]

## Remarks and examples

The cluster-analysis system in Stata has many features that allow you to manage the various cluster analyses that you perform. See [MV] **cluster** for information on all the available cluster-analysis commands; see [MV] **cluster utility** for other cluster commands, including cluster list, that help you manage your analyses. The cluster notes command is modeled after Stata's notes command (see [D] **notes**), but they are different systems and do not interact.

## ▶ Example 1

We illustrate the cluster notes command starting with three cluster analyses that have already been performed. The cluster dir command shows us the names of all the existing cluster analyses; see [MV] cluster utility.

```
. cluster dir
sngeuc
sngabs
kmm3abs
. cluster note sngabs : I used single linkage with absolute value distance
. cluster note sngeuc : Euclidean distance and single linkage
. cluster note kmm3abs : This has the kmeans cluster results for 3 groups
. cluster notes
sngeuc
    notes: 1. Euclidean distance and single linkage
sngabs
    notes: 1. I used single linkage with absolute value distance
kmm3abs
    notes: 1. This has the kmeans cluster results for 3 groups
```

After adding a note to each of the three cluster analyses, we used the cluster notes command without arguments to list all the notes for all the cluster analyses.

The \* and ? characters may be used when referring to cluster names; see [U] 11.2 Abbreviation rules.

recording the information.

cluster notes expanded k\* to kmn3abs, the only cluster name that begins with a k. Notes that extend to multiple lines are automatically wrapped when displayed. When entering long notes, you just continue to type until your note is finished. Pressing *Return* signals that you are done with that note.

After examining the dendrogram (see [MV] cluster dendrogram) for the sngeuc single-linkage cluster analysis and seeing one small group of data that split off from the main body of data at a very large distance, you investigate further and find data problems. You decide to add some notes to the sngeuc analysis.

```
. cluster note *euc : All of Sam's data looks wrong to me.
. cluster note *euc : I think Sam should be fired.
. cluster notes sng?*
sngeuc
     notes:
              1. Euclidean distance and single linkage
              2. All of Sam's data looks wrong to me.
              3. I think Sam should be fired.
sngabs
```

Sam, one of the lab technicians, who happens to be the owner's nephew and is paid more than you, really messed up. After adding these notes, you get second thoughts about keeping the notes attached to the cluster analysis (and the data). You decide you really want to delete those notes and to add a more politically correct note.

1. I used single linkage with absolute value distance

```
. cluster note sngeuc : Ask Jennifer to help Sam reevaluate his data.
```

sngeuc

notes:

. cluster note sngeuc

notes:

1. Euclidean distance and single linkage

- 2. All of Sam's data looks wrong to me.
- 3. I think Sam should be fired.
- 4. Ask Jennifer to help Sam reevaluate his data.
- . cluster note drop sngeuc in 2/3
- . cluster notes kmn3abs s\*

#### kmn3abs

notes:

- 1. This has the kmeans cluster results for 3 groups
- 2. Verify that observation 5 is correct. I am suspicious that there was a typographical error or instrument failure in recording the information.

sngeuc

notes:

1. Euclidean distance and single linkage

2. Ask Jennifer to help Sam reevaluate his data.

sngabs

notes: 1. I used single linkage with absolute value distance

Just for illustration purposes, the new note was added before deleting the two offending notes. cluster notes drop can take an in argument followed by a list of note numbers. The numbers correspond to those shown in the listing provided by the cluster notes command. After the deletions, the note numbers are reassigned to remove gaps. So sngeuc note 4 becomes note 2 after the deletion of notes 2 and 3 as shown above.

Without an in argument, the cluster notes drop command drops all notes associated with the named cluster.

4

Remember that the cluster notes are stored with the data and, as with other updates you make to the data, the additions and deletions are not permanent until you save the data; see [D] save.

#### □ Technical note

Programmers can access the notes (and all the other cluster attributes) by using the cluster query command; see [MV] cluster programming utilities.

## Also see

- [MV] cluster programming utilities Cluster-analysis programming utilities
- [MV] cluster utility List, rename, use, and drop cluster analyses
- [MV] **cluster** Introduction to cluster-analysis commands
- [MV] **clustermat** Introduction to clustermat commands
- [D] **notes** Place notes in data
- [D] save Save Stata dataset

cluster programming subroutines — Add cluster-analysis routines

Description Remarks and examples Reference Also see

## **Description**

This entry describes how to extend Stata's cluster command; see [MV] cluster. Programmers can add subcommands to cluster, add functions to cluster generate (see [MV] cluster generate), add stopping rules to cluster stop (see [MV] cluster stop), and set up an alternative command to be executed when cluster dendrogram is called (see [MV] cluster dendrogram).

The cluster command also provides utilities for programmers; see [MV] cluster programming utilities to learn more.

# Remarks and examples

Remarks are presented under the following headings:

```
Adding a cluster subroutine
Adding a cluster generate function
Adding a cluster stopping rule
Applying an alternate cluster dendrogram routine
```

## Adding a cluster subroutine

You add a cluster subroutine by creating a Stata program with the name cluster\_subcmdname. For example, to add the subcommand xyz to cluster, create cluster\_xyz.ado. Users could then execute the xyz subcommand with

```
cluster xyz ...
```

Everything entered on the command line after cluster xyz is passed to the cluster\_xyz command.

You can add new clustering methods, new cluster-management tools, and new postclustering programs. The cluster command has subcommands that can be helpful to cluster-analysis programmers; see [MV] cluster programming utilities.

## ▶ Example 1

We will add a cluster subroutine by writing a simple postcluster-analysis routine that provides a cross-tabulation of two cluster-analysis grouping variables. The syntax of the new command will be

```
cluster mycrosstab clname1 clname2 [, tabulate_options]
```

Here is the program:

```
program cluster_mycrosstab
    version 14.2
        gettoken clname1 0 : 0 , parse(" ,")
        gettoken clname2 rest : 0 , parse(" ,")
        cluster query 'clname1'
        local groupvar1 'r(groupvar)'
        cluster query 'clname2'
        local groupvar2 'r(groupvar)'
        tabulate 'groupvar1' 'groupvar2' 'rest'
end
```

See [P] gettoken for information on the gettoken command, and see [R] tabulate twoway for information on the tabulate command. The cluster query command is one of the cluster programming utilities that is documented in [MV] cluster programming utilities.

We can demonstrate cluster mycrosstab in action. This example starts with two cluster analyses, cl1 and cl2. The dissimilarity measure and the variables included in the two cluster analyses differ. We want to see how closely the two cluster analyses match.

```
. use http://www.stata-press.com/data/r14/auto
(1978 Automobile Data)
. cluster kmeans gear head tr, L1 k(5) name(cl1) start(krandom(55234))
> gen(cl1gvar)
. cluster kmeans tr tu mpg, L(1.5) k(5) name(cl2) start(krandom(22132))
> gen(gvar2)
. cluster list, type method dissim var
cl2 (type: partition, method: kmeans, dissimilarity: L(1.5))
        vars: gvar2 (group variable)
cl1 (type: partition, method: kmeans, dissimilarity: L1)
```

. cluster mycrosstab cl1 cl2, chi2

vars: cligvar (group variable)

			gvar2			
cl1gvar	1	2	3	4	5	Total
1	10	7	0	0	4	21
2	10	0	0	0	0	10
3	0	0	4	5	2	11
4	0	1	6	4	8	19
5	0	11	1	0	1	13
Total	20	19	11	9	15	74

Pearson chi2(16) = 98.4708 Pr = 0.000

The chi2 option was included to demonstrate that we were able to exploit the existing options of tabulate with little programming effort. We just pass along to tabulate any of the extra arguments received by cluster\_mycrosstab.

## 4

## Adding a cluster generate function

Programmers can add functions to the cluster generate command (see [MV] cluster generate) by creating a command called clusgen\_name. For example, to add a function called abc() to cluster generate, you could create clusgen\_abc.ado. Users could then execute

```
cluster generate newvar = abc( ... ) ...
```

Everything entered on the command line following cluster generate is passed to clusgen\_abc.

## ▶ Example 2

Here is the beginning of a clusgen\_abc program that expects an integer argument and has one option called name(clname), which gives the name of the cluster. If name() is not specified, the name defaults to that of the most recently performed cluster analysis. We will assume, for illustration purposes, that the cluster analysis must be hierarchical and will check for this in the clusgen\_abc program.

```
program clusgen_abc
        version 14.2
        // we use gettoken to work our way through the parsing
        gettoken newvar 0 : 0 , parse(" =")
        gettoken temp 0 : 0 , parse(" =")
        if '"'temp'"' != "=" {
                error 198
        }
        gettoken temp 0 : 0 , parse(" (")
        if '"'temp'", != "abc" {
                error 198
        }
        gettoken funcarg 0 : 0 , parse(" (") match(temp)
        if '"'temp'"' != "(" {
                error 198
        }
        // funcarg holds the integer argument to abc()
        confirm integer number 'funcarg'
        // we can now use syntax to parse the option
        syntax [, Name(str) ]
        // cluster query will give us the list of cluster names
        if '"'name'" == "" {
                cluster query
                local clnames 'r(names)'
                if "'clnames'" == "" {
                        di as err "no cluster solutions defined"
                        exit 198
                }
                // first name in the list is the latest clustering
                local name : word 1 of 'clnames'
        // cluster query followed by name will tell us the type
        cluster query 'name'
        if "'r(type)'," != "hierarchical" {
                di as err "only allowed with hierarchical clustering"
                exit 198
        }
        /*
           you would now pull more information from the call of
                       cluster query 'name'
           and do your computations and generate 'newvar'
end
```

See [MV] cluster programming utilities for details on the cluster query command.

1

## Adding a cluster stopping rule

Programmers can add stopping rules to the rule() option of the cluster stop command (see [MV] cluster stop) by creating a Stata program with the name clstop\_name. For example, to add a stopping rule named mystop so that cluster stop would now have a rule(mystop) option, you could create clstop\_mystop.ado defining the clstop\_mystop program. Users could then execute

```
cluster stop [clname], rule(mystop) ...
```

The clstop\_mystop program is passed the cluster name (*clname*) provided by the user (or the name of the current cluster result if no name is specified), followed by a comma and all the options entered by the user except for the rule(mystop) option.

### Example 3

We will add a rule(stepsize) option to cluster stop. This option implements the simple step-size stopping rule (see Milligan and Cooper 1985), which computes the difference in fusion values between levels in a hierarchical cluster analysis. (A fusion value is the similarity or dissimilarity measure at which clusters are fused or split in the hierarchical cluster structure.) Large values of the step-size stopping rule indicate groupings with more distinct cluster structure.

Examining cluster dendrograms (see [MV] **cluster dendrogram**) to visually determine the number of clusters is equivalent to using a visual approximation to the step-size stopping rule.

Here is the clstop\_stepsize program:

```
program clstop_stepsize, sortpreserve rclass
        version 14.2
        syntax anything(name=clname) [, Depth(integer -1) ]
        cluster query 'clname'
        if "'r(type)," != "hierarchical" {
                di as error ///
                    "rule(stepsize) only allowed with hierarchical clustering"
                exit 198
        if "'r(pseudo_heightvar)'" != "" {
                di as error "dendrogram reversals encountered"
                exit 198
        local hgtvar 'r(heightvar)'
        if '"'r(similarity)'"' != "" {
                sort 'hgtvar'
                local negsign "-"
        }
        else if '"'r(dissimilarity)'"' != "" {
                gsort -'hgtvar'
        }
        else {
                di as error "dissimilarity or similarity not set"
                exit 198
        }
        quietly count if !missing('hgtvar')
        local depth = cond('depth'<=1, r(N), min('depth',r(N)))</pre>
        tempvar diff
        qui gen double 'diff'='negsign'('hgtvar'-'hgtvar'[_n+1]) if _n<'depth'
        di as txt "Depth" _col(10) "Stepsize"
        di as txt "{hline 17}"
        forvalues i = 1/'= 'depth'-1' {
                local j = 'i' + 1
                di as res 'j' _col(10) %8.0g 'diff'['i']
                return scalar stepsize_'j' = 'diff'['i']
        }
        return local rule "stepsize"
end
```

See [P] syntax for information about the syntax command, [P] forvalues for information about the forvalues looping command, and [P] macro for information about the '= ...' macro function. The cluster query command is one of the cluster programming utilities that is documented in [MV] cluster programming utilities.

With this program, users can obtain the step-size stopping rule. We demonstrate this process by using an average-linkage hierarchical cluster analysis on the data found in the second example of [MV] cluster linkage. The dataset contains 30 observations on 60 binary variables. The simple matching coefficient is used as the similarity measure in the average-linkage clustering.

- . use http://www.stata-press.com/data/r14/homework, clear
- . cluster a a1-a60, measure(match) name(alink)
- . cluster stop alink, rule(stepsize) depth(15)

Depth	Stepsize
2	.065167
3	.187333
4	.00625
5	.007639
6	.002778
7	.005952
8	.002381
9	.008333
10	.005556
11	.002778
12	0
13	0
14	.006667
15	.01

In the clstop\_stepsize program, we included a depth() option. cluster stop, when called with the new rule(stepsize) option, can also have the depth() option. Here we specified that it stop at a depth of 15.

The largest step size, .187, happens at the three-group level of the hierarchy. This number, .187, represents the difference between the matching coefficient created when two groups are formed and that created when three groups are formed in this hierarchical cluster analysis.

The clstop\_stepsize program could be enhanced by using a better output table format. An option could also be added that stores the results in a matrix.

4

## Applying an alternate cluster dendrogram routine

Programmers can change the behavior of the cluster dendrogram command (alias cluster tree); see [MV] cluster dendrogram. This task is accomplished by using the other() option of the cluster set command (see [MV] cluster programming utilities) with a tag of treeprogram and with text giving the name of the command to be used in place of the standard Stata program for cluster dendrogram. For example, if you had created a new hierarchical cluster-analysis method for Stata that needed a different algorithm for producing dendrograms, you would use the command

cluster set *clname*, other(treeprogram *progname*)

to set programe as the program to be executed when cluster dendrogram is called.

### Example 4

If we were creating a new hierarchical cluster-analysis method called myclus, we could create a program called cluster\_myclus (see *Adding a cluster subroutine*). If myclus needed a different dendrogram routine from the standard one used within Stata, we could include the following line in cluster\_myclus.ado at the point where we set the cluster attributes.

```
cluster set 'clname', other(treeprogram myclustree)
```

We could then create a program called myclustree in a file called myclustree.ado that implements the particular dendrogram program needed by myclus.

1

### Reference

Milligan, G. W., and M. C. Cooper. 1985. An examination of procedures for determining the number of clusters in a dataset. *Psychometrika* 50: 159–179.

## Also see

[MV] **cluster** — Introduction to cluster-analysis commands

[MV] clustermat — Introduction to clustermat commands

[MV] cluster programming utilities — Cluster-analysis programming utilities

### **Title**

**cluster programming utilities** — Cluster-analysis programming utilities

Description
Options for cluster delete
Stored results

Syntax Options for cluster measures Also see Options for cluster set Remarks and examples

# **Description**

The cluster query, cluster set, cluster delete, cluster parsedistance, and cluster measures commands provide tools for programmers to add their own cluster-analysis subroutines to Stata's cluster command; see [MV] cluster and [MV] cluster programming subroutines. These commands make it possible for the new command to take advantage of Stata's cluster-management facilities.

cluster query provides a way to obtain the various attributes of a cluster analysis in Stata. If *clname* is omitted, cluster query returns in r(names) a list of the names of all currently defined cluster analyses. If *clname* is provided, the various attributes of the specified cluster analysis are returned in r(). These attributes include the type, method, (dis)similarity used, created variable names, notes, and any other information attached to the cluster analysis.

cluster set allows you to set the various attributes that define a cluster analysis in Stata, including naming your cluster results and adding the name to the master list of currently defined cluster results. With cluster set, you can provide information on the type, method, and (dis)similarity measure of your cluster-analysis results. You can associate variables and Stata characteristics (see [P] char) with your cluster analysis. cluster set also allows you to add notes and other specified fields to your cluster-analysis result. These items become part of the dataset and are saved with the data.

cluster delete allows you to delete attributes from a cluster analysis in Stata. This command is the inverse of cluster set.

cluster parsedistance takes the similarity or dissimilarity *measure* name and checks it against the list of those provided by Stata, taking account of allowed minimal abbreviations and aliases. Aliases are resolved (for instance, Euclidean is changed into the equivalent L2).

cluster measures computes the similarity or dissimilarity *measure* between the observations listed in the compare() option and the observations included based on the if and in conditions and places the results in the variables specified by the generate() option. See [MV] matrix dissimilarity for the matrix dissimilarity command that places (dis)similarities in a matrix.

Stata also provides a method for programmers to extend the cluster command by providing subcommands; see [MV] cluster programming subroutines.

## **Syntax**

Obtain various attributes of a cluster analysis

cluster query [clname]

Set various attributes of a cluster analysis

cluster set [clname] [, set\_options]

Delete attributes from a cluster analysis

cluster delete clname [, delete\_options]

Check similarity and dissimilarity measure name

cluster parsedistance measure

Compute similarity and dissimilarity measure

cluster measures varlist [if] [in], compare(numlist) generate(newvarlist) [measures\_options]

set_options	Description
addname	add <i>clname</i> to the master list of cluster analyses
<u>t</u> ype( <i>type</i> )	set the cluster type for <i>clname</i>
$\underline{\mathtt{m}}\mathtt{ethod}(\mathit{method})$	set the name of the clustering method for the cluster analysis
<u>s</u> imilarity( <i>measure</i> )	set the name of the similarity measure used for the cluster analysis
<u>d</u> issimilarity( <i>measure</i> )	set the name of the dissimilarity measure used for the cluster analysis
<u>v</u> ar(tag varname)	set tag that points to varname
<pre>char(tag charname)</pre>	set tag that points to charname
<pre>other(tag text)</pre>	set tag with text attached to the tag marker
$\underline{\mathbf{n}}$ ote( $text$ )	add a note to the clname

delete_options	Description
zap	delete all possible settings for clname
<u>del</u> name	remove clname from the master list of current cluster analyses
<u>t</u> ype	delete the cluster type entry from clname
<u>m</u> ethod	delete the cluster method entry from clname
<u>s</u> imilarity	delete the similarity entries from clname
$\underline{\mathtt{d}}$ issimilarity	delete the dissimilarity entries from clname
$\underline{\mathtt{n}}$ otes( $numlist$ )	delete the specified numbered notes from clname
<u>alln</u> otes	remove all notes from clname
$\underline{\mathbf{v}}$ ar( $tag$ )	remove tag from clname
<u>allv</u> ars	remove all the entries pointing to variables for clname
$\underline{\mathtt{varz}}\mathtt{ap}(\mathit{tag})$	same as var(), but also delete the referenced variable
<u>allvarz</u> ap	same as allvars, but also delete the variables
<u>c</u> har(tag)	remove tag that points to a Stata characteristic from clname
<u>allc</u> hars	remove all entries pointing to Stata characteristics for clname
<pre>charzap(tag)</pre>	same as char(), but also delete the characteristic
<u>allcharz</u> ap	same as allchars, but also delete the characteristics
other(tag)	delete tag and its associated text from clname
allothers	delete all entries from clname that have been set using other()

measures_options	Description
* compare(numlist)	use <i>numlist</i> as the comparison observations
*generate(newvarlist)	create newvarlist variables
measure	(dis)similarity measure; see <i>Options for cluster measures</i> for available measures; default is L2
propvars	interpret observations implied by if and in as proportions of binary observations
<u>propc</u> ompares	interpret comparison observations as proportions of binary observations

<sup>\*</sup>compare(numlist) and generate(newvarlist) are required.

# Options for cluster set

addname adds *clname* to the master list of currently defined cluster analyses. When *clname* is not specified, the addname option is mandatory, and here, cluster set automatically finds a cluster name that is not currently in use and uses this as the cluster name. cluster set returns the name of the cluster in r(name). If addname is not specified, the *clname* must have been added to the master list previously (for instance, through a previous call to cluster set).

type(type) sets the cluster type for clname. type(hierarchical) indicates that the cluster analysis is hierarchical-style clustering, and type(partition) indicates that it is a partition-style clustering. You are not restricted to these types. For instance, you might program some kind of fuzzy partition-clustering analysis, so you then use type(fuzzy).

method(method) sets the name of the clustering method for the cluster analysis. For instance, Stata uses method(kmeans) to indicate a kmeans cluster analysis and uses method(single) to indicate single-linkage cluster analysis. You are not restricted to the names currently used within Stata.

- similarity(measure) and dissimilarity(measure) set the name of the similarity or dissimilarity measure used for the cluster analysis. For example, Stata uses dissimilarity(L2) to indicate the L2 or Euclidean distance. You are not restricted to the names currently used within Stata. See [MV] measure\_option and [MV] cluster for a listing and discussion of (dis)similarity measures.
- var(tag varname) sets a marker called tag in the cluster analysis that points to the variable varname. For instance, Stata uses var(group varname) to set a grouping variable from a kmeans cluster analysis. With single-linkage clustering, Stata uses var(id idvarname), var(order ordervarname), and var(height hgtvarname) to set the id, order, and height variables that define the cluster-analysis result. You are not restricted to the names currently used within Stata. Up to 10 var() options may be specified with a cluster set command.
- char (tag charname) sets a marker called tag in the cluster analysis that points to the Stata characteristic named charname; see [P] char. This characteristic can be either an \_dta[] dataset characteristic or a variable characteristic. Up to 10 char() options may be specified with a cluster set command.
- other(tag text) sets a marker called tag in the cluster analysis with text attached to the tag marker. Stata uses other(k #) to indicate that k (the number of groups) was # in a kmeans cluster analysis. You are not restricted to the names currently used within Stata. Up to 10 other() options may be specified with a cluster set command.
- note(text) adds a note to the clname cluster analysis. The cluster notes command (see [MV] cluster notes) is the command to add, delete, or view cluster notes. The cluster notes command uses the note() option of cluster set to add a note to a cluster analysis. Up to 10 note() options may be specified with a cluster set command.

## Options for cluster delete

- zap deletes all possible settings for cluster analysis *clname*. It is the same as specifying the delname, type, method, similarity, dissimilarity, allnotes, allcharzap, allothers, and allvarzap options.
- delname removes *clname* from the master list of current cluster analyses. This option does not affect the various settings that make up the cluster analysis. To remove them, use the other options of cluster delete.

type deletes the cluster type entry from clname.

method deletes the cluster method entry from clname.

- similarity and dissimilarity delete the similarity and dissimilarity entries, respectively, from *clname*.
- notes (numlist) deletes the specified numbered notes from clname. The numbering corresponds to the returned results from the cluster query clname command. The cluster notes drop command (see [MV] cluster notes) drops a cluster note. It, in turn, calls cluster delete, using the notes () option to drop the notes.
- allnotes removes all notes from the *clname* cluster analysis.
- var(tag) removes from *clname* the entry labeled tag that points to a variable. This option does not delete the variable.
- allvars removes all the entries pointing to variables for *clname*. This option does not delete the corresponding variables.
- varzap(tag) is the same as var() and actually deletes the variable in question.

allvarzap is the same as allvars and actually deletes the variables.

char(tag) removes from *clname* the entry labeled tag that points to a Stata characteristic (see [P] char). This option does not delete the characteristic.

allchars removes all the entries pointing to Stata characteristics for *clname*. This option does not delete the characteristics.

charzap(tag) is the same as char() and actually deletes the characteristics.

allcharzap is the same as allchars and actually deletes the characteristics.

other(tag) deletes from *clname* the tag entry and its associated text, which were set by using the other() option of the cluster set command.

allothers deletes all entries from *clname* that have been set using the other() option of the cluster set command.

## **Options for cluster measures**

compare (numlist) is required and specifies the observations to use as the comparison observations. Each of these observations will be compared with the observations implied by the if and in conditions, using the specified (dis)similarity measure. The results are stored in the corresponding new variable from the generate() option. There must be the same number of elements in numlist as there are variable names in the generate() option.

generate(newvarlist) is required and specifies the names of the variables to be created. There must be as many elements in newvarlist as there are numbers specified in the compare() option.

measure specifies the similarity or dissimilarity measure. The default is L2 (synonym <u>Euclidean</u>).
This option is not case sensitive. See [MV] measure \_option for detailed descriptions of the supported measures.

propvars is for use with binary measures and specifies that the observations implied by the if and in conditions be interpreted as proportions of binary observations. The default action with binary measures treats all nonzero values as one (excluding missing values). With propvars, the values are confirmed to be between zero and one, inclusive. See [MV] measure\_option for a discussion of the use of proportions with binary measures.

propcompares is for use with binary measures. It indicates that the comparison observations (those specified in the compare() option) are to be interpreted as proportions of binary observations. The default action with binary measures treats all nonzero values as one (excluding missing values). With propcompares, the values are confirmed to be between zero and one, inclusive. See [MV] measure\_option for a discussion of the use of proportions with binary measures.

# Remarks and examples

## Example 1

Programmers can determine which cluster solutions currently exist by using the cluster query command without specifying a cluster name to return the names of all currently defined clusters.

```
. use http://www.stata-press.com/data/r14/auto
(1978 Automobile Data)
```

- . cluster k gear turn trunk mpg displ, k(6) name(grpk6L2) measure(L2) gen(g6l2)
- . cluster k gear turn trunk mpg displ, k(7) name(grpk7L2) measure(L2) gen(g712)

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Here there are four cluster solutions. A programmer can further process the r(names) returned macro. For example, to determine which current cluster solutions used kmeans clustering, we would loop through these four cluster solution names and, for each one, call cluster query to determine its properties.

Here we examined r(method), which records the name of the cluster-analysis method. Two of the four cluster solutions used kmeans.

### Example 2

We interactively demonstrate cluster set, cluster delete, and cluster query, though in practice these would be used within a program.

First, we add the name myclus to the master list of cluster analyses and, at the same time, set the type, method, and similarity.

cluster query shows that myclus was successfully added to the master list of cluster analyses and that the attributes that were cluster set can also be obtained.

Now we add a reference to a variable. We will use the word group as the *tag* for a variable mygrpvar. We also add another item called xyz and associate some text with the xyz item.

```
. cluster set myclus, var(group mygrpvar) other(xyz some important info)
. cluster query myclus
. return list
macros:
               r(name) : "myclus"
             r(o1_val) : "some important info"
             r(o1_tag) : "xyz"
           r(groupvar) : "mygrpvar"
            r(v1_name) : "mygrpvar"
             r(v1_tag) : "group"
         r(similarity) : "who knows"
             r(method) : "fake"
               r(type) : "madeup"
```

The cluster query command returned the mygrpvar information in two ways. The first way is with r(v#\_tag) and r(v#\_name). Here there is only one variable associated with myclus, so we have r(v1\_tag) and r(v1\_name). This information allows the programmer to loop over all the stored variable names without knowing beforehand what the tags might be or how many there are. You could loop as follows:

```
local i 1
while "'r(v'i',_tag)'" != "" {
        local ++i
```

The second way the variable information is returned is in an r() result with the tag name appended by var, r(tagvar). In our example, this is r(groupvar). This second method is convenient when, as the programmer, you know exactly which varname information you are seeking.

The same logic applies to characteristic attributes that are cluster set.

Now we continue with our interactive example:

```
. cluster delete myclus, method var(group)
. cluster set myclus, note(a note) note(another note) note(a third note)
. cluster query myclus
. return list
macros:
               r(name) : "myclus"
              r(note3) : "a third note"
              r(note2) : "another note"
              r(note1) : "a note"
             r(o1_val) : "some important info"
             r(o1_tag) : "xyz"
         r(similarity) : "who knows"
               r(type) : "madeup"
```

We used cluster delete to remove the method and the group variable we had associated with myclus. Three notes were then added simultaneously by using the note() option of cluster set. In practice, users will use the cluster notes command (see [MV] cluster notes) to add and delete cluster notes. The cluster notes command is implemented with the cluster set and cluster delete programming commands.

We finish our interactive demonstration of these commands by deleting more attributes from myclus and then eliminating myclus. In practice, users would remove a cluster analysis with the cluster drop command (see [MV] cluster utility), which is implemented with the zap option of the cluster delete command.

4

The cluster attributes that are cluster set become a part of the dataset. They are saved with the dataset when it is saved and are available again when the dataset is used; see [D] save.

### □ Technical note

You may wonder how Stata's cluster-analysis data structures are implemented. Stata data characteristics (see [P] char) hold the information. The details of the implementation are not important, and in fact, we encourage you to use the set, delete, and query subcommands to access the cluster attributes. This way, if we ever decide to change the underlying implementation, you will be protected through Stata's version-control feature.

### Example 3

The cluster parsedistance programming command takes as an argument the name of a similarity or dissimilarity measure. Stata then checks this name against those that are implemented within Stata (and available to you through the cluster measures command). Uppercase or lowercase letters are allowed, and minimal abbreviations are checked. Some of the measures have aliases, which are resolved so that a standard measure name is returned. We demonstrate the cluster parsedistance command interactively:

. sreturn list macros:

> s(drange) : "1 -1" s(dtype) : "similarity" s(unab) : "correlation" s(dist) : "correlation"

. cluster parsedistance jacc

. sreturn list

macros:

s(drange) : "1 0" s(binary) : "binary" s(dtype) : "similarity" s(unab) : "Jaccard" s(dist): "Jaccard"

cluster parsedistance returns s(dtype) as either similarity or dissimilarity. It returns s(dist) as the standard Stata name for the (dis)similarity and returns s(unab) as the unabbreviated standard Stata name. s(drange) gives the range of the measure (most similar to most dissimilar). If the measure is designed for binary variables, s(binary) is returned with the word binary, as seen above.

See [MV] measure\_option for a listing of the similarity and dissimilarity measures and their properties.

1

## Example 4

cluster measures computes the similarity or dissimilarity measure between each comparison observation and the observations implied by the if and in conditions (or all the data if no if or in conditions are specified).

We demonstrate with the auto dataset:

- . use http://www.stata-press.com/data/r14/auto, clear (1978 Automobile Data)
- . cluster measures turn trunk gear in 1/10, compare(3 11) gen(z3 z11) L1
- . format z\* %8.2f
- . list turn trunk gear z3 z11 in 1/11

	turn	trunk	gear_r~o	<b>z</b> 3	z11
1.	40	11	3.58	6.50	14.30
2.	40	11	2.53	6.55	13.25
3.	35	12	3.08	0.00	17.80
4.	40	16	2.93	9.15	8.65
5.	43	20	2.41	16.67	1.13
6.	43	21	2.73	17.35	2.45
7.	34	10	2.87	3.21	20.59
8.	42	16	2.93	11.15	6.65
9.	43	17	2.93	13.15	4.65
10.	42	13	3.08	8.00	9.80
11.	44	20	2.28	•	

Using the three variables turn, trunk, and gear\_ratio, we computed the L1 (or absolute value) distance between the third observation and the first 10 observations and placed the results in the variable z3. The distance between the 11th observation and the first 10 was placed in variable z11.

There are many measures designed for binary data. Below we illustrate cluster measures with the matching coefficient binary similarity measure. We have 8 observations on 10 binary variables, and we will compute the matching similarity measure between the last 3 observations and all 8 observations.

- . use http://www.stata-press.com/data/r14/clprogxmpl1, clear
- . cluster measures x1-x10, compare(6/8) gen(z6 z7 z8) matching
- . format z\* %4.2f
- . list

	x1	x2	х3	x4	x5	х6	х7	х8	х9	x10	<b>z</b> 6	z7	<b>z</b> 8
1. 2.	1 1	0	0	0	1 0	1	0	0	1 1	1 0	0.60	0.80	0.40
3. 4.	0	0	1	0	0	0	1	0	0	1	0.60	0.40	0.70
5.	0	1	0	1	1	0	1	0	0	1	0.40	0.60	0.40
6. 7. 8.	1 0 1	0 0 1	1 0 0	0 1 1	0 1 0	1 1 1	0 0 0	0 0 1	0 1 0	0 1 0	1.00 0.40 0.60	0.40 1.00 0.40	0.60 0.40 1.00

Stata treats all nonzero observations as one (except missing values, which are treated as missing values) when computing these binary measures.

When the similarity measure between binary observations and the means of groups of binary observations is needed, the propours and proposmpares options of cluster measures provide the solution. The mean of binary observations is a proportion. The value 0.2 would indicate that 20% of the values were one and 80% were zero for the group. See [MV] *measure\_option* for a discussion of binary measures. The propours option indicates that the main body of observations should be interpreted as proportions. The proposmpares option specifies that the comparison observations be treated as proportions.

We compare 10 binary observations on five variables to 2 observations holding proportions by using the propcompares option:

- . use http://www.stata-press.com/data/r14/clprogxmpl2, clear
- . cluster measures a\* in 1/10, compare(11 12) gen(c1 c2) matching propcompare
- . list

	a1	a2	<b>a</b> 3	a4	<b>a</b> 5	c1	c2
1.	1	1	1	0	1	.6	.56
2.	0	0	1	1	1	.36	.8
3.	1	0	1	0	0	.76	.56
4.	1	1	0	1	1	.36	.44
5.	1	0	0	0	0	.68	.4
6.	0	0	1	1	1	.36	.8
7.	1	0	1	0	1	.64	.76
8.	1	0	0	0	1	.56	.6
9.	0	1	1	1	1	.32	.6
10.	1	1	1	1	1	.44	.6
11.	.8	.4	.7	. 1	.2		
12.	.5	0	.9	.6	1	•	

### Stored results

```
cluster query with no arguments stores the following in r():
Macros
                         cluster solution names
    r(names)
cluster query with an argument stores the following in r():
                         cluster name
    r(name)
    r(type)
                         type of cluster analysis
    r(method)
                         cluster-analysis method
    r(similarity)
                         similarity measure name
    r(dissimilarity)
                         dissimilarity measure name
    r(note#)
                         cluster note number #
    r(v#_tag)
                         variable tag number #
    r(v#_name)
                         varname associated with r(v#_tag)
    r(tagvar)
                         varname associated with tag
    r(c#_tag)
                         characteristic tag number #
    r(c#_name)
                         characteristic name associated with r(c#_tag)
    r(c#_val)
                         characteristic value associated with r(c#_tag)
    r(tagchar)
                         characteristic name associated with tag
    r(o#_tag)
                         other tag number #
    r(o#_val)
                         other value associated with r(o#_tag)
cluster set stores the following in r():
Macros
    r(name)
                         cluster name
cluster parsedistance stores the following in s():
Macros
    s(dist)
                         (dis)similarity measure name
    s(unab)
                         unabbreviated (dis)similarity measure name (before resolving alias)
    s(darg)
                         argument of (dis)similarities that take them, such as L(#)
    s(dtype)
                         similarity or dissimilarity
                         range of measure (most similar to most dissimilar)
    s(drange)
    s(binary)
                         binary if the measure is for binary observations
cluster measures stores the following in r():
Macros
    r(generate)
                         variable names from the generate() option
    r(compare)
                         observation numbers from the compare() option
    r(dtype)
                         similarity or dissimilarity
    r(distance)
                         the name of the (dis)similarity measure
    r(binary)
                         binary if the measure is for binary observations
```

## Also see

```
[MV] cluster — Introduction to cluster-analysis commands
[MV] clustermat — Introduction to clustermat commands
```

[MV] cluster programming subroutines — Add cluster-analysis routines

#### **Title**

**cluster stop** — Cluster-analysis stopping rules

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

cluster stop and clustermat stop compute the stopping-rule value for each cluster solution. The commands currently provide two stopping rules, the Caliński and Harabasz pseudo-F index and the Duda-Hart Je(2)/Je(1) index. For both rules, larger values indicate more distinct clustering. Presented with the Duda-Hart Je(2)/Je(1) values are pseudo-T-squared values. Smaller pseudo-T-squared values indicate more distinct clustering.

Users can add more stop rules; see [MV] cluster programming subroutines.

### **Quick start**

Cluster analysis of data

Caliński-Harabasz pseudo- ${\cal F}$  index stopping rule for the most recent cluster analysis cluster stop

Duda-Hart Je(2)/Je(1) index stopping rule cluster stop, rule(duda)

As above, but use results for the 5-20-group solutions instead of the default 1-15-group solutions cluster stop, rule(duda) groups(5/20)

As above, but for cluster analysis results named myclus

cluster stop myclus, rule(duda) groups(5/20)

As above, but use variables v1 and v2 to compute the stopping rule instead of the variables used in myclus

cluster stop myclus, rule(duda) groups(5/20) variables(v1 v2)

Cluster analysis of dissimilarity matrix

Caliński-Harabasz pseudo-F index stopping rule computed using v1, v2, and v3 from results named mymatclus

clustermat stop mymatclus, variables(v1 v2 v3)

## Menu

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Cluster analysis stopping rules

## **Syntax**

Cluster analysis of data

```
cluster stop [clname] [, options]
```

Cluster analysis of a dissimilarity matrix

```
clustermat stop [clname] , variables(varlist) [ options ]
```

where *clname* is the name of the cluster analysis. The default is the most recently performed cluster analysis, which can be reset using the cluster use command; see [MV] cluster utility.

options	Description
rule(calinski) rule(duda) rule(rule_name) groups(numlist) matrix(matname)  *variables(varlist)	use Caliński-Harabasz pseudo- $F$ index stopping rule; the default use Duda-Hart Je(2)/Je(1) index stopping rule use $rule\_name$ stopping rule; see $Options$ for details compute stopping rule for specified groups save results in matrix $matname$ compute the stopping rule using $varlist$

<sup>\*</sup> variables(varlist) is required with a clustermat solution and optional with a cluster solution.

rule(rule\_name) is not shown in the dialog box. See [MV] cluster programming subroutines for information on how to add stopping rules to the cluster stop command.

## **Options**

rule(calinski|duda| $rule\_name$ ) indicates the stopping rule. rule(calinski), the default, specifies the Caliński-Harabasz pseudo-F index. rule(duda) specifies the Duda-Hart Je(2)/Je(1) index.

rule(calinski) is allowed for both hierarchical and nonhierarchical cluster analyses. rule(duda) is allowed only for hierarchical cluster analyses.

You can add stopping rules to the cluster stop command (see [MV] cluster programming subroutines) by using the rule(rule\_name) option. [MV] cluster programming subroutines illustrates how to add stopping rules by showing a program that adds a rule(stepsize) option, which implements the simple step-size stopping rule mentioned in Milligan and Cooper (1985).

groups (numlist) specifies the cluster groupings for which the stopping rule is to be computed. groups (3/20) specifies that the measure be computed for the three-group solution, the four-group solution, ..., and the 20-group solution.

With rule(duda), the default is groups(1/15). With rule(calinski) for a hierarchical cluster analysis, the default is groups(2/15). groups(1) is not allowed with rule(calinski) because the measure is not defined for the degenerate one-group cluster solution. The groups() option is unnecessary (and not allowed) for a nonhierarchical cluster analysis.

If there are ties in the hierarchical cluster-analysis structure, some (or possibly all) of the requested stopping-rule solutions may not be computable. cluster stop passes over, without comment, the groups() for which ties in the hierarchy cause the stopping rule to be undefined.

matrix (matname) saves the results in a matrix named matname.

With rule(calinski), the matrix has two columns, the first giving the number of clusters and the second giving the corresponding Caliński-Harabasz pseudo-F stopping-rule index.

With rule(duda), the matrix has three columns: the first column gives the number of clusters, the second column gives the corresponding Duda-Hart Je(2)/Je(1) stopping-rule index, and the third column provides the corresponding pseudo-T-squared values.

variables(varlist) specifies the variables to be used in the computation of the stopping rule. By
default, the variables used for the cluster analysis are used. variables() is required for cluster
solutions produced by clustermat.

# Remarks and examples

Cluster-analysis stopping rules are used to determine the number of clusters. A stopping-rule value (also called an index) is computed for each cluster solution (for example, at each level of the hierarchy in a hierarchical cluster analysis). Larger values (or smaller, depending on the particular stopping rule) indicate more distinct clustering. See [MV] cluster for background information on cluster analysis and on the cluster and clustermat commands.

Everitt et al. (2011) and Gordon (1999) discuss the problem of determining the number of clusters and describe several stopping rules, including the Caliński-Harabasz (1974) pseudo-F index and the Duda-Hart (2001, sec. 10.10) Je(2)/Je(1) index. There are many cluster stopping rules. Milligan and Cooper (1985) evaluate 30 stopping rules, singling out the Caliński-Harabasz index and the Duda-Hart index as two of the best rules.

Large values of the Caliński-Harabasz pseudo-F index indicate distinct clustering. The Duda-Hart Je(2)/Je(1) index has an associated pseudo-T-squared value. A large Je(2)/Je(1) index value and a small pseudo-T-squared value indicate distinct clustering. See *Methods and formulas* at the end of this entry for details.

Example 2 of [MV] clustermat shows the use of the clustermat stop command.

Some stopping rules such as the Duda-Hart index work only with a hierarchical cluster analysis. The Caliński-Harabasz index, however, may be applied to both nonhierarchical and hierarchical cluster analyses.

### Example 1

Previously, you ran kmeans cluster analyses on data where you measured the flexibility, speed, and strength of the 80 students in your physical education class; see example 1 of [MV] **cluster kmeans and kmedians**. Your original goal was to split the class into four groups, though you also examined the three- and five-group kmeans cluster solutions as possible alternatives.

Now out of curiosity, you wonder what the Caliński-Harabasz stopping rule shows for the three-four-, and five-group solutions from a kmedian clustering of this dataset.

- . use http://www.stata-press.com/data/r14/physed
- . cluster kmed flex speed strength, k(3) name(kmed3) measure(abs) start(lastk)
- . cluster kmed flex speed strength, k(4) name(kmed4) measure(abs)
- > start(kr(93947))
- . cluster kmed flex speed strength, k(5) name(kmed5) measure(abs)
- > start(prand(16872))

. cluster stop kmed3

Number of clusters	Calinski/ Harabasz pseudo-F
3	132.75

. cluster stop kmed4

Number of clusters	Calinski/ Harabasz pseudo-F
4	337.10

. cluster stop kmed5

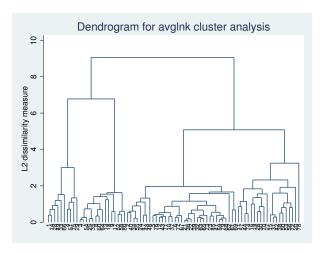
Number of clusters	Calinski/ Harabasz pseudo-F
5	300.45

The four-group solution with a Caliński-Harabasz pseudo-F value of 337.10 is largest, indicating that the four-group solution is the most distinct compared with the three-group and five-group solutions.

The three-group solution has a much lower stopping-rule value of 132.75. The five-group solution, with a value of 300.45, is reasonably close to the four-group solution.

Though you do not think it will change your decision on how to split your class into groups, you are curious to see what a hierarchical cluster analysis might produce. You decide to try an average-linkage cluster analysis using the default Euclidean distance; see [MV] cluster linkage. You examine the resulting cluster analysis with the cluster tree command, which is an easier-to-type alias for the cluster dendrogram command; see [MV] cluster dendrogram.

- . cluster averagelink flex speed strength, name(avglnk)
- . cluster tree avglnk, xlabel(, angle(90) labsize(\*.75))



You are curious to see how the four- and five-group solutions from this hierarchical cluster analysis compare with the four- and five-group solutions from the kmedian clustering.

- . cluster gen avgg = groups(4/5), name(avglnk)
- . table kmed4 avgg4

kmed4	1	avgg 2	3	4
1 2 3 4	10	15	35	20

. table kmed5 avgg5

kmed5	1	a 2	vgg5 3	4	5
1 2		15	15		
3		15		19	1
4 5	10		20		
5	10				

The four-group solutions are identical, except for the numbers used to label the groups. The five-group solutions are different. The kmedian clustering split the 35-member group into subgroups having 20 and 15 members. The average-linkage clustering instead split one member off from the 20-member group.

Now you examine the Caliński-Harabasz pseudo-F stopping-rule values associated with the kmedian hierarchical cluster analysis.

. cluster stop avglnk, rule(calinski)

Number of clusters	Calinski/ Harabasz pseudo-F
2 3 4 5 6 7 8 9 10 11 12 13	131.86 126.62 337.10 269.07 258.40 259.37 290.78 262.86 258.53 249.93 247.85
14 15	236.98 226.51

Because rule(calinski) is the default, you could have obtained this same table by typing

. cluster stop avglnk

or, because avglnk was the most recent cluster analysis performed, by typing

. cluster stop

You did not specify the number of groups to examine from the hierarchical cluster analysis, so it defaulted to examining up to 15 groups. The highest Caliński-Harabasz pseudo-F value is 337.10 for the four-group solution.

What does the Duda–Hart stopping rule produce for this hierarchical cluster analysis?

. cluster stop avglnk, rule(duda) groups(1/10)

Number of clusters	Duda, Je(2)/Je(1)	/Hart pseudo T-squared
1	0.3717	131.86
2	0.1349	147.44
3	0.2283	179.19
4	0.8152	4.08
5	0.2232	27.85
6	0.5530	13.74
7	0.5287	29.42
8	0.6887	3.16
9	0.4888	8.37
10	0.7621	7.80

This time, we asked to see the results for one to 10 groups. The largest Duda-Hart Je(2)/Je(1) stopping-rule value is 0.8152, corresponding to four groups. The smallest pseudo-T-squared value is 3.16 for the eight-group solution, but the pseudo-T-squared value for the four-group solution is also low, with a value of 4.08.

Distinct clustering is characterized by large Caliński-Harabasz pseudo-F values, large Duda-Hart Je(2)/Je(1) values, and small Duda-Hart pseudo-T-squared values.

The conventional wisdom for deciding the number of groups based on the Duda-Hart stopping-rule table is to find one of the largest Je(2)/Je(1) values that corresponds to a low pseudo-T-squared value that has much larger T-squared values next to it. This strategy, combined with the results from the Caliński-Harabasz results, indicates that the four-group solution is the most distinct from this hierarchical cluster analysis.

#### □ Technical note

There is a good reason that the word "pseudo" appears in "pseudo-F" and "pseudo-T-squared". Although these index values are based on well-known statistics, any p-values computed from these statistics would not be valid. Remember that cluster analysis searches for structure.

If you were to generate random observations, perform a cluster analysis, compute these stoppingrule statistics, and then follow that by computing what would normally be the p-values associated with the statistics, you would almost always end up with significant p-values.

Remember that you would expect, on average, five of every 100 groupings of your random data to show up as significant when you use .05 as your threshold for declaring significance. Cluster-analysis methods search for the best groupings, so there is no surprise that p-values show high significance, even when none exists.

Examining the stopping-rule index values relative to one another is useful, however, in finding relatively reasonable groupings that may exist in the data.

4

#### □ Technical note

As mentioned in *Methods and formulas*, ties in the hierarchical cluster structure cause some of the stopping-rule index values to be undefined. Discrete (as opposed to continuous) data tend to cause ties in a hierarchical clustering. The more discrete the data, the more likely it is that ties will occur (and the more of them you will encounter) within a hierarchy.

Even with so-called continuous data, ties in the hierarchical clustering can occur. We say "so-called" because most continuous data are truncated or rounded. For instance, miles per gallon, length, weight, etc., which may really be continuous, may be observed and recorded only to the tens, ones, tenths, or hundredths of a unit.

You can have data with no ties in the observations and still have many ties in the hierarchy. Ties in distances (or similarities) between observations and groups of observations cause the ties in the hierarchy.

Thus, do not be surprised when some (many) of the stopping-rule values that you request are not presented. Stata has decided not to break the ties arbitrarily, because the stopping-rule values may differ widely, depending on which split is made.

#### □ Technical note

The stopping rules also become less informative as the number of elements in the groups becomes small, that is, having many groups, each with few observations. We recommend that if you need to examine the stopping-rule values deep within your hierarchical cluster analysis, you do so skeptically.

### Stored results

```
cluster stop and clustermat stop with rule(calinski) stores the following in r():
Scalars
   r(calinski_#) Caliński-Harabasz pseudo-F for # groups
Macros
   r(rule)
                   calinski
   r(label)
                   C-H pseudo-F
                   Calinski & Harabasz pseudo-F
   r(longlabel)
cluster stop and clustermat stop with rule(duda) stores the following in r():
Scalars
   r(duda_#)
                   Duda-Hart Je(2)/Je(1) value for # groups
   r(dudat2_#)
                   Duda-Hart pseudo-T-squared value for # groups
Macros
   r(rule)
                   duda
   r(label)
                   D-H Je(2)/Je(1)
   r(longlabel)
                   Duda & Hart Je(2)/Je(1)
   r(label2)
                   D-H pseudo-T-squared
```

r(longlabel2) Duda & Hart pseudo-T-squared

### Methods and formulas

The Caliński-Harabasz pseudo-F stopping-rule index for g groups and N observations is

$$\frac{\operatorname{trace}(\mathbf{B})/(g-1)}{\operatorname{trace}(\mathbf{W})/(N-g)}$$

where  $\mathbf{B}$  is the between-cluster sum of squares and cross-products matrix, and  $\mathbf{W}$  is the within-cluster sum of squares and cross-products matrix.

Large values of the Caliński-Harabasz pseudo-F stopping-rule index indicate distinct cluster structure. Small values indicate less clearly defined cluster structure.

The Duda–Hart Je(2)/Je(1) stopping-rule index value is literally Je(2) divided by Je(1). Je(1) is the sum of squared errors within the group that is to be divided. Je(2) is the sum of squared errors in the two resulting subgroups.

Large values of the Duda-Hart pseudo-T-squared stopping-rule index indicate distinct cluster structure. Small values indicate less clearly defined cluster structure.

The Duda-Hart Je(2)/Je(1) index requires hierarchical clustering information. It needs to know at each level of the hierarchy which group is to be split and how. The Duda-Hart index is also local because the only information used comes from the group's being split. The information in the rest of the groups does not enter the computation.

In comparison, the Caliński-Harabasz rule does not require hierarchical information and is global because the information from each group is used in the computation.

A pseudo-T-squared value is also presented with the Duda and Hart Je(2)/Je(1) index. The relationship is

$$\frac{1}{\text{Je}(2)/\text{Je}(1)} = 1 + \frac{T^2}{N_1 + N_2 - 2}$$

where  $N_1$  and  $N_2$  are the numbers of observations in the two subgroups.

Je(2)/Je(1) will be zero when Je(2) is zero, that is, when the two subgroups each have no variability. An example of this is when the cluster being split has two distinct values that are being split into singleton subgroups. Je(1) will never be zero because we do not split groups that have no variability. When Je(2)/Je(1) is zero, the pseudo-T-squared value is undefined.

Ties in splitting a hierarchical cluster analysis create an ambiguity for the Je(2)/Je(1) measure. For example, to compute the measure for the case of going from five clusters to six, you need to identify the one cluster that will be split. With a tie in the hierarchy, you would instead go from five clusters directly to seven (just as an example). Stata refuses to produce an answer in this situation.

### References

Caliński, T., and J. Harabasz. 1974. A dendrite method for cluster analysis. Communications in Statistics—Theory and Methods 3: 1–27.

Duda, R. O., P. E. Hart, and D. G. Stork. 2001. Pattern Classification. 2nd ed. New York: Wiley.

Everitt, B. S., S. Landau, M. Leese, and D. Stahl. 2011. Cluster Analysis. 5th ed. Chichester, UK: Wiley.

Gordon, A. D. 1999. Classification. 2nd ed. Boca Raton, FL: Chapman & Hall/CRC.

Milligan, G. W., and M. C. Cooper. 1985. An examination of procedures for determining the number of clusters in a dataset. *Psychometrika* 50: 159–179.

# Also see

[MV] cluster — Introduction to cluster-analysis commands

[MV] **clustermat** — Introduction to clustermat commands

#### **Title**

cluster utility - List, rename, use, and drop cluster analyses

Description
Options for cluster list

Menu
Options for cluster renamevar

Syntax

Remarks and examples

# **Description**

Also see

These cluster utility commands allow you to view and manipulate the cluster objects that you have created. See [MV] **cluster** for an overview of cluster analysis and for the available cluster commands. If you want even more control over your cluster objects, or if you are programming new cluster subprograms, more cluster programmer utilities are available; see [MV] **cluster programming utilities** for details.

The cluster dir command provides a directory-style listing of all the currently defined clusters. cluster list provides a detailed listing of the specified clusters or of all current clusters if no cluster names are specified. The default action is to list all the information attached to the clusters. You may limit the type of information listed by specifying particular options.

The cluster drop command removes the named clusters. The keyword \_all specifies that all current cluster analyses be dropped.

Stata cluster analyses are referred to by name. Many cluster commands default to using the most recently defined cluster analysis if no cluster name is provided. The cluster use command sets the specified cluster analysis as the most recently executed cluster analysis, so that, by default, this cluster analysis will be used if the cluster name is omitted from many of the cluster commands. You may use the \* and ? name-matching characters to shorten the typing of cluster names; see [U] 11.2 Abbreviation rules.

cluster rename allows you to rename a cluster analysis without changing any of the variable names attached to the cluster analysis. The cluster renamevar command, on the other hand, allows you to rename the variables attached to a cluster analysis and to update the cluster object with the new variable names. Do not use the rename command (see [D] rename) to rename variables attached to a cluster analysis because this would invalidate the cluster object. Use the cluster renamevar command instead.

### Menu

#### cluster list

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Detailed listing of clusters

#### cluster drop

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Drop cluster analyses

#### cluster rename

Statistics > Multivariate analysis > Cluster analysis > Postclustering > Rename a cluster or cluster variables

# **Syntax**

```
Directory-style listing of currently defined clusters
```

cluster dir

Detailed listing of clusters

cluster list [clnamelist] [, list\_options]

Drop cluster analyses

cluster drop { clnamelist | \_all }

Mark a cluster analysis as the most recent one

cluster use clname

Rename a cluster

cluster rename oldclname newclname

Rename variables attached to a cluster

cluster renamevar oldvarname newvar [ ,  $\underline{\mathbf{n}}$ ame(clname)]

cluster renamevar oldstub newstub,  $\underline{\underline{p}}$ refix  $[\underline{\underline{n}}$ ame(clname)

list_options	Description
Options	
<u>n</u> otes	list cluster notes
<u>t</u> ype	list cluster analysis type
$\underline{\mathtt{m}}\mathtt{e}\mathtt{t}\mathtt{h}\mathtt{o}\mathtt{d}$	list cluster analysis method
$\underline{\mathtt{d}}$ issimilarity	list cluster analysis dissimilarity measure
$\underline{\mathtt{s}}\mathtt{imilarity}$	list cluster analysis similarity measure
<u>v</u> ars	list variable names attached to the cluster analysis
<u>c</u> hars	list any characteristics attached to the cluster analysis
<u>o</u> ther	list any "other" information
<u>a</u> ll	list all items and information attached to the cluster; the default

all does not appear in the dialog box.

# **Options for cluster list**

Options

notes specifies that cluster notes be listed.

type specifies that the type of cluster analysis be listed.

method specifies that the cluster analysis method be listed.

dissimilarity specifies that the dissimilarity measure be listed.

similarity specifies that the similarity measure be listed.

vars specifies that the variables attached to the clusters be listed.

chars specifies that any Stata characteristics attached to the clusters be listed.

other specifies that information attached to the clusters under the heading "other" be listed.

The following option is available with cluster list but is not shown in the dialog box:

all, the default, specifies that all items and information attached to the cluster(s) be listed. You may instead pick among the notes, type, method, dissimilarity, similarity, vars, chars, and other options to limit what is presented.

## Options for cluster renamevar

name(clname) indicates the cluster analysis within which the variable renaming is to take place. If name() is not specified, the most recently performed cluster analysis (or the one specified by cluster use) will be used.

prefix specifies that all variables attached to the cluster analysis that have *oldstub* as the beginning of their name be renamed, with *newstub* replacing *oldstub*.

# Remarks and examples

### ▶ Example 1

We demonstrate these cluster utility commands by beginning with four already-defined cluster analyses. The dir and list subcommands provide listings of the cluster analyses.

```
. cluster list
bcx3kmed (type: partition, method: kmedians, dissimilarity: L2)
      vars: bcx3kmed (group variable)
     other: cmd: cluster kmedians b c x, k(3) name(bcx3kmed)
            varlist: b c x
           k · 3
           start: krandom
           range: 0 .
ayz5kmeans (type: partition, method: kmeans, dissimilarity: L2)
      vars: ayz5kmeans (group variable)
     other: cmd: cluster kmeans a y z, k(5) name(ayz5kmeans)
           varlist: a y z
           start: krandom
           range: 0 .
abc_clink (type: hierarchical, method: complete, dissimilarity: L2)
      vars: abc_clink_id (id variable)
            abc_clink_ord (order variable)
            abc_clink_hgt (height variable)
     other: cmd: cluster completelinkage a b c, name(abc_clink)
            varlist: a b c
           range: 0 .
xyz_slink (type: hierarchical, method: single, dissimilarity: L2)
      vars: xyz_slink_id (id variable)
           xyz_slink_ord (order variable)
           xyz_slink_hgt (height variable)
     other: cmd: cluster singlelinkage x y z, name(xyz_slink)
            varlist: x y z
           range: 0 .
. cluster list a*, vars
ayz5kmeans
      vars: ayz5kmeans (group variable)
abc_clink
      vars: abc_clink_id (id variable)
            abc_clink_ord (order variable)
            abc_clink_hgt (height variable)
```

cluster dir listed the names of the four currently defined cluster analyses. cluster list followed by the name of one of the cluster analyses listed the information attached to that cluster analysis. The cluster list command, without an argument, listed the information for all currently defined cluster analyses. We demonstrated the vars option of cluster list to show that we can restrict the information that is listed. Notice also the use of a\* as the cluster name. The \* here indicates that any ending is allowed. For these four cluster analyses, Stata matches the names ayz5kmeans and abc\_clink.

We now demonstrate the use of the renamevar subcommand.

```
. cluster renamevar ayz5kmeans g5km
variable ayz5kmeans not found in bcx3kmed
r(198);
. cluster renamevar ayz5kmeans g5km, name(ayz5kmeans)
. cluster list ayz5kmeans
ayz5kmeans (type: partition, method: kmeans, dissimilarity: L2)
    vars: g5km (group variable)
    other: cmd: cluster kmeans a y z, k(5) name(ayz5kmeans)
        varlist: a y z
        k: 5
        start: krandom
        range: 0 .
```

The first use of cluster renamevar failed because we did not specify which cluster object to use (with the name() option), and the most recent cluster object, bcx3kmed, was not the appropriate one. After specifying the name() option with the appropriate cluster name, the renamevar subcommand changed the name as shown in the cluster list command that followed.

The cluster use command sets a particular cluster object as the default. We show this in conjunction with the prefix option of the renamevar subcommand.

```
. cluster use ayz5kmeans
. cluster renamevar g grp, prefix
. cluster renamevar xyz_slink_ wrk, prefix name(xyz*)
. cluster list ayz* xyz*
ayz5kmeans (type: partition, method: kmeans, dissimilarity: L2)
     vars: grp5km (group variable)
     other: cmd: cluster kmeans a y z, k(5) name(ayz5kmeans)
           varlist: a y z
           start: krandom
           range: 0 .
xyz_slink (type: hierarchical, method: single, dissimilarity: L2)
      vars: wrkid (id variable)
           wrkord (order variable)
           wrkhgt (height variable)
     other: cmd: cluster singlelinkage x y z, name(xyz_slink)
            varlist: x y z
           range: 0 .
```

The cluster use command placed ayz5kmeans as the current cluster object. The cluster renamevar command that followed capitalized on this placement by leaving off the name() option. The prefix option allowed us to change the variable names, as demonstrated in the cluster list of the two changed cluster objects.

cluster rename changes the name of cluster objects. cluster drop allows us to drop some of or all the cluster objects.

```
. cluster rename xyz_slink bob
. cluster rename ayz* sam
. cluster list, type method vars
    (type: partition, method: kmeans)
      vars: grp5km (group variable)
bob (type: hierarchical, method: single)
      vars: wrkid (id variable)
            wrkord (order variable)
            wrkhgt (height variable)
bcx3kmed (type: partition, method: kmedians)
      vars: bcx3kmed (group variable)
abc_clink (type: hierarchical, method: complete)
      vars: abc_clink_id (id variable)
            abc_clink_ord (order variable)
            abc_clink_hgt (height variable)
. cluster drop bcx3kmed abc_clink
. cluster dir
sam
. cluster drop _all
. cluster dir
```

We used options with cluster list to limit what was presented. The \_all keyword with cluster drop removed all currently defined cluster objects.

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### Also see

- [MV] cluster notes Place notes in cluster analysis
- [MV] cluster programming utilities Cluster-analysis programming utilities
- [MV] **cluster** Introduction to cluster-analysis commands
- [MV] **clustermat** Introduction to clustermat commands
- [D] **notes** Place notes in data
- [P] **char** Characteristics

#### Title

```
discrim — Discriminant analysis
```

Description	Syntax	Remarks and examples	Methods and formulas
References	Also see		

# **Description**

discrim performs discriminant analysis, which is also known as classification. kth-nearest-neighbor (KNN) discriminant analysis, linear discriminant analysis (LDA), quadratic discriminant analysis (QDA), and logistic discriminant analysis are available.

# **Syntax**

discrim subcommand ... [, ...]

subcommand	Description
knn	kth-nearest-neighbor discriminant analysis
lda	linear discriminant analysis
logistic	logistic discriminant analysis
qda	quadratic discriminant analysis

# Remarks and examples

Remarks are presented under the following headings:

Introduction
A simple example
Prior probabilities, costs, and ties

#### Introduction

Discriminant analysis is used to describe the differences between groups and to exploit those differences in allocating (classifying) observations of unknown group membership to the groups. Discriminant analysis is also called classification in many references. However, several sources use the word classification to mean cluster analysis.

Some applications of discriminant analysis include medical diagnosis, market research, classification of specimens in anthropology, predicting company failure or success, placement of students (workers) based on comparing pretest results to those of past students (workers), discrimination of natural versus man-made seismic activity, fingerprint analysis, image pattern recognition, and signal pattern classification.

Most multivariate statistics texts have chapters on discriminant analysis, including Rencher (1998), Rencher and Christensen (2012), Johnson and Wichern (2007), Mardia, Kent, and Bibby (1979), Anderson (2003), Everitt and Dunn (2001), Tabachnick and Fidell (2007), and Albert and Harris (1987). Books dedicated to discriminant analysis include Lachenbruch (1975), Klecka (1980), Hand (1981), Huberty (1994), McLachlan (2004), and Afifi, May, and Clark (2012). Of these, McLachlan (2004) gives the most extensive coverage, including 60 pages of references.

If you lack observations with known group membership, use cluster analysis to discover the natural groupings in the data; see [MV] **cluster**. If you have data with known group membership, possibly with other data of unknown membership to be classified, use discriminant analysis to examine the differences between the groups, based on data where membership is known, and to assign group membership for cases where membership is unknown.

Some researchers are not interested in classifying unknown observations and are interested only in the descriptive aspects of discriminant analysis. For others, the classification of unknown observations is the primary consideration. Huberty (1994), Rencher (1998), Rencher and Christensen (2012), and others split their discussion of discrimination into two parts. Huberty labels the two parts descriptive discriminant analysis and predictive discriminant analysis. Rencher and Christensen reserve discriminant analysis for descriptive discriminant analysis and uses the label classification for predictive discriminant analysis.

There are many discrimination methods. discrim has both descriptive and predictive LDA; see [MV] discrim lda. If your interest is in descriptive LDA, candisc computes the same thing as discrim lda, but with output tailored for the descriptive aspects of the discrimination; see [MV] candisc.

The remaining discrim subcommands provide alternatives to LDA for predictive discrimination. [MV] **discrim qda** provides quadratic discriminant analysis (QDA). [MV] **discrim logistic** provides logistic discriminant analysis. [MV] **discrim knn** provides kth-nearest-neighbor (KNN) discrimination.

The discriminant analysis literature uses conflicting terminology for several features of discriminant analysis. For example, in descriptive LDA, what one source calls a classification function another source calls a discriminant function while calling something else a classification function. Check the *Methods and formulas* sections for the discrim subcommands for clarification.

### A simple example

We demonstrate the predictive and descriptive aspects of discriminant analysis with a simple example.

# Example 1: Discriminant analysis for prediction

Johnson and Wichern (2007, 578) introduce the concepts of discriminant analysis with a two-group dataset. A sample of 12 riding-lawnmower owners and 12 nonowners is sampled from a city and the income in thousands of dollars and lot size in thousands of square feet are recorded. A riding-mower manufacturer wants to see if these two variables adequately separate owners from nonowners, and if so to then direct their marketing on the basis of the separation of owners from nonowners.

```
. use http://www.stata-press.com/data/r14/lawnmower2 (Johnson and Wichern (2007) Table 11.1)
```



Do these two variables adequately separate riding-mower owners from nonowners so that the riding-mower manufacturer can base predictions of riding-mower ownership on income and lot size? The graph shows some separation of owners from nonowners, but with overlap. With predictive LDA we can quantify our ability to discriminate between riding-mower owners and nonowners.

. discrim lda lotsize income, group(owner) Linear discriminant analysis Resubstitution classification summary

Key	
Number Percent	

True owner	Classified nonowner	owner	Total
nonowner	10	2	12
	83.33	16.67	100.00
owner	1	11	12
	8.33	91.67	100.00
Total	11	13	24
	45.83	54.17	100.00
Priors	0.5000	0.5000	

The table presented by discrim lda (and the other discrim subcommands) is called a classification table or confusion matrix. It is labeled as a resubstitution classification table because the same observations used in estimating the discriminant model were classified using the model. The diagonal elements in the main body of the table show the number and percent correctly classified into each group. The off-diagonal elements show the misclassified number and percent. One owner and two nonowners were misclassified.

The resubstitution classification table provides an overly optimistic assessment of how well the linear discriminant function will predict the ownership status for observations that were not part of the training sample. A leave-one-out classification table provides a more realistic assessment for future prediction. The leave-one-out classification is produced by holding each observation out, one at a

time; building an LDA model from the remaining training observations; and then classifying the held out observation using this model. The leave-one-out classification table is available at estimation time, at playback, or through the estat classtable postestimation command.

. estat classtable, loo nopriors Leave-one-out classification table

Key
Number Percent

	LOO Classified				
True owner	nonowner	owner	Total		
nonowner	9	3	12		
	75.00	25.00	100.00		
owner	2	10	12		
	16.67	83.33	100.00		
Total	11	13	24		
	45.83	54.17	100.00		

With leave-one-out classification we see that 5, instead of only 3, of the 24 observations are misclassified.

The predict and estat commands provide other predictive discriminant analysis tools. predict generates variables containing the posterior probabilities of group membership or generates a group membership classification variable. estat displays classification tables, displays error-rate tables, and lists classifications and probabilities for the observations.

We now use estat list to show the resubstitution and leave-one-out classifications and posterior probabilities for those observations that were misclassified by our LDA model.

. estat list, class(loo) probabilities(loo) misclassified

	Classification			Probabilities		LOO Probabilities	
Obs.	True	Class.	L00 Cl.	nonowner	owner	nonowner	owner
1 2 13	owner owner nonown	nonown owner	nonown *  owner *	0.7820 0.4945 0.2372	0.2180 0.5055 0.7628	0.8460 0.6177 0.1761	0.1540 0.3823 0.8239
14 17	nonown	nonown owner	owner *  owner *	0.5287 0.3776	0.4713 0.6224	0.4313 0.2791	0.5687 0.7209

\* indicates misclassified observations

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We have used discrim lda to illustrate predictive discriminant analysis. The other discrim subcommands could also be used for predictive discrimination of these data.

Postestimation commands after discrim lda provide descriptive discriminant analysis; see [MV] discrim lda postestimation and [MV] candisc.

#### Example 2: Discriminant analysis for description

The riding-mower manufacturer of the previous example wants to understand how income and lot size affect riding-mower ownership. Descriptive discriminant analysis provides tools for exploring how the groups are separated. Fisher's (1936) linear discriminant functions provide the basis for descriptive LDA; see [MV] **discrim lda** and [MV] **discrim lda postestimation**. The postestimation command estat loadings allows us to view the discriminant function coefficients, which are also called loadings.

. estat loadings, standardized unstandardized Canonical discriminant function coefficients

	function1
lotsize income	.3795228 .0484468
_cons	-11.96094

Standardized canonical discriminant function coefficients

	function1
lotsize income	.7845512 .8058419

We requested both the unstandardized and standardized coefficients. The unstandardized coefficients apply to unstandardized variables. The standardized coefficients apply to variables standardized using the pooled within-group covariance. Standardized coefficients are examined to assess the relative importance of the variables to the discriminant function.

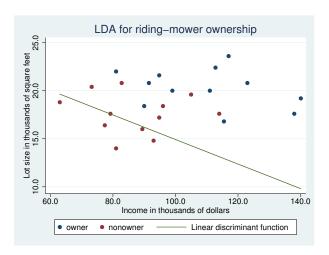
The unstandardized coefficients determine the separating line between riding-mower owners and nonowners.

$$0 = 0.3795228$$
 lotsize  $+0.0484468$  income  $-11.96094$ 

which can be reexpressed as

$$lotsize = -0.1276519 income + 31.51574$$

We now display this line superimposed on the scatterplot of the data.



Other descriptive statistics and summaries are available; see [MV] discrim Ida postestimation.

### Prior probabilities, costs, and ties

Classification is influenced by the selection of prior probabilities, assignment of costs to misclassification, and the method of handling ties in classification criteria.

Prior probabilities are the presumptive or a priori probabilities of group membership. Before you flip a balanced coin 10 times, you know the prior probability of getting heads is the same as getting tails—both are 0.5. Group prior probabilities, commonly called priors, must be taken into account in calculations of posterior probabilities; see *Methods and formulas* for details.

If the cost of misclassification is not equal over the groups, an optimal classification into groups must take misclassification cost into account. When there are two groups, members of the first group can be classified into the second, or members of the second group can be classified into the first. The relative undesirability of these two misclassifications may not be the same. Example 3 of [MV] **discrim knn** classifies poisonous and edible mushrooms. Misclassifying poisonous mushrooms as edible is a big deal at dinnertime.

The expected misclassification cost is the sum of the products of the cost for each misclassification multiplied by the probability of its occurrence. Let  $p_{ij}$  be the probability that an observation from group i is classified into group j, let  $c_{ij}$  be the cost of misclassifying an observation from group i into group j, and let  $q_i$  be the prior probability that the observation is from group i. The expected cost of misclassification is then

$$cost = \sum_{i,j \neq i}^{g} c_{ij} p_{ij} q_i$$

It is this expected cost that we wish to minimize. In the two-group case

$$cost = c_{12}p_{12}q_1 + c_{21}p_{21}q_2$$

and we can use cost-adjusted group prior probabilities,  $\hat{q}_i$ , in the place of the prior probabilities to minimize the cost of misclassification.

$$\widehat{q}_1 = \frac{c_{12}q_1}{c_{12}q_1 + c_{21}q_2}$$

$$\widehat{q}_2 = \frac{c_{21}q_2}{c_{12}q_1 + c_{21}q_2}$$

With more than two groups, there is often not a simple rule to take costs into account. More discussion on this topic is provided by McLachlan (2004, 7–9), Huberty (1994, 68–69), Johnson and Wichern (2007, 606–609), and Anderson (2003, chap. 6).

See example 3 of [MV] discrim knn for an application of costs.

A tie in classification occurs when two or more group posterior probabilities are equal for an observation. Ties are most common with kth-nearest-neighbor discriminant analysis, though they can occur in other forms of discriminant analysis. There are several options for assigning tied observations. The default is to mark the observation as unclassified, that is, classified to a missing value. Ties can also be broken. For most forms of discriminant analysis ties can be broken in two ways—randomly or assigned to the first group that is tied. For kth-nearest-neighbor discriminant analysis, dissimilarities are calculated, and so ties may also be broken by choosing the group of the nearest of the tied observations. If this still results in a tie, the observation is unclassified.

### Methods and formulas

See [MV] discrim Ida for the methods and formulas for descriptive discriminant analysis.

For predictive discriminant analysis, let g be the number of groups,  $n_i$  the number of observations for group i, and  $q_i$  the prior probability for group i. Let  $\mathbf x$  denote an observation measured on p discriminating variables. For consistency with the discriminant analysis literature,  $\mathbf x$  will be a column vector, though it corresponds to a row in your dataset. Let  $f_i(\mathbf x)$  represent the density function for group i, and let  $P(\mathbf x|G_i)$  denote the probability of observing  $\mathbf x$  conditional on belonging to group i. Denote the posterior probability of group i given observation  $\mathbf x$  as  $P(G_i|\mathbf x)$ . With Bayes' theorem, we have

$$P(G_i|\mathbf{x}) = \frac{q_i f_i(\mathbf{x})}{\sum_{j=1}^{g} q_j f_j(\mathbf{x})}$$

Substituting  $P(\mathbf{x}|G_i)$  for  $f_i(\mathbf{x})$ , we have

$$P(G_i|\mathbf{x}) = \frac{q_i P(\mathbf{x}|G_i)}{\sum_{j=1}^g q_j P(\mathbf{x}|G_j)}$$

An observation is classified as belonging to the group with the highest posterior probability.

The difference between the discrim subcommands is in the choice of  $f_i(\mathbf{x})$ . LDA, discrim lda, assumes that the groups are multivariate normal with equal covariance matrices; see [MV] discrim lda. QDA, discrim qda, assumes that the groups are multivariate normal, allowing the groups to have unequal covariance matrices; see [MV] discrim qda. Logistic discriminant analysis, discrim logistic, uses the multinomial logistic model to obtain the posterior probabilities; see [MV] discrim logistic. kth-nearest neighbor, discrim knn, uses a simple nonparametric estimate of  $f_i(\mathbf{x})$ , based on examination of the k closest observations; see [MV] discrim knn.

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### Also see

```
[MV] discrim estat — Postestimation tools for discrim
```

[MV] candisc — Canonical linear discriminant analysis

[MV] cluster — Introduction to cluster-analysis commands

[U] 20 Estimation and postestimation commands

#### Title

discrim	estat	Postestimation	tools for	discrim
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Postestimation commands

Menu for estat

Remarks and examples

References

Description for estat

Syntax for estat

Options for estat

Options for estat

Methods and formulas

#### Postestimation commands

The following postestimation commands are of special interest after candisc, discrim knn, discrim lda, discrim logistic, and discrim qda:

Command	Description
estat classtable	classification table
estat errorrate	classification error-rate estimation
estat grsummarize	group summaries
estat list	classification listing
estat summarize	estimation sample summary

There are more postestimation commands of special interest after discrim lda and discrim qda; see [MV] discrim lda postestimation and [MV] discrim qda postestimation.

### **Description for estat**

estat classtable displays a cross-tabulation of the original groups with the classification groups. Classification percentages, average posterior probabilities, group prior probabilities, totals, and leave-one-out results are available.

estat errorrate displays error-rate estimates for the classification. Count-based estimates and both stratified and unstratified posterior-probability-based estimates of the error rate are available. These estimates can be resubstitution or leave-one-out estimates.

estat grsummarize presents estimation sample summary statistics for the discriminating variables for each group defined by the grouping variable. Means, medians, minimums, maximums, standard deviations, coefficients of variation, standard errors of the means, and group sizes may be displayed. Overall sample statistics are also available.

estat list lists group membership, classification, and probabilities for observations.

estat summarize summarizes the variables in the discriminant analysis over the estimation sample.

### Quick start for estat

Classification table

Classification table computed using proportional prior probabilities estat classtable, priors(proportional)

Leave-one-out classification table showing average posterior probability of classification into each group

estat classtable, looclass probabilities

Classification error-rate estimation

Error-rate table estimated from leave-one-out error count estat errorrate, looclass

Error rates estimated from posterior probabilities using proportional prior probabilities estat errorrate, pp priors(proportional)

Group summaries

Summary statistics by group estat grsummarize

Mean, median, standard deviation, minimum, and maximum by group estat grsummarize, mean median sd min max

Classification listing

Listing of group membership, classification, and probabilities including the leave-one-out results estat list, classification(looclass) probabilities(loopr)

As above, but suppress the resubstitution classification
estat list, classification(looclass noclass) ///
probabilities(loopr nopr)

Estimation sample summary

Summary of variables from the most recent discriminant analysis and displaying variable labels estat summarize, labels

### Menu for estat

Statistics > Postestimation

# Syntax for estat

```
Classification table
    estat classtable [if] [in] [weight] [, classtable_options]
 Classification error-rate estimation
    estat errorrate [if] [in] [weight] [, errorrate_options]
 Group summaries
    estat grsummarize [, grsummarize_options]
 Classification listing
    estat \underline{li}st [if] [in] [, list\_options]
 Estimation sample summary
    estat <u>summarize</u> , <u>lab</u>els <u>nohea</u>der <u>noweights</u>
 classtable_options
                         Description
Main
 class
                         display the classification table; the default
 looclass
                         display the leave-one-out classification table
Options
                         group prior probabilities; defaults to e(grouppriors)
 priors(priors)
 nopriors
                         suppress display of prior probabilities
 ties(ties)
                         how ties in classification are to be handled; defaults to e(ties)
 title(text)
                         title for classification table
                         display the average posterior probability of being classified into each group
 probabilities
 nopercents
                         suppress display of percentages
                         suppress display of row and column totals
 nototals
 norowtotals
                         suppress display of row totals
                         suppress display of column totals
 nocoltotals
 priors
                         Description
                         equal prior probabilities
 equal
 proportional
                         group-size-proportional prior probabilities
                         row or column vector containing the group prior probabilities
 matname
                         matrix expression providing a row or column vector of the group
 matrix_exp
```

prior probabilities

ties	Description
missing	ties in group classification produce missing values
<u>r</u> andom	ties in group classification are broken randomly
<u>f</u> irst	ties in group classification are set to the first tied group
<u>n</u> earest	ties in group classification are assigned based on the closest observation, or missing if this still results in a tie; after discrim knn only
errorrate_options	Description
Main	
<u>cl</u> ass	display the classification-based error-rate estimates table; the default
<u>loo</u> class	display the leave-one-out classification-based error-rate estimates table
count	use a count-based error-rate estimate
pp[ (ppopts) ]	use a posterior-probability-based error-rate estimate
Options	
priors(priors)	group prior probabilities; defaults to e(grouppriors)
nopriors	suppress display of prior probabilities
ties(ties)	how ties in classification are to be handled; defaults to e(ties)
title(text)	title for error-rate estimate table
nototal	suppress display of total column
ppopts	Description
<u>s</u> tratified	present stratified results
<u>uns</u> tratified	present unstratified results
grsummarize_options	Description
n[(% <i>fmt</i> )]	group sizes
mean (%fmt)	means
median (%fmt)	medians
sd[(%fmt)]	standard deviations
cv[(%fmt)]	coefficients of variation
semean (%fmt)	standard errors of the means
min[(%fmt)]	minimums
$\max[(\%fmt)]$	maximums
Options	
nototal	suppress overall statistics
<u>110000</u> 41	suppress overall statistics

list_options	Description	
<u>mis</u> classified	list only misclassified and unclassified observations	
<pre>classification(clopts)</pre>	control display of classification	
<pre>probabilities(propts)</pre>	control display of probabilities	
$\underline{\text{var}}$ list $[(varopts)]$	display discriminating variables	
[ <u>no</u> ] <u>o</u> bs	display or suppress the observation number	
<u>i</u> d(varname [format(%fmt)	) display identification variable	
Options		
$\underline{\mathbf{w}}$ eight[( <i>weightopts</i> )]	display frequency weights	
priors(priors)	group prior probabilities; defaults to e(grouppriors)	
ties(ties)	how ties in classification are to be handled; defaults to e(ties)	
separator(#)	display a horizontal separator every # lines	
1		
clopts	Description	
<u>noc</u> lass	do not display the standard classification	
<u>loo</u> class	display the leave-one-out classification	
<u>not</u> rue	do not show the group variable	
<u>nos</u> tar	do not display stars indicating misclassified observations	
<u>nol</u> abel	suppress display of value labels for the group and classification variables	
<pre>format(%fmt)</pre>	format for group and classification variables; default is %5.0f for unlabeled numeric variables	
propts	Description	
nopr	suppress display of standard posterior probabilities	
loopr	display leave-one-out posterior probabilities	
format(%fmt)	format for probabilities; default is format(%7.4f)	
varopts	Description	
<u>f</u> irst	display input variables before classifications and probabilities	
<u>l</u> ast	display input variables after classifications and probabilities	
format(%fmt)	format for input variables; default is the input variable format	
weightopts	Description	
none	do not display the weights	
format(%fmt)	format for the weight; default is %3.0f for weights < 1,000, %5.0f for 1,000 < weights < 100,000, and %8.0g otherwise	

## **Options for estat**

Options are presented under the following headings:

Options for estat classtable Options for estat errorrate Options for estat grsummarize Options for estat list Options for estat summarize

### Options for estat classtable

( Main )

class, the default, displays the classification table. With in-sample observations, this is called the resubstitution classification table.

looclass displays a leave-one-out classification table, instead of the default classification table. Leave-one-out classification applies only to the estimation sample, and so, in addition to restricting the observations to those chosen with if and in qualifiers, the observations are further restricted to those included in e(sample).

Options

priors(priors) specifies the prior probabilities for group membership. If priors() is not specified, e(grouppriors) is used. If nopriors is specified with priors(), prior probabilities are used for calculation of the classification variable but not displayed. The following priors are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

nopriors suppresses display of the prior probabilities. This option does not change the computations that rely on the prior probabilities specified in priors() or as found by default in e(grouppriors).

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) determines how ties are handled. The following ties are allowed:

 $\verb|ties(\underline{m}| issing)| specifies that ties in group classification produce missing values.$ 

ties(<u>random</u>) specifies that ties in group classification are broken randomly.

 ${\tt ties}(\underline{{\tt first}})$  specifies that ties in group classification are set to the first tied group.

ties(<u>nearest</u>) specifies that ties in group classification are assigned based on the closest observation, or missing if this still results in a tie. ties(nearest) is available after discrim knn only.

title(text) customizes the title for the classification table.

probabilities specifies that the classification table show the average posterior probability of being classified into each group. probabilities implies norowtotals and nopercents.

nopercents specifies that percentages are to be omitted from the classification table.

nototals specifies that row and column totals are to be omitted from the classification table.

norowtotals specifies that row totals are to be omitted from the classification table.

nocoltotals specifies that column totals are to be omitted from the classification table.

### Options for estat errorrate

Main

class, the default, specifies that the classification-based error-rate estimates table be presented. The alternative to class is looclass.

looclass specifies that the leave-one-out classification error-rate estimates table be presented.

count, the default, specifies that the error-rate estimates be based on misclassification counts. The alternative to count is pp().

pp[(ppopts)] specifies that the error-rate estimates be based on posterior probabilities. pp is equivalent
to pp(stratified unstratified). stratified indicates that stratified estimates be presented.
unstratified indicates that unstratified estimates be presented. One or both may be specified.

Options

priors(priors) specifies the prior probabilities for group membership. If priors() is not specified, e(grouppriors) is used. If nopriors is specified with priors(), prior probabilities are used for calculation of the error-rate estimates but not displayed. The following priors are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors (matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

nopriors suppresses display of the prior probabilities. This option does not change the computations that rely on the prior probabilities specified in priors() or as found by default in e(grouppriors).

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) determines how ties are handled. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values.

ties (random) specifies that ties in group classification are broken randomly.

ties ( $\underline{f}$ irst) specifies that ties in group classification are set to the first tied group.

ties(nearest) specifies that ties in group classification are assigned based on the closest observation, or missing if this still results in a tie. ties(nearest) is available after discrim knn only.

title(text) customizes the title for the error-rate estimates table.

nototal suppresses the total column containing overall sample error-rate estimates.

### Options for estat grsummarize

Main

n[(%fmt)] specifies that group sizes be presented. The optional argument provides a display format. The default options are n and mean.

mean[(%fmt)] specifies that means be presented. The optional argument provides a display format. The default options are n and mean.

median[(%fmt)] specifies that medians be presented. The optional argument provides a display format.

- sd[(%fmt)] specifies that standard deviations be presented. The optional argument provides a display format.
- cv[(%fmt)] specifies that coefficients of variation be presented. The optional argument provides a display format.
- semean[(%fmt)) specifies that standard errors of the means be presented. The optional argument
  provides a display format.
- min[(%fmt)] specifies that minimums be presented. The optional argument provides a display format.
- max [ (% fmt) ] specifies that maximums be presented. The optional argument provides a display format.

Options

nototal suppresses display of the total column containing overall sample statistics.

transpose specifies that the groups are to be displayed by row. By default, groups are displayed by column. If you have more variables than groups, you might prefer the output produced by transpose.

### Options for estat list

Main

misclassified lists only misclassified and unclassified observations.

- classification(*clopts*) controls display of the group variable and classification. By default, the standard classification is calculated and displayed along with the group variable in e(groupvar), using labels from the group variable if they exist. *clopts* may be one or more of the following:
  - noclass suppresses display of the standard classification. If the observations are those used in the estimation, classification is called resubstitution classification.
  - looclass specifies that the leave-one-out classification be calculated and displayed. The default is that the leave-one-out classification is not calculated. looclass is not allowed after discrim logistic.
  - notrue suppresses the display of the group variable. By default, e(groupvar) is displayed. notrue implies nostar.
  - nostar suppresses the display of stars indicating misclassified observations. A star is displayed by default when the classification is not in agreement with the group variable. nostar is the default when notrue is specified.
  - nolabel specifies that value labels for the group variable, if they exist, not be displayed for the group or classification or used as labels for the probability column names.
  - format(%fmt) specifies the format for the group and classification variables. If value labels are used, string formats are permitted.
- probabilities (*propts*) controls the display of group posterior probabilities. *propts* may be one or more of the following:
  - nopr suppresses display of the standard posterior probabilities. By default, the posterior probabilities are shown.
  - loopr specifies that leave-one-out posterior probabilities be displayed. loopr is not allowed after discrim logistic.
  - format (% fint) specifies the format for displaying probabilities. The default is format (%7.4f).

varlist[(varopts)] specifies that the discriminating variables found in e(varlist) be displayed and specifies the display options for the variables.

none specifies that discriminating variables are not to be displayed. This is the default.

first specifies variables be displayed before classifications and probabilities.

last specifies variables be displayed after classifications and probabilities.

format (% fmt) specifies the format for the input variables. By default, the variable's format is used.

[no] obs indicates that observation numbers be or not be displayed. Observation numbers are displayed by default unless id() is specified.

id(varname [format(%fmt)]) specifies the identification variable to display and, optionally, the format for that variable. By default, the format of varname is used.

Options

weight [(weightopts)] specifies options for displaying weights. By default, if e(wexp) exists, weights are displayed.

none specifies weights not be displayed. This is the default if weights were not used with discrim.

format(%fmt) specifies a display format for the weights. If the weights are < 1,000, %3.0f is the default, %5.0f is the default if 1,000 < weights < 100,000, else %8.0g is used.

priors(*priors*) specifies the prior probabilities for group membership. If priors() is not specified, e(grouppriors) is used. The following *priors* are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) determines how ties are handled. The following ties are allowed:

 $\verb|ties(\underline{\texttt{m}}issing)| specifies that ties in group classification produce missing values.$ 

ties(<u>random</u>) specifies that ties in group classification are broken randomly.

 $ties(\underline{f}irst)$  specifies that ties in group classification are set to the first tied group.

ties(<u>nearest</u>) specifies that ties in group classification are assigned based on the closest observation, or missing if this still results in a tie. ties(nearest) is available after discrim knn only.

separator(#) specifies a horizontal separator line be drawn every # observations. The default is separator(5).

## Options for estat summarize

labels, noheader, and noweights are the same as for the generic estat summarize; see [R] estat summarize.

## Remarks and examples

Remarks are presented under the following headings:

Discriminating-variable summaries Discrimination listings Classification tables and error rates

There are several estat commands that apply after all the discrim subcommands. estat summarize and estat grsummarize summarize the discriminating variables over the estimation sample and by-group. estat list displays classifications, posterior probabilities, and more for selected observations. estat classtable and estat errorrate display the classification table, also known as a confusion matrix, and error-rate estimates based on the classification table.

### Discriminating-variable summaries

estat summarize and estat grsummarize provide summaries of the variables involved in the preceding discriminant analysis model.

### Example 1

Example 3 of [MV] discrim Ida introduces the famous iris data originally from Anderson (1935) and used by Fisher (1936) in the development of linear discriminant analysis. We continue our exploration of the linear discriminant analysis of the iris data and demonstrate the summary estat tools available after all discrim subcommands.

- . use http://www.stata-press.com/data/r14/iris (Iris data)
- . discrim lda seplen sepwid petlen petwid, group(iris) notable

The notable option of discrim suppressed display of the classification table. We explore the use of estat classtable later.

What can we learn about the underlying discriminating variables? estat summarize gives a summary of the variables involved in the discriminant analysis, restricted to the estimation sample.

. estat summarize

Estimation sample discrim		Nu	Number of obs = 15		
Variable	Mean	Std. Dev.	Min	Max	
groupvar iris	2	.8192319	1	3	
variables seplen sepwid petlen petwid	5.843333 3.057333 3.758 1.199333	.8280661 .4358663 1.765298 .7622377	4.3 2 1	7.9 4.4 6.9 2.5	

estat summarize displays the mean, standard deviation, minimum, and maximum for the group variable, iris, and the four discriminating variables, seplen, sepwid, petlen, and petwid. Also shown is the number of observations. If we had fit our discriminant model on a subset of the data, estat summarize would have restricted its summary to those observations.

More interesting than an overall summary of the discriminating variables is a summary by our group variable, iris.

. estat grsummarize Estimation sample discrim lda Summarized by iris

Mean		iris setosa	versicolor	virginica	Total
	seplen sepwid petlen petwid	5.006 3.428 1.462 .246	5.936 2.77 4.26 1.326	6.588 2.974 5.552 2.026	5.843333 3.057333 3.758 1.199333
	N	50	50	50	150

By default, estat grsummarize displays means of the discriminating variables for each group and overall (the total column), along with group sizes. The summary is restricted to the estimation sample.

The petal length and width of *Iris setosa* appear to be much smaller than those of the other two species. *Iris versicolor* has petal length and width between that of the other two species.

Other statistics may be requested. A look at the minimums and maximums might provide more insight into the separation of the three iris species.

. estat grsummarize, min max Estimation sample discrim lda Summarized by iris

		iris	versicolor	virginica	Total
		setosa	Versicolor	VIIgIIICa	Total
seplen					
	Min	4.3	4.9	4.9	4.3
	Max	5.8	7	7.9	7.9
sepwid					
	Min	2.3	2	2.2	2
	Max	4.4	3.4	3.8	4.4
petlen					
	Min	1	3	4.5	1
	Max	1.9	5.1	6.9	6.9
petwid					
	Min	.1	1	1.4	.1
	Max	.6	1.8	2.5	2.5

Although this table is helpful, an altered view of it might make comparisons easier. estat grsummarize allows a format to be specified with each requested statistic. We can request a shorter format for the minimum and maximum and specify a fixed format so that the decimal point lines up. estat grsummarize also has a transpose option that places the variables and requested statistics as columns and the groups as rows. If you have fewer discriminating variables than groups, this might be the most natural way to view the statistics. Here we have more variables, but with a narrow display format, the transposed view still works well.

. estat grsummarize,  $\min(\%4.1f)$   $\max(\%4.1f)$  transpose Estimation sample discrim lda

Summarized by iris

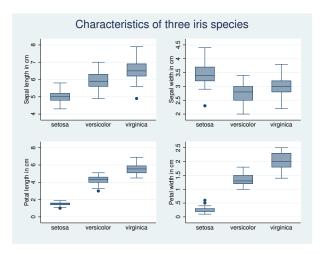
	seplen		sepwid		petlen		petwid	
iris	Min	Max	Min	Max	Min	Max	Min	Max
setosa versicolor virginica	4.3 4.9 4.9	5.8 7.0 7.9	2.3 2.0 2.2	4.4 3.4 3.8	1.0 3.0 4.5	1.9 5.1 6.9	0.1 1.0 1.4	0.6 1.8 2.5
Total	4.3	7.9	2.0	4.4	1.0	6.9	0.1	2.5

The maximum petal length and width for *Iris setosa* are much smaller than the minimum petal length and width for the other two species. The petal length and width clearly separate *Iris setosa* from the other two species.

You are not limited to one or two statistics with estat grsummarize, and each statistic may have different requested display formats. The total column, or row if the table is transposed, can also be suppressed.

Using Stata's graph box command is another way of seeing the differences among the three iris species for the four discriminating variables.

- . graph box seplen, over(iris) name(sl)
- . graph box sepwid, over(iris) name(sw)
- . graph box petlen, over(iris) name(pl)
- . graph box petwid, over(iris) name(pw)
- . graph combine sl sw pl pw, title(Characteristics of three iris species)



The box plots confirm the lack of overlap in the petal lengths and widths for *Iris setosa* compared with the other two iris species. Other differences between the species are also seen.

More summary estat commands are available after discrim 1da; see [MV] discrim Ida postestimation.

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### **Discrimination listings**

Listing the true group, classified group, group posterior probabilities, and discriminating variables for observations of interest after discrim is easy with the estat list command.

### Example 2

Example 1 of [MV] **discrim** introduced the riding-mower data of Johnson and Wichern (2007) and presented a linear discriminant analysis that concluded with the use of estat list displaying the misclassified observations.

- . use http://www.stata-press.com/data/r14/lawnmower2 (Johnson and Wichern (2007) Table 11.1)
- . discrim lda income lotsize, group(owner) notable
- . estat list, class(loo) pr(loo) misclassified

	Classif	ication		Probabilities		LOO Probabilities	
Obs.	True	Class.	L00 Cl.	nonowner	owner	nonowner	owner
1	owner	nonown >	* nonown *	0.7820	0.2180	0.8460	0.1540
2	owner	owner	nonown *	0.4945	0.5055	0.6177	0.3823
13	nonown	owner >	* owner *	0.2372	0.7628	0.1761	0.8239
14	nonown	nonown	owner *	0.5287	0.4713	0.4313	0.5687
17	nonown	owner	* owner *	0.3776	0.6224	0.2791	0.7209

\* indicates misclassified observations

The misclassified option limited the listing to those observations that were misclassified by the linear discriminant model. class(loo) and pr(loo) added leave-one-out (LOO) classifications and probabilities to the resubstitution classifications and probabilities.

We demonstrate a few other options available with estat list. We can limit which observations are displayed with if and in qualifiers and can add the display of the discriminating variables with the varlist option. Here we limit the display to those observations that have income greater than \$110.000.

. estat list if income > 110, varlist

	Data		Classifica	tion	Probabilities		
Obs.	income	lotsize	True	Class.	nonowner	owner	
2	115.5	16.8	owner	owner	0.4945	0.5055	
5	117.0	23.6	owner	owner	0.0040	0.9960	
6	140.1	19.2	owner	owner	0.0125	0.9875	
7	138.0	17.6	owner	owner	0.0519	0.9481	
8	112.8	22.4	owner	owner	0.0155	0.9845	
10	123.0	20.8	owner	owner	0.0196	0.9804	
12	111.0	20.0	owner	owner	0.1107	0.8893	
17	114.0	17.6	nonowner	owner *	0.3776	0.6224	

\* indicates misclassified observations

Starting with the command above, we specify sep(0) to suppress the separator line that, by default, displays after every 5 observations. We eliminate the observation numbers with the noobs option. With the class() option: the looclass suboption adds the LOO classification; the noclass suboption suppress the resubstitution classification; and the nostar suboption eliminates the marking

of misclassified observations with asterisks. With pr(loopr nopr) we specify that LOO probabilities are to be displayed and resubstitution probabilities are to be suppressed.

- . estat list if income > 110, sep(0) class(looclass noclass nostar)
- > pr(loopr nopr) varlist noobs

Data		Classification		LOO Probabilities	
income lo	tsize	True	L00 C1	nonowner	owner
115.5 117.0 140.1 138.0 112.8 123.0 111.0	16.8 23.6 19.2 17.6 22.4 20.8 20.0	owner owner owner owner owner owner	nonowner owner owner owner owner owner owner	0.6177 0.0029 0.0124 0.0737 0.0168 0.0217 0.1206 0.2791	0.3823 0.9971 0.9876 0.9263 0.9832 0.9783 0.8794 0.7209

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Use the if e(sample) qualifier to restrict the listing from estat list to the estimation sample. Out-of-sample listings are obtained if your selected observations are not part of the estimation sample.

As an alternative to estat list, you can use predict after discrim to obtain the classifications, posterior probabilities, or whatever else is available for prediction from the discrim subcommand that you ran, and then use list to display your predictions; see [D] list and see example 2 of [MV] discrim knn postestimation for an example.

#### Classification tables and error rates

Classification tables (also known as confusion matrices) and error-rate estimate tables are available with the estat classtable and estat errorrate commands after discrim.

## Example 3

Example 2 of [MV] **discrim knn** introduces a head measurement dataset from Rencher and Christensen (2012, 291) with six discriminating variables and three groups. We perform a quadratic discriminant analysis (QDA) on the dataset to illustrate classification tables and error-rate estimation.

- . use http://www.stata-press.com/data/r14/head (Table 8.3 Head measurements, Rencher and Christensen (2012))
- . discrim qda wdim circum fbeye eyehd earhd jaw, group(group)

Quadratic discriminant analysis Resubstitution classification summary

Key
Number Percent

True group	Classified high school	college	nonplayer	Total
high school	27	1	2	30
	90.00	3.33	6.67	100.00
college	2	21	7	30
	6.67	70.00	23.33	100.00
nonplayer	1	4	25	30
	3.33	13.33	83.33	100.00
Total	30	26	34	90
	33.33	28.89	37.78	100.00
Priors	0.3333	0.3333	0.3333	

By default, discrim displayed the resubstitution classification table. A resubstitution classification table is obtained by classifying the observations used in building the discriminant model. The resubstitution classification table is overly optimistic as an indicator of how well you might classify other observations.

This resubstitution classification table shows that from the high school group 27 observations were correctly classified, 1 observation was classified as belonging to the college group, and 2 observations were classified as belonging to the nonplayer group. The corresponding percentages were also presented: 90%, 3.33%, and 6.67%. The college and nonplayer rows are read in a similar manner. For instance, there were 7 observations from the college group that were misclassified as nonplayers. Row and column totals are presented along with the group prior probabilities. See table 9.4 of Rencher and Christensen (2012, 321) for this same classification table.

There are various ways of estimating the error rate for a classification. estat errorrate presents the overall (total) error rate and the error rate for each group. By default, it uses a count-based estimate of the error rate.

. estat errorrate

Error rate estimated by error count

	group high school	college	nonplayer	Total
Error rate	.1	.3	.166666667	.188888889
Priors	.333333333	.333333333	.333333333	

This is a resubstitution count-based error-rate estimate corresponding to the classification table previously presented. Three of the 30 high school observations were misclassified—a proportion of 0.1; 9 of the 30 college observations were misclassified—a proportion of 0.3; and 5 of the 30 nonplayers were misclassified—a proportion of 0.1667. The total error rate is computed as the sum of the group error rates times their prior probabilities—here 0.1889.

An error-rate estimate based on the posterior probabilities is also available with estat errorrate.

. estat errorrate, pp

Error rate estimated from posterior probabilities

Error Rate	group high school	college	nonplayer	Total
Stratified	.08308968	.337824355	.2030882	.208000745
Unstratified	.08308968	.337824355	.2030882	.208000745
Priors	.333333333	.333333333	.333333333	

Because we did not specify otherwise, we obtained resubstitution error-rate estimates. By default both the stratified and unstratified estimates are shown. The stratified estimates give less weight to probabilities where the group sample size is large compared with the group prior probabilities; see Methods and formulas for details. Here the stratified and unstratified estimates are the same. This happens when the prior probabilities are proportional to the sample sizes—here we have equal prior probabilities and equal group sizes.

For this example, the count-based and posterior-probability-based estimates are similar to one another.

Leave-one-out (LOO) estimation provides a more realistic assessment of your potential classification success with observations that were not used in building the discriminant analysis model. The loo option of estat classtable and estat errorrate specify a LOO estimation.

. estat classtable, loo nopercents nopriors nototals Leave-one-out classification table

Key	
Number	

True group	LOO Classified high school	college	nonplayer
high school	26	2	2
college	3	16	11
nonplayer	4	9	17

To demonstrate some of the available options, we specified the nopercents option to suppress the display of percentages; the nopriors option to suppress the display of the prior probabilities; and the nototals option to suppress row and column totals.

If you compare this LOO classification table with the resubstitution classification table, you will see that fewer observations appear on the diagonal (were correctly classified) in the LOO table. The LOO estimates are less biased than the resubstitution estimates.

We now examine the LOO error-rate estimates by using the loo option with the estat error command. We first produce the count-based estimates and then request the posterior-probability-based estimates. In the first case, we use the nopriors option to demonstrate that you can suppress the display of the prior probabilities. Suppressing the display does not remove their effect on the computations. In the second estat errorrate call, we specify that only the unstratified estimates be presented. (Because the prior probabilities and samples sizes match [are equal], the stratified results will be the same.)

. estat err, loo nopriors

Error rate estimated by leave-one-out error count

	group high school	college	nonplayer	Total
Error rate	.133333333	.466666667	.433333333	.34444444

. estat err, loo pp(unstratified)

Error rate estimated from leave-one-out posterior probabilities

Error Rate	group high school	college	nonplayer	Total
Unstratified	.049034154	.354290969	.294376541	.232567222
Priors	.333333333	.333333333	.333333333	

Instead of displaying percentages below the counts in the classification table, we can display average posterior probabilities. The probabilities option requests the display of average posterior probabilities. We add the nopriors option to demonstrate that the prior probabilities can be suppressed from the table. The classifications are still based on the prior probabilities; they are just not displayed.

. estat classtable, probabilities nopriors

Resubstitution average-posterior-probabilities classification table

Key		
Number Average	posterior	probability

True group	Classified high school	college	nonplayer
high school	27	1	2
	0.9517	0.6180	0.5921
college	2	21	7
	0.6564	0.8108	0.5835
nonplayer	1 0.4973	0.5549	25 0.7456
Total	30	26	34
	0.9169	0.7640	0.7032

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Both estat classtable and estat errorrate allow if and in qualifiers so that you can select the observations to be included in the computations and displayed. If you want to limit the table to the estimation sample, use if e(sample). You can also do out-of-sample classification tables and error-rate estimation by selecting observations that were not part of the estimation sample.

## □ Technical note

As noted by Huberty (1994, 92), the posterior-probability-based error-rate estimates for the individual groups may be negative. This may happen when there is a discrepancy between group prior probabilities and relative sample size.

Continuing with our last example, if we use prior probabilities of 0.2, 0.1, and 0.7 for the high school, college, and nonplayer groups, the nonplayer stratified error-rate estimate and the high school group unstratified error-rate estimate are negative.

. estat error, pp priors(.2, .1, .7)

Error rate estimated from posterior probabilities

Error Rate	group high school	college	nonplayer	Total
Stratified	.19121145	.737812235	001699715	.110833713
Unstratified	36619243	.126040785	.29616143	.146678593
Priors	.2	.1	.7	

More examples of the use of estat list, estat classtable, and estat errorrate can be found in the other discrim-related manual entries.

# Stored results

estat classtable stores the following in r():

#### Matrices

r(counts) group counts

r(percents) percentages for each group (unless nopercents specified)

r(avgpostprob) average posterior probabilities classified into each group (probabilities only)

estat errorrate stores the following in r():

#### Matrices

r(grouppriors) row vector of group prior probabilities used in the calculations r(erate\_count) matrix of error rates estimated from error counts (count only)

r(erate\_strat) matrix of stratified error rates estimated from posterior probabilities (pp only)
r(erate\_unstrat) matrix of unstratified error rates estimated from posterior probabilities (pp only)

estat grsummarize stores the following in r():

Matrices r(count) group counts r(mean) means (mean only) r(median) medians (median only) r(sd) standard deviations (sd only) r(cv) coefficients of variation (cv only) r(semean) standard errors of the means (semean only) r(min) minimums (min only) r(max) maximums (max only)

## Methods and formulas

Let  ${\bf C}$  denote the classification table (also known as the confusion matrix), with rows corresponding to the true groups and columns corresponding to the assigned groups. Let  $C_{ij}$  denote the element from row i and column j of  ${\bf C}$ .  $C_{ij}$  represents the number of observations from group i assigned to group j.  $n_i$  is the number of observations from group i and  $N = \sum_{i=1}^g n_i$  is the total sample size.  ${\cal N}_i = \sum_{j=1}^g C_{ij}$  is the number of observations from group i that were classified into one of the g groups. If some observations from group i are unclassified (because of ties),  ${\cal N}_i \neq n_i$  and  ${\cal N} \neq N$  (where  ${\cal N} = \sum {\cal N}_i$ ). Let  $q_i$  be the prior probability of group i.

estat classtable displays C, with options controlling the display of cell percentages by row, average posterior probabilities, prior probabilities, row totals, and column totals.

McLachlan (2004, chap. 10) devotes a chapter to classification error-rate estimation. The estat errorrate command provides several popular error-rate estimates. Smith (1947) introduced the count-based apparent error-rate estimate. The count-based error-rate estimate for group i is

$$\widehat{E}_i^{(C)} = 1 - C_{ii} / \mathcal{N}_i$$

The overall (total) count-based error-rate estimate is

$$\widehat{E}^{(C)} = \sum_{i=1}^{g} q_i \widehat{E}_i^{(C)}$$

In general,  $\widehat{E}^{(C)} \neq 1 - \sum_{i=1}^{g} C_{ii}/\mathcal{N}$ , though some sources, Rencher and Christensen (2012, 319), appear to report this latter quantity.

If C is based on the same data used in the estimation of the discriminant analysis model, the error rates are called apparent error rates. Leave-one-out (LOO) error rates are obtained if C is based on a leave-one-out analysis where each observation to be classified is classified based on the discriminant model built excluding that observation; see Lachenbruch and Mickey (1968) and McLachlan (2004, 342).

Error rates can also be estimated from the posterior probabilities. Huberty (1994, 90–91) discusses hit rates (one minus the error rates) based on posterior probabilities and shows two versions of the posterior-probability based estimate—stratified and unstratified.

Let  $\mathcal{P}_{ji}$  be the sum of the posterior probabilities for all observations from group j assigned to group i. The posterior-probability-based unstratified error-rate estimate for group i is

$$\widehat{E}_i^{(Pu)} = 1 - \frac{1}{\mathcal{N}q_i} \sum_{i=1}^g \mathcal{P}_{ji}$$

The overall (total) posterior-probability-based unstratified error-rate estimate is

$$\widehat{E}^{(Pu)} = \sum_{i=1}^{g} q_i \widehat{E}_i^{(Pu)}$$

The posterior-probability-based stratified error-rate estimate for group i is

$$\widehat{E}_i^{(Ps)} = 1 - \frac{1}{q_i} \sum_{j=1}^g \frac{q_j}{\mathcal{N}_j} \mathcal{P}_{ji}$$

The overall (total) posterior-probability-based stratified error-rate estimate is

$$\widehat{E}^{(Ps)} = \sum_{i=1}^{g} q_i \widehat{E}_i^{(Ps)}$$

## References

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## Also see

[MV] **discrim** — Discriminant analysis

[MV] discrim knn postestimation — Postestimation tools for discrim knn

[MV] discrim Ida postestimation — Postestimation tools for discrim Ida

[MV] discrim logistic postestimation — Postestimation tools for discrim logistic

[MV] discrim qda postestimation — Postestimation tools for discrim qda

[MV] candisc — Canonical linear discriminant analysis

[U] 20 Estimation and postestimation commands

### **Title**

discrim knn — kth-nearest-neighbor discriminant analysis

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# **Description**

 $\operatorname{discrim}$  knn performs kth-nearest-neighbor discriminant analysis. A wide selection of similarity and dissimilarity measures is available.

kth-nearest neighbor must retain the training data and search through the data for the k nearest observations each time a classification or prediction is performed. Consequently for large datasets, kth-nearest neighbor is slow and uses a lot of memory.

See [MV] discrim for other discrimination commands.

### **Quick start**

kth-nearest-neighbor discriminant analysis of v1, v2, v3, and v4 for groups defined by catvar and k=5

```
discrim knn v1 v2 v3 v4, k(5) group(catvar)
```

As above, but use prior probabilities proportional to group size

```
discrim knn v1 v2 v3 v4, k(5) group(catvar) priors(proportional)
```

Display only the leave-one-out classification table

```
discrim knn v1 v2 v3 v4, k(5) group(catvar) lootable notable
```

Use absolute-value distance

```
discrim knn v1 v2 v3 v4, k(5) group(catvar) measure(absolute)
```

#### Menu

Statistics > Multivariate analysis > Discriminant analysis > Kth-nearest neighbor (KNN)

# **Syntax**

options	Description
Model	
*group(groupvar)	variable specifying the groups
* k (#)	number of nearest neighbors
<pre>priors(priors)</pre>	group prior probabilities
ties(ties)	how ties in classification are to be handled
Measure	
<pre>measure(measure)</pre>	similarity or dissimilarity measure; default is measure(L2)
s2d( <u>st</u> andard)	convert similarity to dissimilarity: $d(ij) = \sqrt{s(ii) + s(jj) - 2s(ij)}$ , the default
s2d( <u>one</u> minus)	convert similarity to dissimilarity: $d(ij) = 1 - s(ij)$
<u>mah</u> alanobis	Mahalanobis transform continuous data before computing dissimilarities
Reporting	
<u>not</u> able	suppress resubstitution classification table
<u>loo</u> table	display leave-one-out classification table
priors	Description
equal	equal prior probabilities; the default
$\underline{\mathtt{prop}}\mathtt{ortional}$	group-size-proportional prior probabilities
matname	row or column vector containing the group prior probabilities
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities
ties	Description
$\underline{\mathtt{m}}\mathtt{issing}$	ties in group classification produce missing values; the default
$\underline{\mathtt{r}}\mathtt{andom}$	ties in group classification are broken randomly
<u>f</u> irst	ties in group classification are set to the first tied group
$\underline{\mathtt{n}}\mathtt{earest}$	ties in group classification are assigned based on the closest observation, or missing if this still results in a tie

<sup>\*</sup>group() and k() are required.

statsby and xi are allowed; see [U] 11.1.10 Prefix commands.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

# **Options**

group(groupvar) is required and specifies the name of the grouping variable. groupvar must be a numeric variable.

k(#) is required and specifies the number of nearest neighbors on which to base computations. In the event of ties, the next largest value of k() is selected. Suppose that k(3) is selected. For a given observation, one must go out a distance d to find three nearest neighbors, but if, say, there are five data points all within distance d, then the computation will be based on all five nearest points.

priors(*priors*) specifies the prior probabilities for group membership. The following *priors* are allowed:

priors (equal) specifies equal prior probabilities. This is the default.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors (matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties (ties) specifies how ties in group classification will be handled. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values. This is the default.

ties(random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

ties(<u>nearest</u>) specifies that ties in group classification are assigned based on the closest observation, or missing if this still results in a tie.

Measure

measure(measure) specifies the similarity or dissimilarity measure. The default is measure(L2); all measures in [MV] measure\_option are supported except for measure(Gower).

s2d(standard oneminus) specifies how similarities are converted into dissimilarities.

The available s2d() options, standard and oneminus, are defined as

standard 
$$d(ij) = \sqrt{s(ii) + s(jj) - 2s(ij)} = \sqrt{2\{1 - s(ij)\}}$$
 oneminus 
$$d(ij) = 1 - s(ij)$$

s2d(standard) is the default.

mahalanobis specifies performing a Mahalanobis transformation on continuous data before computing dissimilarities. The data is transformed via the Cholesky decomposition of the within-group covariance matrix, and then the selected dissimilarity measure is performed on the transformed data. If the L2 (Euclidean) dissimilarity is chosen, this is the Mahalanobis distance. If the within-group covariance matrix does not have sufficient rank, an error is returned.

Reporting

notable suppresses the computation and display of the resubstitution classification table.

lootable displays the leave-one-out classification table.

# Remarks and examples

Remarks are presented under the following headings:

Introduction
A first example
Mahalanobis transformation
Binary data

#### Introduction

kth-nearest-neighbor (KNN) discriminant analysis dates at least as far back as Fix and Hodges (1951). An introductory treatment is available in Rencher and Christensen (2012). More advanced treatments are in Hastie, Tibshirani, and Friedman (2009) and McLachlan (2004).

KNN is a nonparametric discrimination method based on the k nearest neighbors of each observation. KNN can deal with binary data via one of the binary measures; see [MV] *measure\_option*.

## A first example

What distinguishes kth-nearest-neighbor analysis from other methods of discriminant analysis is its ability to distinguish irregular-shaped groups, including groups with multiple modes. We create a dataset with unusual boundaries that lends itself to KNN analysis and graphical interpretation.

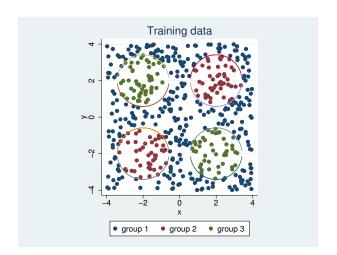
## Example 1

We create a two-dimensional dataset on the plane with x and y values in [-4,4]. In each quadrant we consider points within a circle with a square root of two radii, centered around the points (2,2), (-2,2), (-2,-2), and (2,-2). We set the group value to 1 to start and then replace it in the circles. In the first and third circles we set the group value to 2, and in the second and fourth circles we set the group value to 3. Outside the circles, the group value remains 1.

```
. set seed 98712321
. set obs 500
number of observations (_N) was 0, now 500
. generate x = 8*runiform() - 4
. generate y = 8*runiform() - 4
. generate group = 1
. replace group = 2 if (y+2)^2 + (x+2)^2 <= 2
(45 real changes made)
. replace group = 2 if (y-2)^2 + (x-2)^2 <= 2
(50 real changes made)
. replace group = 3 if (y+2)^2 + (x-2)^2 <= 2
(45 real changes made)
. replace group = 3 if (y-2)^2 + (x+2)^2 <= 2
(51 real changes made)</pre>
```

Next we define some local macros for function plots of the circles. This makes it easier to graph the boundary circles on top of the data. We set the graph option aspectratio(1) to force the aspect ratio to be 1; otherwise, the circles might appear to be ovals.

```
. local rp : di %12.10f 2+sqrt(2)
. local rm : di %12.10f 2-sqrt(2)
. local functionplot
> (function y = sqrt(2-(x+2)^2) - 2, lpat(solid) range(-'rp' -'rm'))
> (function y = -sqrt(2-(x+2)^2) - 2, lpat(solid) range(-'rp' -'rm'))
> (function y = sqrt(2-(x-2)^2) + 2, lpat(solid) range(-'rm'
> (function y = -sqrt(2-(x-2)^2) + 2, lpat(solid) range(-'rm'
\Rightarrow (function y = sqrt(2-(x+2)^2) + 2, lpat(solid) range(-'rp' -'rm'))
> (function y = -sqrt(2-(x+2)^2) + 2, lpat(solid) range(-'rp' -'rm'))
> (function y = sqrt(2-(x-2)^2) - 2, lpat(solid) range( 'rm'
> (function y = -sqrt(2-(x-2)^2) - 2, lpat(solid) range('rm'
. local graphopts
> aspectratio(1) legend(order(1 "group 1" 2 "group 2" 3 "group 3") rows(1))
 twoway (scatter y x if group==1)
         (scatter y x if group==2)
>
         (scatter y x if group==3)
         'functionplot', 'graphopts' name(original, replace)
         title("Training data")
```



We perform three discriminant analyses on these data for comparison. We use linear discriminant analysis (LDA), quadratic discriminant analysis (QDA) and KNN. The results from logistic discriminant analysis are similar to those of LDA and are not included. With all three models, we use proportional probabilities, priors(proportional). The probability of landing in a given group is proportional to the geometric area of that group; they are certainly not equal. Rather than doing geometric calculations for the prior probabilities, we use priors(proportional) to approximate this. We suppress the standard classification table with notable. Instead we look at the lootable, that is, leave-one-out (LOO) table, where the observation in question is omitted and its result is predicted from the rest of the data. Likewise, we predict the LOO classification (looclass). With KNN we get to choose a measure(); here we want the straight line distance between the points. This is the default, Euclidean distance, so we do not have to specify measure().

We choose k=7 for this run with 500 observations. See *Methods and formulas* for more information on choosing k.

. discrim lda x y, group(group) notable lootable priors(proportional)

Linear discriminant analysis Leave-one-out classification summary

> Key Number Percent

	Classif	ied		
True group	1	2	3	Total
1	309 100.00	0.00	0.00	309 100.00
2	95 100.00	0.00	0.00	95 100.00
3	96 100.00	0.00	0.00	96 100.00
Total	500 100.00	0.00	0.00	500 100.00
Priors	0.6180	0.1900	0.1920	

LDA classifies all observations into group one, the group with the highest prior probability.

. discrim qda x y, group(group) notable lootable priors(proportional)

Quadratic discriminant analysis Leave-one-out classification summary

> Key Number Percent

	Classified			
True group	1	2	3	Total
1	258 83.50	31 10.03	20 6.47	309 100.00
2	57 60.00	38 40.00	0.00	95 100.00
3	77 80.21	0.00	19 19.79	96 100.00
Total	392 78.40	69 13.80	39 7.80	500 100.00
Priors	0.6180	0.1900	0.1920	

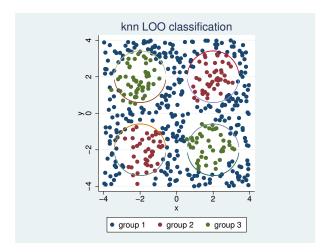
QDA has 185 (31 + 20 + 57 + 77) misclassified observations of 500, but it correctly classifies 38 of the 95 observations from group 2 and 19 of the 96 observations from group 3.

. discrim knn x y, group(group) k(7) notable lootable priors(proportional) Kth-nearest-neighbor discriminant analysis Leave-one-out classification summary



	Classified			
True group	1	2	3	Total
1	299 96.76	4 1.29	6 1.94	309 100.00
2	13 13.68	82 86.32	0.00	95 100.00
3	10 10.42	0.00	86 89.58	96 100.00
Total	322 64.40	86 17.20	92 18.40	500 100.00
Priors	0.6180	0.1900	0.1920	

In contrast to the other two models, KNN has only 33 (4+6+13+10) misclassified observations. We can see how points are classified by KNN by looking at the following graph.



KNN has some resolution of the circles and correctly classifies most of the points. Its misclassified observations are near the boundaries of the circles, where nearest points fall on both sides of the boundary line.

#### Mahalanobis transformation

The Mahalanobis transformation eliminates the correlation between the variables and standardizes the variance of each variable, as demonstrated in example 2 of [MV] **discrim lda**. When the Mahalanobis transformation is used in conjunction with Euclidean distance, it is called Mahalanobis distance. The Mahalanobis transformation may be applied when any continuous measure is chosen, not just measure (Euclidean). See [MV] *measure\_option* for a description of the available measures.

# Example 2

We will reproduce an example from Rencher and Christensen (2012, 290–292) that uses the Mahalanobis distance. Rencher and Christensen present data collected by G. R. Bryce and R. M. Barker of Brigham Young University as part of a preliminary study of a possible link between football helmet design and neck injuries. Six head dimensions were measured for each subject. Thirty subjects were sampled in each of three groups: high school football players (group 1), college football players (group 2), and nonfootball players (group 3). The six variables are wdim, head width at its widest dimension; circum, head circumference; fbeye, front-to-back measurement at eye level; eyehd, eye to top of head measurement; earhd, ear to top of head measurement; and jaw, jaw width.

These measurements will not have the same ranges. For example, the head circumference should be much larger than eye to top of head measurement. Mahalanobis distance is used to standardize the measurements.

- . use http://www.stata-press.com/data/r14/head, clear (Table 8.3 Head measurements, Rencher and Christensen (2012))
- . discrim knn wdim-jaw, k(5) group(group) mahalanobis

Kth-nearest-neighbor discriminant analysis Resubstitution classification summary

Key
Number Percent

True group	Classified high school	college	nonplayer	Unclassified
high school	26 86.67	0.00	1 3.33	3 10.00
college	1 3.33	19 63.33	9 30.00	1 3.33
nonplayer	1 3.33	4 13.33	22 73.33	3 10.00
Total	28 31.11	23 25.56	32 35.56	7 7.78
Priors	0.3333	0.3333	0.3333	
True group	Classified Total			
high school	30 100.00			
college	30 100.00			
nonplayer	30 100.00			
Total	90			
Priors				

A subset of this result is in Rencher and Christensen (2012, 331-332). Of the 90 original observations, 16 were misclassified and 7 observations were unclassified. Rencher and Christensen also state the error rate for this example is 0.193. We use estat errorrate to get the error rate.

. estat errorrate

Error rate estimated by error count

Note: 7 observations were not classified and are not included in the table

	group high school	college	nonplayer	Total
Error rate	.037037037	.344827586	.185185185	.189016603
Priors	.333333333	.333333333	.333333333	

Our error rate of 0.189 does not match that of Rencher and Christensen. Why is this? Rencher and Christensen calculates the error rate as the number of misclassified observations over the total

number of observations classified. This is  $16/83 \approx 0.193$ . We use the standard error-rate definition that takes into account the prior probabilities. From the high school group, there is one misclassified observation of 27 total observations classified from this group, so its error rate is  $(1/27) \approx 0.037$ , and its contribution to the total is (1/27)(1/3). Likewise, the error rates for the college and nonplayer group are  $(10/29) \approx 0.345$  and  $(5/27) \approx 0.185$  respectively, with contributions of (10/29)(1/3) and (5/27)(1/3). Adding all contributions, we get the displayed error rate of 0.189. See

Methods and formulas of [MV] discrim estat for details.

The unclassified observations are those that resulted in ties. We can force ties to be classified by changing the ties() option. The default is ties(missing), which says that ties are to be classified as missing values. Here we choose ties(nearest), which breaks the tie by classifying to the group of the nearest tied observation.

. discrim knn wdim-jaw, k(5) group(group) mahalanobis ties(nearest) Kth-nearest-neighbor discriminant analysis Resubstitution classification summary

Key
Number Percent

True group	Classified high school	college	nonplayer	Total
high school	28 93.33	0.00	2 6.67	30 100.00
college	1	20	9	30
	3.33	66.67	30.00	100.00
nonplayer	1	4	25	30
	3.33	13.33	83.33	100.00
Total	30	24	36	90
	33.33	26.67	40.00	100.00
Priors	0.3333	0.3333	0.3333	

Compare this with example 1 in [MV] candisc, example 3 in [MV] discrim estat, and example 2 of [MV] discrim logistic.

1

# Binary data

In addition to the measures for continuous data, a variety of binary measures are available for KNN. Binary data can be created from any categorical dataset by using xi; see [R] xi.

# ➤ Example 3

You have invited some scientist friends over for dinner, including Mr. Mushroom (see vignette below), a real "fun guy". Mr. Mushroom is a researcher in mycology. He not only enjoys studying mushrooms; he is also an enthusiastic mushroom gourmand who likes nothing better than to combine his interests in classification and cookery. His current research is identification of poisonous mushrooms from photographs. From the photographs, he can identify the shape of a mushroom's cap, the cap's surface, the cap's color, the population of mushrooms, and, with some careful attention to detail in the surrounding area, the habitat.

William Alphonso Murrill (1867–1957) was a famous mycologist, taxonomist, and writer from the New York Botanical Gardens and was nicknamed "Mr. Mushroom". Although we borrowed his nickname, Mr. Mushroom and the events portrayed in this example are entirely fictitious. William Murrill's many scientific accomplishments include the 1916 book Edible and Poisonous Mushrooms.

Knowing your friend, you imagine that he will insist on bringing a mushroom dish to be unveiled and served at dinnertime—perhaps his experimental subjects. Although you know that he is a careful scientist and a gifted cook, you are stalked with worries about poisoning your other guests.

Late at night you cannot sleep for worrying about poisonous mushrooms, and you decide to do a little research into mushroom classification. You do a Google search online and find mushroom data at http://archive.ics.uci.edu/ml/datasets/Mushroom. For reference, these records are drawn from Lincoff (1981).

This is a large dataset of 8,124 observations on the Agaricus and Lepiota. Each species is identified as definitely edible, definitely poisonous, or of unknown edibility and not recommended. This last class was combined with the poisonous one. Lincoff (1981) clearly states that there is no simple rule for determining the edibility of a mushroom; no rule like "leaflets three, let it be" for Poison Oak and Ivy, a fact that does not seem comforting. Twenty-two attributes are collected, including those that Mr. Mushroom can identify from his photographs.

The mushroom data is a set of 23 variables that describe the cap of the mushroom, whether or not it has bruises, the gills, the veil, the stalk, the ring, the spores, the population, and the habitat. The variables that describe the cap, for example, are capshape, capsurface, and capcolor. The capshape variable, for example, has categories bell, conical, convex, flat, knobbed, and sunken. Other variables and categories are similar.

You read in this dataset by using infile and make some modifications, attaching notes to this dataset to describe what you did to the original mushroom data. Modifications include dropping categories of the variables of interest that completely determine whether a mushroom is poisonous. The full mushroom data are also available; webuse mushroom\_full to obtain it.

. use http://www.stata-press.com/data/r14/mushroom (Lincoff (1981) Audubon Guide; http://archive.ics.uci.edu/ml/datasets/Mushroom)

. tabulate habitat poison

	poison			
habitat	edible	poisonous	Total	
grasses	752	680	1,432	
leaves	240	585	825	
meadows	128	24	152	
paths	136	1,008	1,144	
urban	64	224	288	
woods	1,848	1,268	3,116	
Total	3,168	3,789	6,957	

You can see by tabulating two of the variables, habitat and poison, that in each habitat you have some mushrooms that are poisonous as well as some that are edible. The other descriptive variables of interest produce similar results.

Each variable is a set of unordered categories. You can use xi to create indicator (binary) variables from the categorical data; see [R] xi. xi, by default, does not create collinear variables; it omits one of the categories. You want to take all categories into account, and so you use the noomit option.

With KNN you can choose a measure that is suited to this data. You expect data with many zeroes and few ones. A match of two ones is far more significant than two matching zeroes. Looking through the binary similarity measures in [MV] *measure\_option*, you see that the Jaccard binary similarity coefficient reports the proportion of matches of ones when at least one of the observations contains a one, and the Dice binary similarity measure weighs matches of ones twice as heavily as the Jaccard measure. Either suits the situation, and you choose the Dice measure. The conversion from a similarity to a dissimilarity measure will be s2d(standard) by default.

The poisonous and edible mushrooms are split about half and half in the original dataset, and in the current subset of these data the ratio is still approximately half and half, so you do not specify priors, obtaining priors(equal), the default.

Because of the size of the dataset and the number of indicator variables created by xi, KNN analysis is slow. You decide to discriminate based on 2,000 points selected at random, approximately a third of the data.

- . set seed 12345678
- . generate u = runiform()
- . sort u
- . xi, noomit: discrim knn i.population i.habitat i.bruises i.capshape
- > i.capsurface i.capcolor in 1/2000, k(15) group(poison) measure(dice)

Kth-nearest-neighbor discriminant analysis Resubstitution classification summary

Key
Number Percent

True poison	Classified edible	poisonous	Total
edible	848	65	913
	92.88	7.12	100.00
poisonous	29	1,058	1,087
	2.67	97.33	100.00
Total	877	1,123	2,000
	43.85	56.15	100.00
Priors	0.5000	0.5000	

In some settings, these results would be considered good. Of the original 2,000 mushrooms, you see that only 29 poisonous mushrooms have been misclassified as edible. However, even sporadic classification of a poisonous mushroom as edible is a much bigger problem than classifying an edible mushroom as poisonous. This does not take the cost of misclassification into account. You decide that calling a poisonous mushroom edible is at least 10 times worse than calling an edible mushroom poisonous. In the two-group case, you can easily use the priors() option to factor in this cost; see [MV] discrim or McLachlan (2004, 9). We set the prior probability of poisonous mushrooms 10 times higher than that of the edible mushrooms.

. estat classtable in 1/2000, priors(.09, .91) Resubstitution classification table

Key
Number Percent

True poison	Classified edible	poisonous	Total
edible	728 79.74	185 20.26	913 100.00
poisonous	0.00	1,087 100.00	1,087 100.00
Total	728 36.40	1,272 63.60	2,000 100.00
Priors	0.0900	0.9100	

These results are reassuring. There are no misclassified poisonous mushrooms, although 185 edible mushrooms of the total 2,000 mushrooms in our model are misclassified.

You now check to see how this subsample of the data performs in predicting the poison status of the rest of the data. This takes a few minutes of computer time, but unlike using estat classtable above, the variable predicted will stay with your dataset until you drop it. tabulate can be used instead of estat classtable.

- . predict cpoison, classification priors(.09, .91)
- . label values cpoison poison
- . tabulate poison cpoison

poison	classif edible	ication poisonous	Total
edible poisonous	2,450 0	718 3,789	3,168 3,789
Total	2,450	4,507	6,957

This is altogether reassuring. Again, no poisonous mushrooms were misclassified. Perhaps there is no need to worry about dinnertime disasters, even with a fungus among us. You are so relieved that you plan on serving a Jello dessert to cap off the evening—your guests will enjoy a mold to behold. Under the circumstances, you think doing so might just be a "morel" imperative.

4

#### Stored results

discrim knn stores the following in e():

```
Scalars
                          number of observations
    e(N)
    e(N_groups)
                          number of groups
    e(k_nn)
                          number of nearest neighbors
    e(k)
                          number of discriminating variables
Macros
                          discrim
    e(cmd)
    e(subcmd)
                          knn
    e(cmdline)
                          command as typed
    e(groupvar)
                          name of group variable
    e(grouplabels)
                          labels for the groups
    e(measure)
                          similarity or dissimilarity measure
    e(measure_type)
                          dissimilarity or similarity
    e(measure_binary)
                          binary, if binary measure specified
    e(s2d)
                          standard or oneminus, if s2d() specified
    e(varlist)
                          discriminating variables
    e(wtype)
                          weight type
                          weight expression
    e(wexp)
                          title in estimation output
    e(title)
    e(ties)
                          how ties are to be handled
                          mahalanobis, if Mahalanobis transform is performed
    e(mahalanobis)
    e(properties)
                          nob noV
    e(estat_cmd)
                          program used to implement estat
    e(predict)
                          program used to implement predict
    e(marginsnotok)
                          predictions disallowed by margins
Matrices
    e(groupcounts)
                          number of observations for each group
    e(grouppriors)
                          prior probabilities for each group
    e(groupvalues)
                          numeric value for each group
    e(means)
                          group means on discriminating variables
    e(SSCP_W)
                          pooled within-group SSCP matrix
    e(W_eigvals)
                          eigenvalues of e(SSCP_W)
                          eigenvectors of e(SSCP_W)
    e(W_eigvecs)
    e(S)
                          pooled within-group covariance matrix
    e(Sinv)
                          inverse of e(S)
    e(sqrtSinv)
                          Cholesky (square root) of e(Sinv)
    e(community)
                          community of neighbors for prediction
Functions
    e(sample)
                          marks estimation sample
```

# Methods and formulas

Let g be the number of groups,  $n_i$  the number of observations for group i, and  $q_i$  the prior probability for group i. Let  $\mathbf{x}$  denote an observation measured on p discriminating variables. For consistency with the discriminant analysis literature,  $\mathbf{x}$  will be a column vector, though it corresponds to a row in your dataset. Let  $f_i(\mathbf{x})$  represent the density function for group i, and let  $P(\mathbf{x}|G_i)$  denote the probability of observing  $\mathbf{x}$  conditional on belonging to group i. Denote the posterior probability of group i given observation  $\mathbf{x}$  as  $P(G_i|\mathbf{x})$ . With Bayes' theorem, we have

$$P(G_i|\mathbf{x}) = \frac{q_i f_i(\mathbf{x})}{\sum_{j=1}^g q_j f_j(\mathbf{x})}$$

Substituting  $P(\mathbf{x}|G_i)$  for  $f_i(\mathbf{x})$ , we have

$$P(G_i|\mathbf{x}) = \frac{q_i P(\mathbf{x}|G_i)}{\sum_{j=1}^g q_j P(\mathbf{x}|G_j)}$$

For KNN discrimination, we let  $k_i$  be the number of the k nearest neighbors from group i, and the posterior-probability formula becomes

$$P(G_i|\mathbf{x}) = \frac{\frac{q_i k_i}{n_i}}{\sum_{j=1}^g \frac{q_j k_j}{n_j}}$$

In the event that there are ties among the nearest neighbors, k is increased to accommodate the ties. If five points are all nearest and equidistant from a given x, then an attempt to calculate the three nearest neighbors of x will actually obtain five nearest neighbors.

Determining the nearest neighbors depends on a dissimilarity or distance calculation. The available dissimilarity measures are described in [MV] *measure\_option*. Continuous and binary measures are available. If a similarity measure is selected, it will be converted to a dissimilarity by either

standard 
$$d(ij) = \sqrt{s(ii) + s(jj) - 2s(ij)} = \sqrt{2\{1 - s(ij)\}}$$
 oneminus 
$$d(ij) = 1 - s(ij)$$

With any of the continuous measures, a Mahalanobis transformation may be performed before computing the dissimilarities. For details on the Mahalanobis transformation, see *Methods and formulas* of [MV] **discrim Ida**. The Mahalanobis transformation with Euclidean distance is called Mahalanobis distance.

Optimal choice of k for KNN is not an exact science. With two groups, k should be chosen as an odd integer to avoid ties. Rencher and Christensen (2012, 331) cites the research of Loftsgaarden and Quesenberry (1965), which suggests that an optimal k is  $\sqrt{n_i}$ , where  $n_i$  is a typical group size. Rencher and Christensen also suggest running with several different values of k and choosing the one that gives the best error rate. McLachlan (2004) cites Enas and Choi (1986), which suggests that when there are two groups of comparable size that k should be chosen approximately between  $N^{3/8}$  or  $N^{2/8}$ , where N is the number of observations.

## References

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## Also see

[MV] discrim knn postestimation — Postestimation tools for discrim knn

[MV] **discrim** — Discriminant analysis

[U] 20 Estimation and postestimation commands

# **Title**

discrim knn postestimation —	- Postestimation	tools for	discrim	knn
------------------------------	------------------	-----------	---------	-----

Postestimation commands predict Remarks and examples Methods and formulas Also see

# **Postestimation commands**

The following postestimation commands are of special interest after discrim knn:

Command	Description
estat classtable	classification table
estat errorrate	classification error-rate estimation
estat grsummarize	group summaries
estat list	classification listing
estat summarize	estimation sample summary

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results
predict	group classification and posterior probabilities

<sup>\*</sup>All estimates subcommands except table and stats are available; see [R] estimates.

# predict

## **Description for predict**

predict creates a new variable containing predictions such as group classifications, probabilities, leave-one-out group classifications, and leave-one-out probabilities.

## Menu for predict

Statistics > Postestimation

# Syntax for predict

matname

matrix\_exp

```
predict [type] newvar [if] [in] [, statistic options]
    predict [type] { stub* | newvarlist } [if] [in] [, statistic options]
 statistic
                            Description
Main
 classification
                            group membership classification; the default when one variable is
                              specified and group() is not specified
                            probability of group membership; the default when group() is
 pr
                              specified or when multiple variables are specified
                            leave-one-out group membership classification; may be used only
^stlooclass
                              when one new variable is specified
                            leave-one-out probability of group membership
 loopr
 options
                            Description
Main
 group(group)
                            the group for which the statistic is to be calculated
Options
                            group prior probabilities; defaults to e(grouppriors)
 priors(priors)
                            how ties in classification are to be handled; defaults to e(ties)
 ties(ties)
 noupdate
                            do not update the within-group covariance matrix with leave-one-out
                              predictions
 priors
                            Description
                            equal prior probabilities
 equal
 proportional
                            group-size-proportional prior probabilities
```

row or column vector containing the group prior probabilities

prior probabilities

matrix expression providing a row or column vector of the group

ties	Description
missing	ties in group classification produce missing values
$\underline{\mathtt{r}}\mathtt{andom}$	ties in group classification are broken randomly
<u>f</u> irst	ties in group classification are set to the first tied group
<u>n</u> earest	ties in group classification are assigned based on the closest observation, or missing if this still results in a tie

You specify one new variable with classification or looclass and specify either one or e(N\_groups) new variables with pr or loopr.

Unstarred statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample. Starred statistics are calculated only for the estimation sample, even when if e(sample) is not specified.

group() is not allowed with classification or looclass.

noupdate is an advanced option and does not appear in the dialog box.

## Options for predict

Main

classification, the default, calculates the group classification. Only one new variable may be specified.

pr calculates group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.

looclass calculates the leave-one-out group classifications. Only one new variable may be specified. Leave-one-out calculations are restricted to e(sample) observations.

loopr calculates the leave-one-out group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables. Leave-one-out calculations are restricted to e(sample) observations.

group(group) specifies the group for which the statistic is to be calculated and can be specified using

#1, #2, ..., where #1 means the first category of the e(groupvar) variable, #2 the second category, etc.;

the values of the e(groupvar) variable; or

the value labels of the e(groupvar) variable if they exist.

group() is not allowed with classification or looclass.

Options

priors(*priors*) specifies the prior probabilities for group membership. If priors() is not specified, e(grouppriors) is used. The following *priors* are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities. ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) is used. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values.

ties(random) specifies that ties in group classification are broken randomly.

ties ( $\underline{f}$ irst) specifies that ties in group classification are set to the first tied group.

ties(nearest) specifies that ties in group classification are assigned based on the closest observation, or missing if this still results in a tie.

The following option is available with predict after discrim knn but is not shown in the dialog box:

noupdate causes the within-group covariance matrix not to be updated with leave-one-out predictions. noupdate is an advanced, rarely used option that is valid only if a Mahalanobis transformation is specified.

# Remarks and examples

kth-nearest-neighbor (KNN) discriminant analysis and postestimation can be time consuming for large datasets. The training data must be retained and then searched to find the nearest neighbors each time a classification or prediction is performed.

You can find more examples of postestimation with KNN in [MV] discrim knn, and more examples of the common estat subcommands in [MV] discrim estat.

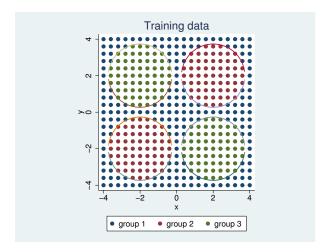
## Example 1: Leave-one-out classification after KNN

Recall example 1 of [MV] discrim knn. We use a similar idea here, creating a two-dimensional dataset on the plane with x and y variables in [-4,4]. Instead of random data, we choose data on a regular grid to make things easy to visualize, and once again, we assign groups on the basis of geometric calculations. To start, we assign all points a group value of one, then within four circles of radius 3, one in each quadrant, we change the group value to two in the circles in the first and third quadrants, and we change the group value to three in the circles in the second and fourth quadrants.

Instructions for creating this dataset and definitions for local macros associated with it are contained in its notes.

```
. use http://www.stata-press.com/data/r14/circlegrid
(Gridded circle data)
. local rp: di %12.10f 2+sqrt(3)
. local rm: di %12.10f 2-sqrt(3)
. local functionplot
> (function y = sqrt(3-(x+2)^2) - 2, lpat(solid) range(-'rp' -'rm'))
> (function y = -sqrt(3-(x+2)^2) - 2, lpat(solid) range(-'rp' -'rm'))
> (function y = sqrt(3-(x-2)^2) + 2, lpat(solid) range(-'rm' 'rp'))
> (function y = sqrt(3-(x-2)^2) + 2, lpat(solid) range(-'rm' 'rp'))
> (function y = sqrt(3-(x-2)^2) + 2, lpat(solid) range(-'rm' 'rp'))
> (function y = -sqrt(3-(x+2)^2) + 2, lpat(solid) range(-'rp' -'rm'))
> (function y = sqrt(3-(x-2)^2) + 2, lpat(solid) range(-'rp' -'rm'))
> (function y = -sqrt(3-(x-2)^2) - 2, lpat(solid) range('rm' 'rp'))
> (function y = -sqrt(3-(x-2)^2) - 2, lpat(solid) range('rm' 'rp'))
. local graphopts
> aspectratio(1) legend(order(1 "group 1" 2 "group 2" 3 "group 3") rows(1))
```

```
. twoway (scatter y x if group==1)
>          (scatter y x if group==2)
>          (scatter y x if group==3)
>          'functionplot', 'graphopts' name(original, replace)
>          title("Training data")
```



We do a KNN discriminant analysis, choosing k(3). We elect to omit the standard classification table and instead take a look at the leave-one-out (LOO) classification table.

. discrim knn x y, group(group) k(3) priors(proportional) notable lootable Kth-nearest-neighbor discriminant analysis Leave-one-out classification summary

Key
Number Percent

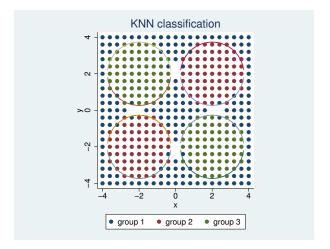
	Classif	ied		
True group	1	2	3	Total
1	173 87.82	12 6.09	12 6.09	197 100.00
2	8 6.56	114 93.44	0.00	122 100.00
3	8 6.56	0.00	114 93.44	122 100.00
Total	189 42.86	126 28.57	126 28.57	441 100.00
Priors	0.4467	0.2766	0.2766	

We will predict the LOO classification, changing to priors (equal), and look at the plot.

```
. predict cknn, looclass priors(equal) warning: 8 ties encountered ties are assigned to missing values (8 missing values generated)
```

4

```
. twoway (scatter y x if cknn==1)
>          (scatter y x if cknn==2)
>          (scatter y x if cknn ==3)
>          'functionplot', 'graphopts' name(KNN, replace)
>          title("KNN classification")
```



We see several empty spots on the grid. In our output, changing to priors(equal) created several ties that were assigned to missing values. Missing values are the blank places in our graph.

# Example 2: Listing misclassified observations

Continuing where we left off, we use estat list to display LOO probabilities for the misclassified observations, but this produces a lot of output.

. estat list, misclass class(noclass looclass) pr(nopr loopr) priors(equal)

	Classification		LOO Pro	babiliti	es
Obs.	True LOO	Cl.	1	2	3
24 28 34 38 50	1 1 1 1 2	2 * 2 * 3 * 3 *	0.3836 0.2374 0.2374 0.3836 0.5513	0.6164 0.7626 0.0000 0.0000 0.4487	0.0000 0.0000 0.7626 0.6164 0.0000
54 (outpu	3 t omitted)	1 *	0.5513	0.0000	0.4487

\* indicates misclassified observations

Instead, we predict the LOO probabilities and list only those where the LOO classification is missing.

- . predict pr\*, loopr priors(equal)
- . list group cknn pr\* if missing(cknn)

	group	cknn	pr1	pr2	pr3
94.	1		.2373541	.381323	.381323
115.	1		.2373541	.381323	.381323
214.	1		.2373541	.381323	.381323
215.	1		.2373541	.381323	.381323
225.	1		.2373541	.381323	.381323
226.	1		. 2373541	.381323	.381323
325.	1		. 2373541	.381323	.381323
346.	1		. 2373541	.381323	.381323

The missing LOO classifications represent ties for the largest probability.

4

# Example 3: Out-of-sample KNN classification

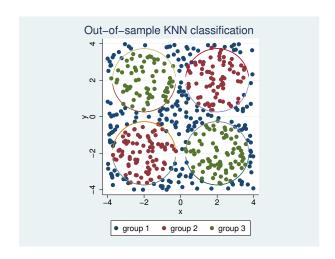
LOO classification and LOO probabilities are available only in sample, but standard probabilities can be obtained out of sample. To demonstrate this, we continue where we left off, with the KNN model of example 2 still active. We drop our current data and generate some new data. We predict the standard classification with the new data and graph our results.

- . clear
- . set obs 500

number of observations (\_N) was 0, now 500

- . set seed 314159265
- . generate x = 8\*runiform() 4
- . generate y = 8\*runiform() 4
- . predict cknn, class

```
. twoway (scatter y x if cknn==1)
>
         (scatter y x if cknn==2)
         (scatter y x if cknn ==3)
         'functionplot', 'graphopts' name(KNN2, replace)
         title("Out-of-sample KNN classification", span)
```



# Methods and formulas

See [MV] discrim knn for methods and formulas.

#### Also see

[MV] discrim knn — kth-nearest-neighbor discriminant analysis

[MV] discrim estat — Postestimation tools for discrim

[MV] **discrim** — Discriminant analysis

[U] 20 Estimation and postestimation commands

#### **Title**

discrim Ida — Linear discriminant analysis

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# **Description**

discrim 1da performs linear discriminant analysis. See [MV] discrim for other discrimination commands.

If you want canonical linear discriminant results displayed, see [MV] candisc.

### **Quick start**

Linear discriminant analysis of v1, v2, v3, and v4 for groups defined by catvar discrim lda v1 v2 v3 v4, group(catvar)

As above, but use prior probabilities proportional to group size discrim lda v1 v2 v3 v4, group(catvar) priors(proportional)

Display the leave-one-out and the resubstitution classification tables discrim lda v1 v2 v3 v4, group(catvar) lootable

As above, but suppress the resubstitution classification table discrim lda v1 v2 v3 v4, group(catvar) lootable notable

## Menu

Statistics > Multivariate analysis > Discriminant analysis > Linear (LDA)

# **Syntax**

discrim lda varlist [if] [in] [weight], group(groupvar) [options]

options	Description	
Model		
group( <i>groupvar</i> )	variable specifying the groups	
priors(priors)	group prior probabilities	
$\overline{\underline{\text{tie}}}$ s(ties)	how ties in classification are to be handled	
Reporting		
<u>not</u> able	suppress resubstitution classification table	
lootable	display leave-one-out classification table	
priors	Description	
equal	equal prior probabilities; the default	
proportional	group-size-proportional prior probabilities	
matname	row or column vector containing the group prior probabilities	
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities	
ties	Description	
missing	ties in group classification produce missing values; the default	
random	ties in group classification are broken randomly	
first	ties in group classification are set to the first tied group	

<sup>\*</sup>group() is required.

statsby and xi are allowed; see [U] 11.1.10 Prefix commands.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

# **Options**

Model

group(groupvar) is required and specifies the name of the grouping variable. groupvar must be a numeric variable.

priors(priors) specifies the prior probabilities for group membership. The following priors are allowed:

priors (equal) specifies equal prior probabilities. This is the default.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties (ties) specifies how ties in group classification will be handled. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values. This is the default

ties(random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

Reporting

notable suppresses the computation and display of the resubstitution classification table.

lootable displays the leave-one-out classification table.

# Remarks and examples

discrim lda computes the same things as candisc, but candisc displays more information. The same information can be displayed after discrim lda by using the estat suite of commands; see [MV] discrim lda postestimation.

Remarks are presented under the following headings:

Introduction
Descriptive LDA
Predictive LDA
A classic example

#### Introduction

Linear discriminant analysis (LDA) was developed by different researchers, Fisher (1936) and Mahalanobis (1936), starting with different approaches to the problem of discriminating between groups. Kshirsagar and Arseven (1975), Green (1979), and Williams (1982) demonstrate the mathematical relationship between Fisher's linear discriminant functions and the classification functions from the Mahalanobis approach to LDA; see Rencher (1998, 239).

Fisher's approach to LDA forms the basis of descriptive LDA but can be used for predictive LDA. The Mahalanobis approach to LDA more naturally handles predictive LDA, allowing for prior probabilities and producing estimates of the posterior probabilities. The Mahalanobis approach to LDA also extends to quadratic discriminant analysis (QDA); see [MV] discrim qda.

# **Descriptive LDA**

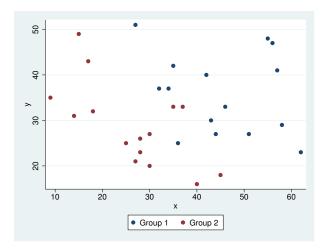
Fisher (1936) approached linear discriminant analysis by seeking the linear combination of the discriminating variables that provides maximal separation between the groups (originally two groups, but later extended to multiple groups). Maximal separation of groups is determined from an eigen analysis of  $\mathbf{W}^{-1}\mathbf{B}$ , where  $\mathbf{B}$  is the between-group sum-of-squares and cross-products (SSCP) matrix, and  $\mathbf{W}$  is the within-group SSCP matrix. The eigenvalues and eigenvectors of  $\mathbf{W}^{-1}\mathbf{B}$  provide what are called Fisher's linear discriminant functions.

The first linear discriminant function is the eigenvector associated with the largest eigenvalue. This first discriminant function provides a linear transformation of the original discriminating variables into one dimension that has maximal separation between group means. The eigenvector associated with the second-largest eigenvalue is the second linear discriminant function and provides a dimension uncorrelated with (but usually not orthogonal to) the first discriminant function. The second discriminant function provides the maximal separation of groups in a second dimension. The third discriminant function provides the maximum separation of groups in a third dimension.

### Example 1

Two groups measured on two variables illustrate Fisher's approach to linear discriminant analysis.

. use http://www.stata-press.com/data/r14/twogroup
(Two Groups)



Splitting the two groups on the basis of y or x alone would leave a great deal of overlap between the groups. By eye it appears that a line with a slope of about -1 could be positioned between the two groups with only a few of the observations falling on the wrong side of the line.

Fisher's approach to LDA helps us find the best separating line.

. discrim lda y x, group(group) notable

discrim lda computes the information needed for both a predictive and descriptive linear discriminant analysis. We requested notable, which suppressed the display of the resubstitution classification table. We will examine this feature of discrim lda when we discuss predictive LDA. The descriptive features of LDA are available through postestimation commands.

. estat loadings, unstandardized
Canonical discriminant function coefficients

	function1
y	.0862145
x	.0994392
_cons	-6.35128

Fisher's linear discriminant functions provide the basis for what are called the canonical discriminant functions; see Methods and formulas. The canonical discriminant function coefficients are also called unstandardized loadings because they apply to the unstandardized discriminating variables (x and y). Because we have only two groups, there is only one discriminant function. From the coefficients or loadings of this discriminant function, we obtain a one-dimensional projection of the data that gives maximal separation between the two groups relative to the spread within the groups. The estat loadings postestimation command displayed these loadings; see [MV] discrim Ida postestimation. After estat loadings, the unstandardized loadings are available in matrix  $r(L\_unstd)$ . We take these values and determine the equation of the separating line between the groups and a line perpendicular to the separating line.

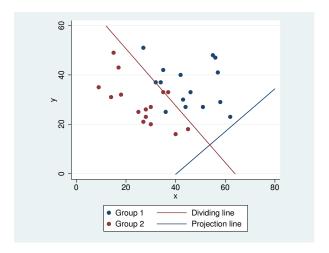
The unstandardized canonical discriminant function coefficients indicate that

$$0 = 0.0862145y + 0.0994392x - 6.35128$$

which in standard y = mx + b form is

$$y = -1.1534x + 73.6684$$

which is the dividing line for classifying observations into the two groups for this LDA. A line perpendicular to this dividing line has slope -1/-1.153=0.867. The following graph shows the data with this dividing line and a perpendicular projection line.



Another way of thinking about the discriminant function is that it projects the data from the original two dimensions down to one dimension—the line perpendicular to the dividing line. Classifications are based on which side of the separating line the observations fall.

Researchers often wish to know which of the discriminating variables is most important or helpful in discriminating between the groups. They want to examine the standardized loadings—the loadings that apply to standardized variables.

. estat loadings, standardized

Standardized canonical discriminant function coefficients

	function1
y	.7798206
x	1.057076

These coefficients or loadings apply to x and y that have been standardized using the pooled within-group covariance matrix. The loading for x is larger than that for y, indicating that it contributes more to the discrimination between the groups. Look back at the scatterplot to see that there is more separation between the groups in the x dimension than the y dimension. See [MV] **discrim lda postestimation** for more details of the estat loadings command.

Some researchers prefer to examine what are called structure coefficients.

. estat structure

Canonical structure

	function1
y	.3146309
x	.7138982

The estat structure command provides structure coefficients, which measure the correlation between each discriminating variable and the discriminant function; see [MV] **discrim lda postestimation**. Here the canonical structure coefficient for x is larger than that for y, leading to the same conclusion as with standardized loadings. There is disagreement in the literature concerning the use of canonical structure coefficients versus standardized loadings; see Rencher and Christensen (2012, 300–301) and Huberty (1994, 262–264).

4

In addition to loading and structure coefficients, there are other descriptive LDA features available after discrim lda. These include canonical correlations and tests of the canonical correlations, classification functions, scree plots, loading plots, score plots, and various group summaries; see [MV] discrim lda postestimation.

If your main interest is in descriptive LDA, you may find the candisc command of interest; see [MV] candisc. discrim lda and candisc differ only in their default output. discrim lda shows classification tables. candisc shows canonical correlations, standardized coefficients (loadings), structure coefficients, and more. All the features found in [MV] discrim lda postestimation are available for both commands.

#### Predictive LDA

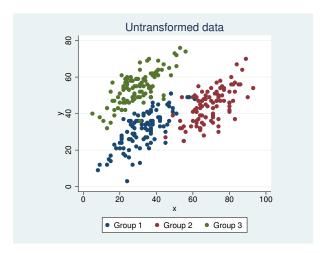
Another approach to linear discriminant analysis starts with the assumption that the observations from each group are multivariate normal with the groups having equal covariance matrices but different means. Mahalanobis (1936) distance plays an important role in this approach. An observation with unknown group membership is classified as belonging to the group with smallest Mahalanobis distance between the observation and group mean. Classification functions for classifying observations of unknown group membership can also be derived from this approach to LDA and formulas for the posterior probability of group membership are available.

As shown in *Methods and formulas*, Mahalanobis distance can be viewed as a transformation followed by Euclidean distance. Group membership is assigned based on the Euclidean distance in this transformed space.

# Example 2

We illustrate the Mahalanobis transformation and show some of the features of predictive discriminant analysis with a simple three-group example dataset.

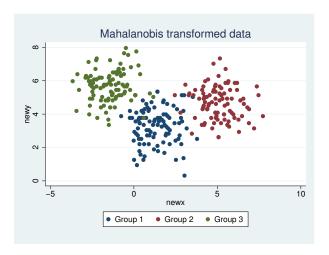
. use http://www.stata-press.com/data/r14/threegroup
(Three Groups)



These three groups appear to have similar covariance structure—showing a positive correlation between x and y. There is some overlap of the three groups, but general identification of the groups does not appear difficult by human eye.

If we were to apply Euclidean distance for classifying this untransformed data, we would misclassify some observations that clearly should not be misclassified when judged by eye. For example, in the graph above, the observations from group 3 that have y values below 40 (found in the lower left of the group 3 cloud of points) are closer in Euclidean distance to the center of group 1.

The following graph shows the Mahalanobis-transformed data.



With the transformed data, using Euclidean distance between observations and group means works well.

Now let's see how well discrim lda can distinguish between the groups. By default, a resubstitution classification table is presented. The rows correspond to the known group and the columns to the grouping as assigned by the discrim model. The word resubstitution is used because the same observations that built the model are being classified by the model.

. discrim lda y x, group(group) Linear discriminant analysis Resubstitution classification summary

Key
Number Percent

	Classif	ied		
True group	1	2	3	Total
1	93 93.00	4 4.00	3 3.00	100
2	3 3.00	97 97.00	0.00	100 100.00
3	3 3.00	0.00	97 97.00	100 100.00
Total	99 33.00	101 33.67	100 33.33	300 100.00
Priors	0.3333	0.3333	0.3333	

For these 300 observations, group 1 had 93 observations correctly classified, 4 observations misclassified into group 2, and 3 observations misclassified into group 3. Group 2 had 3 observations misclassified into group 1 and 97 observations correctly classified. Group 3 had 3 observations misclassified into group 1 and 97 observations correctly classified.

Generally, resubstitution classification tables give an overly optimistic view of how well you would classify an unknown observation. Leave-one-out (LOO) classification tables provide a more realistic assessment for classification success. With this 300-observation dataset, the LOO classification table gives the same results. We could see the LOO classification table by requesting it at estimation, by requesting it at replay, or by using the estat classtable command.

We now list the misclassified observations.

. estat list, varlist misclassified

	Data		Classif	ication	Probabi	lities	
Obs.	У	х	True	Class.	1	2	3
19 29 47 55 70	49 49 49 24 48	37 57 37 45 61	1 1 1 1	3 * 2 * 3 * 2 *	0.2559 0.4245 0.2559 0.4428 0.0661	0.0000 0.5750 0.0000 0.5572 0.9339	0.7441 0.0005 0.7441 0.0000 0.0000
74 92 143 161 185	49 37 27 39 49	58 22 45 49 54	1 1 2 2 2	2 * 3 * 1 * 1 *	0.3041 0.3969 0.6262 0.8026 0.7782	0.6957 0.0000 0.3738 0.1973 0.2187	0.0003 0.6031 0.0000 0.0001 0.0030
238 268 278	48 50 36	44 44 31	3 3 3	1 * 1 * 1 *	0.8982 0.7523 0.9739	0.0017 0.0009 0.0000	0.1001 0.2469 0.0261

<sup>\*</sup> indicates misclassified observations

The posterior probabilities for each displayed observation for each of the three groups is presented along with the true group and the classified group. The observation number is also shown. We added the discriminating variables x and y to the list with the varlist option. By default, estat list would list all the observations. The misclassified option restricts the list to those observations that were misclassified.

With predict we could generate classification variables, posterior probabilities, Mahalanobis squared distances from observations to group means, classification function scores (see Methods and formulas), and more. Fifteen estat commands provide more predictive and descriptive tools after discrim lda; see [MV] discrim lda postestimation.

4

# A classic example

We use the iris data from Fisher's (1936) pioneering LDA article to demonstrate the discrim lda command.

# Example 3

Fisher obtained the iris data from Anderson (1935). The data consist of four features measured on 50 samples from each of three iris species. The four features are the length and width of the sepal and petal. The three species are Iris setosa, Iris versicolor, and Iris virginica. Morrison (2005, app. B.2) is a modern source of the data.

```
. use http://www.stata-press.com/data/r14/iris
(Iris data)
```

Running discrim 1da produces the resubstitution classification table.

. discrim lda seplen sepwid petlen petwid, group(iris)

Linear discriminant analysis
Resubstitution classification summary

Key
Number Percent

True iris	Classified setosa	versicolor	virginica	Total
setosa	50 100.00	0.00	0.00	50 100.00
versicolor	0.00	48 96.00	2 4.00	50 100.00
virginica	0.00	1 2.00	49 98.00	50 100.00
Total	50 33.33	49 32.67	51 34.00	150 100.00
Priors	0.3333	0.3333	0.3333	

One *Iris virginica* observation was misclassified as a *versicolor*, two *Iris versicolor* observations were misclassified as *virginica*, and no *Iris setosa* observations were misclassified in our resubstitution classification.

Which observations were misclassified?

. estat list, misclassified

	Classification		Probabi	lities	
Obs.	True	Class.	setosa	versicolor	virginica
71 84 134	versicol	virginic * virginic * versicol *	0.0000 0.0000 0.0000	0.2532 0.1434 0.7294	0.7468 0.8566 0.2706

<sup>\*</sup> indicates misclassified observations

Postestimation command estat list shows that observations 71, 84, and 134 were misclassified and shows the estimated posterior probabilities for the three species for the misclassified observations.

We now examine the canonical discriminant functions for this LDA. The number of discriminant functions will be one fewer than the number of groups or will be the number of discriminating variables, whichever is less. With four discriminating variables and three species, we will have two discriminant functions. estat loadings displays the discriminant coefficients or loadings.

. estat loadings, unstandardized standardized Canonical discriminant function coefficients

	function1	function2
seplen	8293776	0241021
sepwid	-1.534473	-2.164521
petlen	2.201212	.9319212
petwid	2.81046	-2.839188
_cons	-2.105106	6.661473

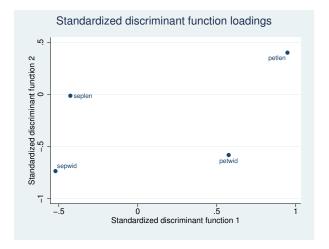
Standardized canonical discriminant function coefficients

	function1	function2
seplen	4269548	0124075
sepwid	5212417	7352613
petlen	.9472572	.4010378
petwid	.5751608	5810399

We requested the display of both unstandardized and standardized loadings. The two unstandardized discriminant functions provide linear combinations of the seplen, sepwid, petlen, and petwid discriminating variables—producing two new dimensions. The standardized canonical discriminant function coefficients indicate the relative importance and relationship between the discriminating variables and the discriminant functions. The first discriminant function compares seplen and sepwid, which have negative standardized coefficients, to petlen and petwid, which have positive standardized coefficients. The second discriminant function appears to be contrasting the two width variables from the two length variables, though this is not as distinct of a difference as found in the first discriminant function because the seplen variable in the second standardized discriminant function is close to zero.

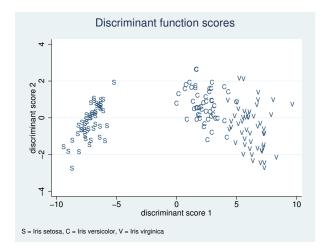
Understanding the composition of the discriminant functions is aided by plotting the coefficients. loadingplot graphs the discriminant function coefficients (loadings); see [MV] discrim lda postestimation and [MV] scoreplot.

#### . loadingplot



We now show a scatterplot of our three species projected onto the two dimensions of our discriminant solution. The scoreplot command takes care of most of the graphing details for us; see [MV] discrim lda postestimation and [MV] scoreplot. However, by default, scoreplot uses the full value labels for the three iris species and the resulting graph is busy. The iris dataset has two label languages

predefined. The default label language has the full value labels. The other predefined label language is called oneletter, and it uses a one-letter code as value labels for the three iris species. The label language command will switch between these two label languages; see [D] label language. We also use the msymbol(i) graph option so that the points will not be displayed—only the one-letter value labels will be displayed for each observation.



The *Iris setosa* are well separated from the other two species. *Iris versicolor* and *Iris virginica* show some overlap.

See example 1 of [MV] discrim estat and examples 6, 7, and 8, of [MV] discrim Ida postestimation for more examples of what can be produced after discrim Ida for this iris dataset.

4

# Stored results

discrim 1da stores the following in e():

```
Scalars
                           number of observations
    e(N)
    e(N_groups)
                           number of groups
                           number of discriminating variables
    e(k)
    e(f)
                           number of nonzero eigenvalues
Macros
    e(cmd)
                           discrim
    e(subcmd)
                           lda
    e(cmdline)
                           command as typed
    e(groupvar)
                           name of group variable
    e(grouplabels)
                           labels for the groups
    e(varlist)
                           discriminating variables
    e(wtype)
                           weight type
    e(wexp)
                           weight expression
    e(title)
                           title in estimation output
    e(ties)
                           how ties are to be handled
    e(properties)
                           nob noV eigen
                           program used to implement estat
    e(estat_cmd)
    e(predict)
                           program used to implement predict
    e(marginsnotok)
                           predictions disallowed by margins
Matrices
    e(groupcounts)
                           number of observations for each group
                           prior probabilities for each group
    e(grouppriors)
                           numeric value for each group
    e(groupvalues)
                           group means on discriminating variables
    e(means)
    e(SSCP_W)
                           pooled within-group SSCP matrix
    e(SSCP_B)
                           between-groups SSCP matrix
    e(SSCP_T)
                           total SSCP matrix
    e(SSCP_W#)
                           within-group SSCP matrix for group #
    e(W_eigvals)
                           eigenvalues of e(SSCP_W)
    e(W_eigvecs)
                           eigenvectors of e(SSCP_W)
    e(S)
                           pooled within-group covariance matrix
    e(Sinv)
                           inverse of e(S)
    e(sqrtSinv)
                           Cholesky (square root) of e(Sinv)
    e(Ev)
                           eigenvalues of W^{-1}B
    e(L_raw)
                           eigenvectors of W^{-1}B
    e(L_unstd)
                           unstandardized canonical discriminant function coefficients
                           within-group standardized canonical discriminant function coefficients
    e(L_std)
                           total-sample standardized canonical discriminant function coefficients
    e(L_totalstd)
    e(C)
                           classification coefficients
    e(cmeans)
                           unstandardized canonical discriminant functions evaluated at group means
    e(canstruct)
                           canonical structure matrix
    e(candisc_stat)
                           canonical discriminant analysis statistics
Functions
    e(sample)
                           marks estimation sample
```

# Methods and formulas

Methods and formulas are presented under the following headings:

Predictive LDA Descriptive LDA

#### Predictive LDA

Let g be the number of groups,  $n_i$  the number of observations for group i, and  $q_i$  the prior probability for group i. Let  $\mathbf{x}$  denote an observation measured on p discriminating variables. For consistency with the discriminant analysis literature,  $\mathbf{x}$  will be a column vector, though it corresponds to a row in your dataset. Let  $f_i(\mathbf{x})$  represent the density function for group i, and let  $P(\mathbf{x}|G_i)$  denote the probability of observing  $\mathbf{x}$  conditional on belonging to group i. Denote the posterior probability of group i given observation  $\mathbf{x}$  as  $P(G_i|\mathbf{x})$ . With Bayes's theorem, we have

$$P(G_i|\mathbf{x}) = \frac{q_i f_i(\mathbf{x})}{\sum_{j=1}^g q_j f_j(\mathbf{x})}$$

Substituting  $P(\mathbf{x}|G_i)$  for  $f_i(\mathbf{x})$ , we have

$$P(G_i|\mathbf{x}) = \frac{q_i P(\mathbf{x}|G_i)}{\sum_{j=1}^g q_j P(\mathbf{x}|G_j)}$$

LDA assumes that the groups are multivariate normal with equal covariance matrices. Let S denote the pooled within-group sample covariance matrix and  $\bar{\mathbf{x}}_i$  denote the sample mean of group i. The  $\bar{\mathbf{x}}_i$  are returned as the columns of the e(means) matrix. The squared Mahalanobis distance between observation  $\mathbf{x}$  and  $\bar{\mathbf{x}}_i$  is

$$D_i^2 = (\mathbf{x} - \bar{\mathbf{x}}_i)' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}_i)$$

Plugging these sample estimates into the multivariate normal density gives

$$P(\mathbf{x}|G_i) = (2\pi)^{-p/2}|\mathbf{S}|^{-1/2}e^{-D_i^2/2}$$

Substituting this into the formula for  $P(G_i|\mathbf{x})$  and simplifying gives

$$P(G_i|\mathbf{x}) = \frac{q_i e^{-D_i^2/2}}{\sum_{j=1}^g q_j e^{-D_j^2/2}}$$

as the LDA posterior probability of observation x belonging to group i.

Computation of Mahalanobis distance can be broken down into two steps. Step one: transform the data by using the Mahalanobis transformation. Step two: compute the Euclidean distance of the transformed data.

Let L be the Cholesky factorization of  $S^{-1}$  such that  $S^{-1} = L'L$  and L is lower triangular. L is returned in matrix e(sqrtSinv). Squared Mahalanobis distance can be expressed in terms of L.

$$D_i^2 = (\mathbf{x} - \bar{\mathbf{x}}_i)' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}_i)$$

$$= (\mathbf{x} - \bar{\mathbf{x}}_i)' \mathbf{L}' \mathbf{L} (\mathbf{x} - \bar{\mathbf{x}}_i)$$

$$= (\mathbf{L} \mathbf{x} - \mathbf{L} \bar{\mathbf{x}}_i)' (\mathbf{L} \mathbf{x} - \mathbf{L} \bar{\mathbf{x}}_i)$$

$$= (\mathbf{z} - \bar{\mathbf{z}}_i)' (\mathbf{z} - \bar{\mathbf{z}}_i)$$

which is the squared Euclidean distance between z and  $\bar{z}_i$ . We call z = Lx the Mahalanobis transformation.

The squared Mahalanobis distance between group means is produced by estat grdistances; see [MV] discrim Ida postestimation.

Classification functions can be derived from the Mahalanobis formulation for LDA; see Rencher and Christensen (2012, 315–316) and Huberty (1994, 59). Let  $L_i(\mathbf{x})$  denote the linear classification function for the *i*th group applied to observation  $\mathbf{x}$ .  $L_i(\mathbf{x}) = \mathbf{c}_i'\mathbf{x} + c_{i0}$ , where  $\mathbf{c}_i = \bar{\mathbf{x}}_i'\mathbf{S}^{-1}$  and  $c_{i0} = -(1/2)\bar{\mathbf{x}}_i'\mathbf{S}^{-1}\bar{\mathbf{x}}_i + \ln(q_i)$ . The g linear classification functions are returned as the columns of matrix  $\mathbf{e}(\mathbf{C})$  and through the estat classfunction command; see [MV] discrim Ida postestimation. An observation can be classified based on largest posterior probability or based on largest classification function score.

### Descriptive LDA

As with predictive LDA, let g be the number groups,  $n_i$  the number of training (sample) observations for group i, p the number of discriminating variables, and  $N = \sum_{i=1}^g n_i$  the total number of observations. Also, let W be the within-group sums-of-squares and cross-products (SSCP) matrix and let B be the between-groups SSCP matrix. Fisher's (1936) linear discriminant functions are based on the eigenvalues and eigenvectors of  $W^{-1}B$ .

There are  $s = \min(g-1,p)$  nonzero eigenvalues of  $\mathbf{W}^{-1}\mathbf{B}$ . Let  $\lambda_1, \lambda_2, \ldots, \lambda_s$  denote the s eigenvalues in decreasing order. The eigenvalues are returned in e(Ev). Let  $v_1, v_2, \ldots, v_s$ denote the corresponding eigenvectors. Rencher and Christensen (2012, 289) outlines the approach for obtaining the eigenvalues and eigenvectors of the nonsymmetric  ${f W}^{-1}{f B}$  matrix. Because  ${f W}^{-1}{f B}$ is nonsymmetric, the resulting eigenvectors are not orthogonal but merely uncorrelated; see Rencher and Christensen (2012, 289). A matrix with the  $v_i$  as columns is returned in  $e(L_raw)$ . The phrase raw coefficients is used by Klecka (1980, 22) to describe the v vectors.

Any constant multiple of the eigenvector  $\mathbf{v}_i$  is still an eigenvector of  $\mathbf{W}^{-1}\mathbf{B}$  associated with eigenvalue  $\lambda_i$ . Typically,  $\mathbf{vu}_i = \mathbf{v}_i \sqrt{N-g}$  are used as the eigenvectors (discriminant functions) and are called unstandardized canonical discriminant functions because they correspond to the unstandardized discriminating variables. An extra element is added to the bottom of the vu vectors for the constant, so that if the vu vectors are applied as linear combinations of the discriminating variables, the resulting variables have mean zero; see Klecka (1980, 21–23). A matrix with the  $\mathbf{vu}_i$  as columns is returned in e(L\_unstd).

The means of the discriminating variables for each group are returned as the columns of the matrix e (means). These group means multiplied by the unstandardized discriminant-function coefficients,  $\mathbf{v}\mathbf{u}_i$ , produce what are called group means on canonical variables and are returned in the matrix e(cmeans) and displayed with the command estat grmeans, canonical.

Standardized discriminant functions are obtained as  $\mathbf{v}\mathbf{s}_i = \mathbf{v}_i \sqrt{W_{ii}}$ . The *i*th raw eigenvector is standardized by the square root of the ith diagonal element of the W matrix. These within-group standardized discriminant functions are used in assessing the importance and relationship of the original discriminating variables to the discriminant functions. A matrix with the  $vs_i$  as columns is returned in e(L\_std).

Let T denote the total sample SSCP matrix. Total-sample standardized discriminant functions are computed as  $\mathbf{vt}_i = \mathbf{v}_i \sqrt{T_{ii}(N-g)/(N-1)}$ . A matrix with the  $\mathbf{vt}_i$  as columns is returned in e(L\_totalstd). There is debate as to which of vs and vt should be used for interpretation; see Mueller and Cozad (1988), Nordlund and Nagel (1991), and Mueller and Cozad (1993).

The estat loadings command displays e(L\_unstd), e(L\_std), and e(L\_totalstd); see [MV] discrim Ida postestimation.

The canonical structure matrix measures the correlation between the discriminating variables and the discriminant function and is returned in matrix e(canstruct). The canonical structure matrix is equal to WV with the ith row divided by  $\sqrt{W_{ii}}$ , where V contains the  $\mathbf{v}_i$  eigenvectors as columns. Rencher and Christensen (2012, 300) warns against the use of structure coefficients for interpretation, but Huberty (1994, 262–264) contends otherwise.

The returned matrix e(candisc\_stat) contains columns for the information shown by estat canontest, including the eigenvalues, canonical correlations, proportion of variance, cumulative proportion of variance, likelihood-ratio test statistics, and the corresponding F tests, degrees of freedom, and p-values. See [MV] canon.

As noted in the *Introduction* section of *Remarks and examples*, Kshirsagar and Arseven (1975), Green (1979), and Williams (1982) demonstrate the mathematical relationship between Fisher's linear discriminant functions (the basis for descriptive LDA) and the classification functions from the Mahalanobis approach to LDA (the basis for predictive LDA); see Rencher (1998, 239).

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#### Also see

[MV] discrim lda postestimation — Postestimation tools for discrim lda

[MV] **discrim** — Discriminant analysis

[MV] candisc — Canonical linear discriminant analysis

[U] 20 Estimation and postestimation commands

# **Title**

discrim Ida postestimation — Postestimation tools for discrim Ida

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

# **Postestimation commands**

The following postestimation commands are of special interest after discrim lda:

Command	Description
estat anova	ANOVA summaries table
estat canontest	tests of the canonical discriminant functions
estat classfunctions	classification functions
estat classtable	classification table
estat correlations	correlation matrices and p-values
estat covariance	covariance matrices
estat errorrate	classification error-rate estimation
estat grdistances	Mahalanobis and generalized squared distances between the group means
estat grmeans	group means and variously standardized or transformed means
estat grsummarize	group summaries
estat list	classification listing
estat loadings	canonical discriminant-function coefficients (loadings)
estat manova	MANOVA table
estat structure	canonical structure matrix
estat summarize	estimation sample summary
loadingplot	plot standardized discriminant-function loadings
scoreplot	plot discriminant-function scores
screeplot	plot eigenvalues

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results
predict	group classification and posterior probabilities

<sup>\*</sup>All estimates subcommands except table and stats are available; see [R] estimates.

# predict

### **Description for predict**

predict creates a new variable containing predictions such as group classifications, probabilities, Mahalanobis squared distances, discriminant function scores, leave-one-out probabilities, leave-one-out group classifications, and leave-one-out Mahalanobis squared distances.

# Menu for predict

Statistics > Postestimation

# Syntax for predict

```
predict [type] newvar [if] [in] [, statistic options]
    predict [type] { stub* | newvarlist } [if] [in] [, statistic options]
 statistic
                            Description
Main
 classification
                            group membership classification; the default when one variable is
                              specified and group() is not specified
                            probability of group membership; the default when group() is
 pr
                              specified or when multiple variables are specified
 mahalanobis
                            Mahalanobis squared distance between observations and groups
 dscore
                            discriminant function score
                            group classification function score
 clscore
                            leave-one-out group membership classification; may be used only
*looclass
                              when one new variable is specified
                            leave-one-out probability of group membership
^stloopr
*loomahal
                            leave-one-out Mahalanobis squared distance between observations and
                              groups
                            Description
 options
Main
 group(group)
                            the group for which the statistic is to be calculated
Options
 priors(priors)
                            group prior probabilities; defaults to e(grouppriors)
 ties(ties)
                            how ties in classification are to be handled; defaults to e(ties)
```

#### 260 discrim Ida postestimation — Postestimation tools for discrim Ida

Description
equal prior probabilities
group-size-proportional prior probabilities
row or column vector containing the group prior probabilities
matrix expression providing a row or column vector of the group prior probabilities
Description
ties in group classification produce missing values
ties in group classification are broken randomly
ties in group classification are set to the first tied group

You specify one new variable with classification or looclass; either one or e(N\_groups) new variables with pr, loopr, mahalanobis, loomahal, or clscore; and one to e(f) new variables with dscore.

Unstarred statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample. Starred statistics are calculated only for the estimation sample, even when if e(sample) is not specified.

group() is not allowed with classification, dscore, or looclass.

### Options for predict

Main

- classification, the default, calculates the group classification. Only one new variable may be specified.
- pr calculates group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- mahalanobis calculates the squared Mahalanobis distance between the observations and group means. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- dscore produces the discriminant function score. Specify as many variables as leading discriminant functions that you wish to score. No more than e(f) variables may be specified.
- clscore produces the group classification function score. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- looclass calculates the leave-one-out group classifications. Only one new variable may be specified. Leave-one-out calculations are restricted to e(sample) observations.
- loopr calculates the leave-one-out group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables. Leave-one-out calculations are restricted to e(sample) observations.
- loomahal calculates the leave-one-out squared Mahalanobis distance between the observations and group means. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables. Leave-one-out calculations are restricted to e(sample) observations.

group(group) specifies the group for which the statistic is to be calculated and can be specified using

#1, #2, ..., where #1 means the first category of the e(groupvar) variable, #2 the second category, etc.;

the values of the e(groupvar) variable; or

the value labels of the e(groupvar) variable if they exist.

group() is not allowed with classification, dscore, or looclass.

Options

priors(*priors*) specifies the prior probabilities for group membership. If priors() is not specified, e(grouppriors) is used. The following *priors* are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors (matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) is used. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values.

ties(<u>random</u>) specifies that ties in group classification are broken randomly.

 $ties(\underline{f}irst)$  specifies that ties in group classification are set to the first tied group.

# **Description for estat**

estat anova presents a table summarizing the one-way ANOVAs for each variable in the discriminant analysis.

estat canontest presents tests of the canonical discriminant functions. Presented are the canonical correlations, eigenvalues, proportion and cumulative proportion of variance, and likelihood-ratio tests for the number of nonzero eigenvalues.

estat classfunctions displays the classification functions.

estat correlations displays the pooled within-group correlation matrix, between-groups correlation matrix, total-sample correlation matrix, and/or the individual group correlation matrices. Two-tailed p-values for the correlations may also be requested.

estat covariance displays the pooled within-group covariance matrix, between-groups covariance matrix, total-sample covariance matrix, and/or the individual group covariance matrices.

estat grdistances provides Mahalanobis squared distances between the group means along with the associated F statistics and significance levels. Also available are generalized squared distances.

estat grmeans provides group means, total-sample standardized group means, pooled within-group standardized means, and canonical functions evaluated at the group means.

estat loadings present the canonical discriminant-function coefficients (loadings). Unstandardized, pooled within-class standardized, and total-sample standardized coefficients are available.

estat manova presents the MANOVA table associated with the discriminant analysis.

estat structure presents the canonical structure matrix.

#### Menu for estat

Statistics > Postestimation

#### Syntax for estat

```
ANOVA summaries table
    estat anova
 Tests of the canonical discriminant functions
    estat canontest
 Classification functions
    estat classfunctions [, classfunctions_options]
 Correlation matrices and p-values
    estat correlations [, correlations_options]
 Covariance matrices
    estat covariance [, covariance_options]
 Mahalanobis and generalized squared distances between the group means
    estat grdistances [, grdistances_options]
 Group means and variously standardized or transformed means
    estat grmeans [, grmeans_options]
 Canonical discriminant-function coefficients (loadings)
    estat loadings [, loadings_options]
 MANOVA table
    estat manova
 Canonical structure matrix
    estat structure [, format(%fmt)]
 classfunctions_options
                          Description
Main
 adjustequal
                          adjust the constant even when priors are equal
 format(% fmt)
                          numeric display format; default is %9.0g
Options
 priors(priors)
                          group prior probabilities; defaults to e(grouppriors)
                          suppress display of prior probabilities
 nopriors
```

correlations_options	Description
Main	
within	display pooled within-group correlation matrix; the default
- between	display between-groups correlation matrix
total	display total-sample correlation matrix
groups	display the correlation matrix for each group
all	display all the above
p	display two-sided p-values for requested correlations
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g
nohalf	display full matrix even if symmetric
covariance_options	Description
Main	
within	display pooled within-group covariance matrix; the default
- between	display between-groups covariance matrix
_ total	display total-sample covariance matrix
groups	display the covariance matrix for each group
all	display all the above
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g
nohalf	display full matrix even if symmetric
grdistances_options	Description
Main	
mahalanobis (f p)	display Mahalanobis squared distances between group means; the default
generalized	display generalized Mahalanobis squared distances between group means
all	equivalent to mahalanobis(f p) generalized
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g
Options	
priors(priors)	group prior probabilities; defaults to e(grouppriors)
grmeans_options	Description
Main	
$\underline{\mathbf{r}}$ aw	display untransformed and unstandardized group means
$\underline{\mathtt{t}}\mathtt{otalstd}$	display total-sample standardized group means
$\underline{\mathbf{w}}$ ithinstd	display pooled within-group standardized group means
<u>c</u> anonical	display canonical functions evaluated at group means
all	display all the mean tables

loadings_options	Description
Main	
<u>st</u> andardized	display pooled within-group standardized canonical discriminant function coefficients; the default
<u>tot</u> alstandardized	display the total-sample standardized canonical discriminant function coefficients
$\underline{\mathtt{unst}}$ andardized	display unstandardized canonical discriminant function coefficients
all	display all the above
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g

# **Options for estat**

Options for estat are presented under the following headings:

Options for estat classfunctions Options for estat correlations Options for estat covariance Options for estat grdistances Options for estat grmeans Options for estat loadings Option for estat structure

# Options for estat classfunctions

Main

adjustequal specifies that the constant term in the classification function be adjusted for prior probabilities even though the priors are equal. By default, equal prior probabilities are not used in adjusting the constant term. adjustequal has no effect with unequal prior probabilities.

format(%fmt) specifies the matrix display format. The default is format(%9.0g).

∫ Options ໄ

priors (priors) specifies the group prior probabilities. The prior probabilities affect the constant term in the classification function. By default, priors is determined from e(grouppriors). See Options for predict for the priors specification. By common convention, when there are equal prior probabilities the adjustment of the constant term is not performed. See adjustequal to override this convention.

nopriors specifies that the prior probabilities not be displayed. By default, the prior probabilities used in determining the constant in the classification functions are displayed as the last row in the classification functions table.

# Options for estat correlations

(Main

within specifies that the pooled within-group correlation matrix be displayed. This is the default. between specifies that the between-groups correlation matrix be displayed.

total specifies that the total-sample correlation matrix be displayed.

groups specifies that the correlation matrix for each group be displayed.

all is the same as specifying within, between, total, and groups.

p specifies that two-sided p-values be computed and displayed for the requested correlations.

format(% fmt) specifies the matrix display format. The default is format(%8.5f).

nohalf specifies that, even though the matrix is symmetric, the full matrix be printed. The default is to print only the lower triangle.

# Options for estat covariance

Main

within specifies that the pooled within-group covariance matrix be displayed. This is the default.

between specifies that the between-groups covariance matrix be displayed.

total specifies that the total-sample covariance matrix be displayed.

groups specifies that the covariance matrix for each group be displayed.

all is the same as specifying within, between, total, and groups.

format(%fmt) specifies the matrix display format. The default is format(%9.0g).

nohalf specifies that, even though the matrix is symmetric, the full matrix be printed. The default is to print only the lower triangle.

# Options for estat grdistances

Main

mahalanobis [(f p)] specifies that a table of Mahalanobis squared distances between group means be presented. mahalanobis(f) adds F tests for each displayed distance and mahalanobis(p) adds the associated p-values. mahalanobis(f p) adds both. The default is mahalanobis.

generalized specifies that a table of generalized Mahalanobis squared distances between group means be presented. generalized starts with what is produced by the mahalanobis option and adds a term accounting for prior probabilities. Prior probabilities are provided with the priors() option, or if priors() is not specified, by the values in e(grouppriors). By common convention, if prior probabilities are equal across the groups, the prior probability term is omitted and the results from generalized will equal those from mahalanobis.

all is equivalent to specifying mahalanobis(f p) and generalized.

 ${\tt format(\% \it fmt)}$  specifies the matrix display format. The default is  ${\tt format(\%9.0g)}$ .

Options

priors (*priors*) specifies the group prior probabilities and affects only the output of the generalized option. By default, *priors* is determined from e(grouppriors). See *Options for predict* for the *priors* specification.

### Options for estat grmeans

Main

raw, the default, displays a table of group means.

totalstd specifies that a table of total-sample standardized group means be presented.

withinstd specifies that a table of pooled within-group standardized group means be presented.

canonical specifies that a table of the unstandardized canonical discriminant functions evaluated at the group means be presented.

all is equivalent to specifying raw, totalstd, withinstd, and canonical.

# **Options for estat loadings**

∫ Main ໄ

standardized specifies that the pooled within-group standardized canonical discriminant function coefficients be presented. This is the default.

totalstandardized specifies that the total-sample standardized canonical discriminant function coefficients be presented.

unstandardized specifies that the unstandardized canonical discriminant function coefficients be presented.

all is equivalent to specifying standardized, totalstandardized, and unstandardized.

format(% fmt) specifies the matrix display format. The default is format(%9.0g).

# Option for estat structure

Main

format(%fmt) specifies the matrix display format. The default is format(%9.0g).

# Remarks and examples

Remarks are presented under the following headings:

Classification tables, error rates, and listings ANOVA, MANOVA, and canonical correlations Discriminant and classification functions Scree, loading, and score plots Means and distances Covariance and correlation matrices Predictions

# Classification tables, error rates, and listings

After discrim, including discrim lda, you can obtain classification tables, error-rate estimates, and listings; see [MV] discrim estat.

#### Example 1: Predictive linear discriminant analysis

Example 1 of [MV] manova introduces the apple tree rootstock data from Andrews and Herzberg (1985, 357–360) and used in Rencher and Christensen (2012, 184). Descriptive linear discriminant analysis is often used after a multivariate analysis of variance (MANOVA) to explore the differences between groups found to be significantly different in the MANOVA.

We first examine the predictive aspects of the linear discriminant model on these data by examining classification tables, error-rate estimate tables, and classification listings.

To illustrate the ability of discrim lda and the postestimation commands of handling unequal prior probabilities, we perform our LDA using prior probabilities of 0.2 for the first four rootstock groups and 0.1 for the last two rootstock groups.

```
. use http://www.stata-press.com/data/r14/rootstock
(Table 6.2 Rootstock Data, Rencher and Christensen (2012))
```

. discrim lda y1 y2 y3 y4, group(rootstock) priors(.2, .2, .2, .2, .1, .1)

Linear discriminant analysis
Resubstitution classification summary

Key
Number Percent

True	Classif	ied					
rootstock	1	2	3	4	5	6	Total
1	7 87.50	0.00	0.00	1 12.50	0.00	0.00	8 100.00
2	0.00	4 50.00	2 25.00	1 12.50	1 12.50	0.00	8 100.00
3	0.00	1 12.50	6 75.00	1 12.50	0.00	0.00	8 100.00
4	3 37.50	0.00	1 12.50	4 50.00	0.00	0.00	8 100.00
5	0.00	3 37.50	2 25.00	0.00	2 25.00	1 12.50	8 100.00
6	3 37.50	0.00	0.00	0.00	2 25.00	3 37.50	8 100.00
Total	13 27.08	8 16.67	11 22.92	7 14.58	5 10.42	4 8.33	48 100.00
Priors	0.2000	0.2000	0.2000	0.2000	0.1000	0.1000	

The prior probabilities are reported at the bottom of the table. The classification results are based, in part, on the selection of prior probabilities.

With only 8 observations per rootstock and six rootstock groups, we have small cell counts in our table, with many zero cell counts. Because resubstitution classification tables give an overly optimistic view of classification ability, we use the estat classtable command to request a leave-one-out (LOO) classification table and request the reporting of average posterior probabilities in place of percentages.

. estat classtable, probabilities loo

Leave-one-out average-posterior-probabilities classification table

Key		
Number Average	posterior	probability

True	LOO Cla	ssified				
rootstock	1	2	3	4	5	6
1	5	0	0	2	0	1
	0.6055		•	0.6251	•	0.3857
2	0	4	2	1	1	0
		0.6095	0.7638	0.3509	0.6607	•
3	0	1	6	1	0	0
		0.5520	0.7695	0.4241	•	•
4	4	0	1	3	0	0
	0.5032	•	0.7821	0.5461	•	•
5	0	3	2	0	2	1
		0.7723	0.5606	•	0.4897	0.6799
6	3	0	0	0	2	3
	0.6725	•	•	•	0.4296	0.5763
Total	12	8	11	7	5	5
	0.5881	0.6634	0.7316	0.5234	0.4999	0.5589
Priors	0.2000	0.2000	0.2000	0.2000	0.1000	0.1000

Zero cell counts report a missing value for the average posterior probability. We did not specify the priors() option with estat classtable, so the prior probabilities used in our LDA model were used.

estat errorrate estimates the error rates for each group. We use the pp option to obtain estimates based on the posterior probabilities instead of the counts.

. estat errorrate, pp

Error rate estimated from posterior probabilities

Error Rate	rootstock 1	2	3	4	5
Stratified	.2022195	.431596	.0868444	.4899799	.627472
Unstratified	.2404022	.41446	.1889412	.5749832	.4953118
Priors Error Rate	.2 rootstock	.2 Total	.2	.2	.1
Stratified	.6416429	.3690394			
Unstratified	.4027382	.3735623			
Priors	.1				

We did not specify the priors() option, and estat errorrate defaulted to using the prior probabilities from the LDA model. Both stratified and unstratified estimates are shown for each rootstock group and for the overall total. See [MV] **discrim estat** for an explanation of the error-rate estimation.

We can list the classification results and posterior probabilities from our discriminant analysis model by using the estat list command. estat list allows us to specify which observations we wish to examine and what classification and probability results to report.

We request the LOO classification and LOO probabilities for all misclassified observations from the fourth rootstock group. We also suppress the resubstitution classification and probabilities from being displayed.

00+2+	lie+	i f	rootetock==/	misclassified	clace(	1 ^^	noclace)	nr(1	$\sim$	nonr)	

	Classific	ation	LOO Pro	babiliti	es			
Obs.	True LO	0 Cl.	1	2	3	4	5	6
25 26 27 29 32	4 4 4 4	1 * 3 * 1 * 1 *	0.5433 0.0216 0.3506 0.6134 0.5054	0.1279 0.0199 0.1860 0.0001 0.0011	0.0997 0.7821 0.0583 0.0005 0.0017	0.0258 0.1458 0.2342 0.2655 0.4856	0.0636 0.0259 0.0702 0.0002 0.0002	0.1397 0.0048 0.1008 0.1202 0.0059

<sup>\*</sup> indicates misclassified observations

Four of the five misclassifications for rootstock group 4 were incorrectly classified as belonging to rootstock group 1.

# 4

# ANOVA, MANOVA, and canonical correlations

There is a mathematical relationship between Fisher's LDA and one-way MANOVA. They are both based on the eigenvalues and eigenvectors of the same matrix,  $\mathbf{W}^{-1}\mathbf{B}$  (though in MANOVA the matrices are labeled  $\mathbf{E}$  and  $\mathbf{H}$  for error and hypothesis instead of  $\mathbf{W}$  and  $\mathbf{B}$  for within and between). See [MV] **manova** and [R] **anova** for more information on MANOVA and ANOVA. Researchers often wish to examine the MANOVA and univariate ANOVA results corresponding to their LDA model.

Canonical correlations are also mathematically related to Fisher's LDA. The canonical correlations between the discriminating variables and indicator variables constructed from the group variable are based on the same eigenvalues and eigenvectors as MANOVA and Fisher's LDA. The information from a canonical correlation analysis gives insight into the importance of each discriminant function in the discrimination. See [MV] canon for more information on canonical correlations.

The estat manova, estat anova, and estat canontest commands display MANOVA, ANOVA, and canonical correlation information after discrim lda.

# Example 2: MANOVA, ANOVA, and canonical correlation corresponding to LDA

Continuing with the apple tree rootstock example, we examine the MANOVA, ANOVA, and canonical correlation results corresponding to our LDA.

. estat manova

	Nτ	umber of obs	=	48					
	•••	= Wilks' la = Pillai's		L = Lawley-Hotelling trace R = Roy's largest root					
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F		
rootstock	W P L R	0.1540 1.3055 2.9214 1.8757	5	20.0 20.0 20.0 5.0	130.3 168.0 150.0 42.0	4.07 5.48	0.0000 0.0000 0.0000 0.0000	a	
Residual			42						
Total			47					_	

e = exact, a = approximate, u = upper bound on F

. estat anova

Univariate ANOVA summaries

Variable	Model MS	Resid MS	Total MS	R-sq	Adj. R-sq	F	Pr > F
y1 y2 y3 y4	4.1996621 6.1139358	.31998754 12.14279 4.2908128 1.7225248	11.297777 4.484762	0.2570 0.5876	0.1685 0.5385	2.9052 11.969	0.0243 0.0000

Number of obs = 48 Model df = 5 Residual df = 42

All four of the MANOVA tests reject the null hypothesis that the six rootstock groups have equal means. See example 1 of [MV] manova for an explanation of the MANOVA table.

estat anova presents a concise summary of univariate ANOVAs run on each of our four discriminating variables. Variables y3, trunk girth at 15 years, and y4, weight of tree above ground at 15 years, show the highest level of significance of the four variables.

estat canontest displays the canonical correlations and associated tests that correspond to our LDA model.

. estat canontest

Canonical linear discriminant analysis

Canon.	Eigen- value			Like- lihood Ratio	F	df1	df2	Prob>F
0.8076	1.87567	0.6421	0.6421	0.1540	4.9369	20	130.3	0.0000 a
				0.4429	3.1879			
0.4317	.229049	0.0784	0.9911	0.7931	1.6799	6	82	0.1363 e
0.1591	.025954	0.0089	1.0000	0.9747	.54503	2	42	0.5839 e
	0.8076 0.6645 0.4317	Corr. value  0.8076 1.87567 0.6645 .790694 0.4317 .229049	Corr.     value     Prop.       0.8076     1.87567     0.6421       0.6645     .790694     0.2707       0.4317     .229049     0.0784	Corr.         value         Prop.         Cumul.           0.8076         1.87567         0.6421         0.6421           0.6645         .790694         0.2707         0.9127           0.4317         .229049         0.0784         0.9911	Canon.         Eigen-value         Variance Prop.         lihood Ratio           0.8076         1.87567         0.6421         0.6421         0.1540           0.6645         .790694         0.2707         0.9127         0.4429           0.4317         .229049         0.0784         0.9911         0.7931	Canon.         Eigen-value         Variance Prop.         1ihood Ratio         F           0.8076         1.87567         0.6421         0.6421         0.1540         4.9369           0.6645         .790694         0.2707         0.9127         0.4429         3.1879           0.4317         .229049         0.0784         0.9911         0.7931         1.6799	Canon.         Eigen-Corr.         Variance Variance         lihood Ratio         F         df1           0.8076         1.87567         0.6421         0.6421         0.1540         4.9369         20           0.6645         .790694         0.2707         0.9127         0.4429         3.1879         12           0.4317         .229049         0.0784         0.9911         0.7931         1.6799         6	Canon.         Eigen-Corr.         Variance Value         1ihood Ratio         F         df1         df2           0.8076         1.87567         0.6421         0.6421         0.1540         4.9369         20         130.3           0.6645         .790694         0.2707         0.9127         0.4429         3.1879         12         106.1           0.4317         .229049         0.0784         0.9911         0.7931         1.6799         6         82

Ho: this and smaller canon. corr. are zero; e = exact F, a = approximate F

The number of nonzero eigenvalues in Fisher's LDA is  $\min(g-1,p)$  With g=6 groups, and p=4 discriminating variables, there are four nonzero eigenvalues. The four eigenvalues and the corresponding canonical correlations of  $\mathbf{W}^{-1}\mathbf{B}$ , ordered from largest to smallest, are reported along with the proportion and cumulative proportion of variance accounted for by each of the discriminant functions. Using one discriminant dimension is insufficient for capturing the variability of our four-dimensional data. With two dimensions we account for 91% of the variance. Using three of the four dimensions accounts for 99% of the variance. Little is gained from the fourth discriminant dimension.

Also presented are the likelihood-ratio tests of the null hypothesis that each canonical correlation and all smaller canonical correlations from this model are zero. The letter a is placed beside the p-values of the approximate F tests, and the letter e is placed beside the p-values of the exact F tests. The first two tests are highly significant, indicating that the first two canonical correlations are likely not zero. The third test has a p-value of 0.1363, so that we fail to reject that the third and fourth canonical correlation are zero.

4

#### Discriminant and classification functions

See [MV] discrim lda for a discussion of linear discriminant functions and linear classification functions for LDA.

Discriminant functions are produced from Fisher's LDA. The discriminant functions provide a set of transformations from the original p-dimensional (the number of discriminating variables) space to the minimum of p and g-1 (the number of groups minus 1) dimensional space. The discriminant functions are ordered in importance.

Classification functions are by-products of the Mahalanobis approach to LDA. There are always g classification functions—one for each group. They are not ordered by importance, and you cannot use a subset of them for classification.

A table showing the discriminant function coefficients is available with estat loadings (see example 3), and a table showing the classification function coefficients is available with estat classfunctions (see example 4).

#### Example 3: Canonical discriminant functions and canonical structures

We continue with the apple tree rootstock example. The canonical discriminant function coefficients (loadings) are available through the estat loadings command. Unstandardized, pooled within-group standardized, and total-sample standardized coefficients are available. The all option requests all three, and the format() option provides control over the numeric display format used in the tables.

. estat loadings, all format(%6.2f)

Canonical discriminant function coefficients

	func~1	func~2	func~3	func~4
y1	-3.05	-1.14	-1.00	23.42
y2	1.70	-1.22	1.67	-3.08
у3	-4.23	7.17	3.05	-2.01
у4	0.48	-11.52	-5.51	3.10
_cons	15.45	-12.20	-9.99	-12.47

Standardized canonical discriminant function coefficients

	func~1	func~2	func~3	func~4
y1	-0.27	-0.10	-0.09	2.04
у2	0.92	-0.65	0.90	-1.65
у3	-1.35	2.29	0.97	-0.64
у4	0.10	-2.33	-1.12	0.63

Total-sample standardized canonical discriminant function coefficients

	func~1	func~2	func~3	func~4
y1 y2 y3 y4	1.00 -1.99	-0.10 -0.72 3.37 -3.45	0.99 1.43	-1.81 -0.95

The unstandardized canonical discriminant function coefficients shown in the first table are the function coefficients that apply to the unstandardized discriminating variables—y1 through y4 and a constant term. See example 5 for a graph, known as a score plot, that plots the observations transformed by these unstandardized canonical discriminant function coefficients.

The standardized canonical discriminant function coefficients are the coefficients that apply to the discriminating variables after they have been standardized by the pooled within-group covariance. These coefficients are appropriate for interpreting the importance and relationship of the discriminating variables within the discriminant functions. See example 5 for a graph, known as a loading plot, that plots these standardized coefficients.

The total-sample standardized canonical discriminant function coefficients are the coefficients that apply to the discriminating variables after they have been standardized by the total-sample covariance. See *Methods and formulas* of [MV] **discrim lda** for references discussing which of within-group and total-sample standardization is most appropriate.

For both styles of standardization, variable y1 has small (in absolute value) coefficients for the first three discriminant functions. This indicates that y1 does not play an important part in these discriminant functions. Because the fourth discriminant function accounts for such a small percentage of the variance, we ignore the coefficients from the fourth function when assessing the importance of the variables.

Some sources, see Huberty (1994), advocate the interpretation of structure coefficients, which measure the correlation between the discriminating variables and the discriminant functions, instead of standardized discriminant function coefficients; see the discussion in example 1 of [MV] discrim lda for references to this dispute. The estat structure command displays structure coefficients.

. estat structure, format(%9.6f)

#### Canonical structure

	function1	function2	function3	function4
у3	-0.086765 -0.836986	-0.281362	0.898063 0.457902	0.006158 -0.103031
у4	-0.793621	-0.572890	0.162901	-0.124206

Using structure coefficients for interpretation, we conclude that y1 is important for the second and third discriminant functions.

4

# Example 4: LDA classification functions

Switching from Fisher's approach to LDA to Mahalanobis's approach to LDA, we examine what are called classification functions with the estat classfunctions command. Classification functions are applied to the unstandardized discriminating variables. The classification function that results in the largest value for an observation indicates the group to assign the observation.

Continuing with the rootstock LDA, we specify the format() option to control the display format of the classification coefficients.

. estat classfunctions, format(%8.3f)

Classification functions

	rootstock 1	2	3	4	5	6
y1 y2 y3	314.640 -59.417 149.610	317.120 -63.981 168.161	324.589 -65.152 154.910	307.260 -59.373 147.652	316.767 -65.826 168.221	311.301 -63.060 160.622
y4 _cons	-161.178 -301.590	-172.644	-150.356 -330.103	-153.387	-172.851	-175.477 -318.099
Priors	0.200	0.200	0.200	0.200	0.100	0.100

The prior probabilities, used in constructing the coefficient for the constant term, are displayed as the last row in the table. We did not specify the priors() option, so the prior probabilities defaulted to those in our LDA model, which has rootstock group 5 and 6 with prior probabilities of 0.1, whereas the other groups have prior probabilities of 0.2.

See example 10 for applying the classification function to data by using the predict command.

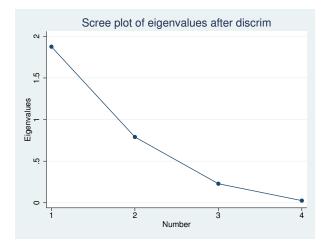
# Scree, loading, and score plots

Examples of discriminant function loading plots and score plots (see [MV] scoreplot) can be found in example 3 of [MV] discrim lda and example 1 of [MV] candisc. Also available after discrim lda are scree plots; see [MV] screeplot.

# Example 5: Scree, loading, and score plots

Continuing with our rootstock example, the scree plot of the four nonzero eigenvalues we previously saw in the output of estat canontest in example 2 are graphed using the screeplot command.

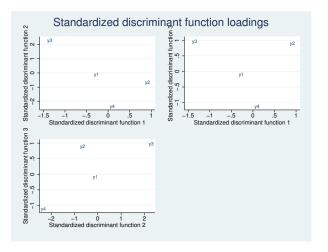
. screeplot



The Remarks and examples in [MV] screeplot concerning the use of scree plots for selecting the number of components in the context of pca apply also for selecting the number of discriminant functions after discrim lda. With these four eigenvalues, it is not obvious whether to choose the top two or three eigenvalues. From the estat canontest output of example 2, the first two discriminant functions account for 91% of the variance, and three discriminant functions account for 99% of the variance.

The loadingplot command (see [MV] scoreplot) allows us to graph the pooled within-group standardized discriminant coefficients (loadings) that we saw in tabular form from the estat loadings command of example 3. By default only the loadings from the first two functions are graphed. We override this setting with the components(3) option, obtaining graphs of the first versus second, first versus third, and second versus third function loadings. The combined option switches from a matrix graph to a combined graph. The msymbol(i) option removes the plotting points, leaving the discriminating variable names in the graph, and the option mlabpos(0) places the discriminating variable names in the positions of the plotted points.

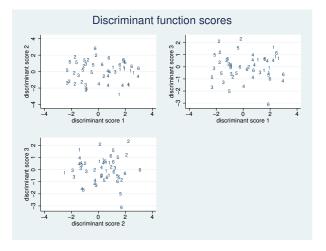
. loadingplot, components(3) combined msymbol(i) mlabpos(0)



Variable y1, trunk girth at 4 years, is near the origin in all three graphs, indicating that it does not play a strong role in discriminating among our six rootstock groups. y4, weight of tree above ground at 15 years, does not play much of a role in the first discriminant function but does in the second and third discriminant functions.

The corresponding three score plots are easily produced with the scoreplot command; see [MV] scoreplot. Score plots graph the discriminant function—transformed observations (called scores).

. scoreplot, components(3) combined msymbol(i)



There is a lot of overlap, but some separation of the rootstock groups is apparent. One of the observations from group 6 seems to be sitting by itself in the bottom of the two graphs that have discriminant function 3 as the y axis. In example 11, we identify this point by using the predict command.

1

#### Means and distances

The estat grsummarize command is available after all discrim commands and will display means, medians, minimums, maximums, standard deviations, group sizes, and more for the groups; see [MV] discrim estat. After discrim 1da, the estat grmeans command will also display group means. It, however, has options for displaying the within-group standardized group means, the totalsample standardized group means, and the canonical discriminant functions evaluated at the group means.

#### Example 6: Standardized group means and canonical discriminant functions at the means

We introduce the estat grmeans command with the iris data originally from Anderson (1935), introduced in example 3 of [MV] discrim lda.

```
. use http://www.stata-press.com/data/r14/iris
(Iris data)
```

. discrim lda seplen sepwid petlen petwid, group(iris) notable

The notable option of discrim suppressed the classification table.

By default, estat grmeans displays a table of the means of the discriminating variables for each group. You could obtain the same information along with other statistics with the estat grsummarize command: see [MV] discrim estat.

. estat grmeans Group means

	iris setosa	versico~r	virginica
seplen	5.006	5.936	6.588
sepwid	3.428	2.77	2.974
petlen	1.462	4.26	5.552
petwid	.246	1.326	2.026

Differences in the iris species can be seen within these means. For instance, the petal lengths and widths of the *Iris setosa* are smaller than those of the other two species. See example 1 of [MV] **discrim estat** for further exploration of these differences.

The main purpose of estat grmeans is to present standardized or transformed means. The totalstd and withinstd options request the two available standardizations.

. estat grmeans, totalstd withinstd Total-sample standardized group means

	iris setosa	versico~r	virginica
seplen	-1.011191	.1119073	.8992841
sepwid	.8504137	6592236	1911901
petlen	-1.30063	.2843712	1.016259
petwid	-1.250704	.1661774	1.084526

Pooled within-group standardized group means

	iris setosa	versico~r	virginica
seplen	-1.626555	.1800089	1.446546
sepwid	1.091198	8458749	2453234
petlen	-5.335385	1.166534	4.16885
petwid	-4.658359	.6189428	4.039416

The first table presents the total-sample standardized group means on the discriminating variables. These are the means for each group on the total-sample standardized discriminating variables.

The second table presents the pooled within-group standardized means on the discriminating variables. Instead of using the total-sample variance, the pooled within-group variance is used to standardize the variables. Of most interest in the context of an LDA is the within-group standardization.

The canonical option of estat grmeans displays the discriminant functions evaluated at the group means and gives insight into what the functions do to the groups.

. estat grmeans, canonical Group means on canonical variables

iris	function1	function2
setosa	-7.6076	215133
versicolor	1.825049	.7278996
virginica	5.78255	5127666

The first function places *Iris setosa* strongly negative and *Iris virginica* strongly positive with *Iris versicolor* in between. The second function places *Iris virginica* and *Iris setosa* negative and *Iris versicolor* positive.

1

The Mahalanobis distance between the groups in an LDA helps in assessing which groups are similar and which are different.

#### Example 7: Mahalanobis distance between groups

Continuing with the iris example, we use the estat grdistances command to view the squared Mahalanobis distances between the three iris species.

. estat grdistances

Mahalanobis squared distances between groups

iris	iris setosa	versicolor	virginica
setosa	0		
versicolor	89.864186	0	
virginica	179.38471	17.201066	0

*Iris setosa* is farthest from *Iris virginica* with a squared Mahalanobis distance of 179. *Iris versicolor* and *Iris virginica* are closest with a squared Mahalanobis distance of 17.

Are these distances significant? Requesting F statistics and p-values associated with these Mahalanobis squared distances between means will help answer that question. The mahalanobis() option requests F tests, p-values, or both.

. estat grdistances, mahalanobis(f p)

Mahalanobis squared distances between groups

Key	
Mahalanobis squared F with 4 and 144 df p-value	distance

iris	iris setosa	versicolor	virginica
setosa	0 0 1		
versicolor	89.864186 550.18889 3.902e-86	0 0 1	
virginica	179.38471 1098.2738 9.20e-107	17.201066 105.31265 9.515e-42	0 0 1

All three of the means are statistically significantly different from one another.

The generalized squared distance between groups starts with the Mahalanobis squared distance between groups and adjusts for prior probabilities when they are not equal. With equal prior probabilities there will be no difference between the generalized squared distance and Mahalanobis squared distance. The priors() option specifies the prior probabilities for calculating the generalized squared distances.

To illustrate, we select prior probabilities of 0.2 for *I. setosa*, 0.3 for *I. versicolor*, and 0.5 for *I. virginica*.

. estat grdistances, generalized priors(.2, .3, .5) Generalized squared distances between groups

iris	iris setosa	versicolor	virginica
setosa	3.2188758	92.272131	180.77101
versicolor	93.083061	2.4079456	18.587361
virginica	182.60359	19.609012	1.3862944

This matrix is not symmetric and does not have zeros on the diagonal.

1

#### Covariance and correlation matrices

Equal group covariance matrices is an important assumption underlying LDA. The estat covariance command displays the group covariance matrices, the pooled within-group covariance matrix, the between-groups covariance matrix, and the total-sample covariance matrix. The estat correlation command provides the corresponding correlation matrices, with an option to present *p*-values with the correlations.

### Example 8: Group covariances and correlations

Continuing our examination of LDA on the iris data, we request to see the pooled within-group covariance matrix and the covariance matrices for the three iris species.

. estat covariance, within groups
Pooled within-group covariance matrix

	seplen	sepwid	petlen	petwid
seplen sepwid petlen petwid	.2650082 .0927211 .1675143 .0384014	.1153878 .0552435 .0327102	.1851878	.0418816
Poomia	.0001011	.0021102	.0120000	.0110010

Group covariance matrices

petwid

iris: setosa

		seplen	sepwid	petlen	petwid
	seplen	.124249			
	sepwid	.0992163	.1436898		
	petlen	.0163551	.011698	.0301592	
	petwid	.0103306	.009298	.0060694	.0111061
iris:	versicolor	•			
		seplen	sepwid	petlen	petwid
	seplen	. 2664327			
	sepwid	.0851837	.0984694		
	petlen	.182898	.0826531	.2208163	
	petwid	.0557796	.0412041	.073102	.0391061
iris:	virginica				
		seplen	sepwid	petlen	petwid
	seplen	.4043429			
	sepwid	.0937633	.1040041		
	petlen	.3032898	.0713796	.3045878	
	r - 32-022				

.0476286

.0488245

.0754327

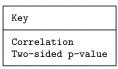
.0490939

All variables have positive covariance—not surprising for physical measurements (length and width).

We could have requested the between-groups covariance matrix and the total-sample covariance matrix. Options of estat covariance control how the covariance matrices are displayed.

Correlation matrices are also easily displayed. With estat correlations we show the pooled within-group correlation matrix, and add the p option to request display of p-values with the correlations. The p-values help us evaluate whether the correlations are statistically significant.

. estat corr, p
Pooled within-group correlation matrix



	seplen	sepwid	petlen	petwid
seplen	1.00000			
sepwid	0.53024 0.00000	1.00000		
petlen	0.75616 0.00000	0.37792 0.00000	1.00000	
petwid	0.36451 0.00001	0.47053 0.00000	0.48446 0.00000	1.00000

All correlations are statistically significant. The largest correlation is between the petal length and the sepal length.

1

#### **Predictions**

The predict command after discrim lda has options for obtaining classifications, probabilities, Mahalanobis squared distances from observations to group means, and the leave-one-out (LOO) estimates of all of these. You can also obtain the discriminant scores and classification scores for observations. The predictions can be obtained in or out of sample.

# Example 9: Out-of-sample LDA classification and probabilities

We use the riding-mower data from Johnson and Wichern (2007) introduced in example 1 of [MV] **discrim** to illustrate out-of-sample prediction of classification and probabilities after an LDA.

- . use http://www.stata-press.com/data/r14/lawnmower2 (Johnson and Wichern (2007) Table 11.1)
- . discrim lda lotsize income, group(owner) notable

Now we see how the LDA model classifies observations with income of \$90,000, \$110,000, and \$130,000, each with a lot size of 20,000 square feet. We add 3 observations to the bottom of our dataset containing these values and then use predict to obtain the classifications and probabilities.

. input

```
owner income lots~e
```

25. . 90 20

26. . 110 20

27. . 130 20

28. end

. predict grp in 25/L, class (24 missing values generated)

. predict pr\* in 25/L, pr

(24 missing values generated)

. list in 25/L

	owner income lot		lotsize	grp	pr1	pr2
25.		90.0	20.0	0	.5053121	.4946879
26.		110.0	20.0	1	.1209615	.8790385
27.		130.0	20.0	1	.0182001	.9818

The observation with income of \$90,000 was classified as a nonowner, but it was a close decision with probabilities of 0.505 for nonowner and 0.495 for owner. The two other observations, with \$110,000 and \$130,000 income, were classified as owners, with higher probability of ownership for the higher income.

4

The estat list, estat classtable, and estat errorrate commands (see [MV] **discrim estat**) obtain their information by calling predict. The LOO listings and tables from these commands are obtained by calling predict with the looclass and loopr options.

In addition to predictions and probabilities, we can obtain the classification scores for observations.

# Example 10: Classification scores

In example 4, we used the estat classfunctions command to view the classification functions for the LDA of the apple tree rootstock data. We can use predict to obtain the corresponding classification scores—the classification function applied to observations.

- . use http://www.stata-press.com/data/r14/rootstock, clear (Table 6.2 Rootstock Data, Rencher and Christensen (2012))
- . discrim lda y1 y2 y3 y4, group(rootstock) priors(.2,.2,.2,.2,.1,.1) notable
- . predict clscr\*, clscore
- . format clscr\* %6.1f
- . list rootstock clscr\* in 1/3, noobs

rootst~k	clscr1	clscr2	clscr3	clscr4	clscr5	clscr6
1	308.1	303.7	303.1	307.1	303.5	307.1
1	327.6	324.1	322.9	326.1	323.3	326.0
1	309.5	308.2	306.3	309.3	307.5	309.0

We did not specify the priors() option, so predict used the prior probabilities that were specified with our LDA model in determining the constant term in the classification function; see example 4 for a table of the classification functions. Observations may be classified to the group with

largest score. The first 3 observations belong to rootstock group 1 and are successfully classified as belonging to group 1 because the classification score in clscr1 is larger than the classification scores for the other groups.

4

Scoring the discriminating variables by using Fisher's canonical discriminant functions is accomplished with the dscore option of predict.

### Example 11: Scoring the discriminant variables

Using the rootstock data in example 5, we noticed 1 observation, from group 6, near the bottom of the score plot where the third discriminant function was the y axis. The observation has a score for the third discriminant function that appears to be below -3. We will use the dscore option of predict to find the observation.

- . predict ds\*, dscore
- . format ds\* %5.0g
- . list rootstock y\* ds\* if ds3 < -3

	rootst~k	у1	у2	у3	у4	ds1	ds2	ds3	ds4
42.	6	0.75	0.840	3.14	0.606	1.59	1.44	-3.11	-1.93

Observation 42 is the one producing that third discriminant score.

4

# Stored results

estat anova stores the following in r():

Scalars

r(N) number of observations r(df\_m) model degrees of freedom r(df\_r) residual degrees of freedom

Matrices

r(anova\_stats) ANOVA statistics for the model

estat canontest stores the following in r():

Scalars

r(N) number of observations r(N\_groups) number of groups r(k) number of variables

r(f) number of canonical discriminant functions

Matrices

r(stat) canonical discriminant statistics

estat classfunction stores the following in r():

Matrices

r(C) classification function matrix r(priors) group prior probabilities

#### estat correlations stores the following in r():

```
Matrices
    r(Rho)
                          pooled within-group correlation matrix (within only)
    r(P)
                          two-sided p-values for pooled within-group correlations (within and p only)
    r(Rho_between)
                          between-groups correlation matrix (between only)
    r(P_between)
                          two-sided p-values for between-groups correlations (between and p only)
    r(Rho_total)
                          total-sample correlation matrix (total only)
    r(P_total)
                          two-sided p-values for total-sample correlations (total and p only)
    r(Rho_#)
                          group # correlation matrix (groups only)
    r(P_#)
                          two-sided p-values for group # correlations (groups and p only)
estat covariance stores the following in r():
Matrices
    r(S)
                          pooled within-group covariance matrix (within only)
    r(S_between)
                          between-groups covariance matrix (between only)
    r(S_total)
                          total-sample covariance matrix (total only)
    r(S_#)
                          group # covariance matrix (groups only)
estat grdistances stores the following in r():
Scalars
    r(df1)
                          numerator degrees of freedom (mahalanobis only)
    r(df2)
                          denominator degrees of freedom (mahalanobis only)
Matrices
                          Mahalanobis squared distances between group means (mahalanobis only)
    r(sqdist)
    r(F_sqdist)
                          F statistics for tests that the Mahalanobis squared distances between group means
                            are zero (mahalanobis only)
    r(P_sqdist)
                          p-value for tests that the Mahalanobis squared distances between group means are
                            zero (mahalanobis only)
                          generalized squared distances between group means (generalized only)
    r(gsqdist)
estat grmeans stores the following in r():
Matrices
    r(means)
                          group means (raw only)
    r(stdmeans)
                          total-sample standardized group means (totalstd only)
    r(wstdmeans)
                          pooled within-group standardized group means (withinstd only)
    r(cmeans)
                          group means on canonical variables (canonical only)
estat loadings stores the following in r():
Matrices
    r(L_std)
                          within-group standardized canonical discriminant function coefficients
                            (standardized only)
                          total-sample standardized canonical discriminant function coefficients
    r(L_totalstd)
                            (totalstandardized only)
                          unstandardized canonical discriminant function coefficients
    r(L_unstd)
                            (unstandardized only)
estat manova stores the following in r():
```

Scalars	
r(N)	number of observations
$r(df_m)$	model degrees of freedom
$r(df_r)$	residual degrees of freedom
Matrices	
r(stat_m)	multivariate statistics for the model

#### Methods and formulas

See Methods and formulas of [MV] discrim Ida for background on what is produced by predict, estat classfunctions, estat grdistances, estat grmeans, estat loadings, and estat structure. See [MV] discrim estat for more information on estat classtable, estat errorrate, estat grsummarize, and estat list. See [R] anova for background information on the ANOVAs summarized by estat anova; see [MV] manova for information on the MANOVA shown by estat manova; and see [MV] canon for background information on canonical correlations and related tests shown by estat canontest.

### References

Anderson, E. 1935. The irises of the Gaspe Peninsula. Bulletin of the American Iris Society 59: 2-5.

Andrews, D. F., and A. M. Herzberg, ed. 1985. Data: A Collection of Problems from Many Fields for the Student and Research Worker. New York: Springer.

Huberty, C. J. 1994. Applied Discriminant Analysis. New York: Wiley.

Johnson, R. A., and D. W. Wichern. 2007. Applied Multivariate Statistical Analysis. 6th ed. Englewood Cliffs, NJ: Prentice Hall.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.

#### Also see

- [MV] discrim lda Linear discriminant analysis
- [MV] **discrim estat** Postestimation tools for discrim
- [MV] **scoreplot** Score and loading plots
- [MV] screeplot Scree plot
- [MV] candisc Canonical linear discriminant analysis
- [MV] canon Canonical correlations
- [MV] discrim Discriminant analysis
- [MV] manova Multivariate analysis of variance and covariance
- [U] 20 Estimation and postestimation commands

#### **Title**

discrim logistic — Logistic discriminant analysis

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

## **Description**

discrim logistic performs logistic discriminant analysis. See [MV] discrim for other discrimination commands.

### **Quick start**

```
Logistic discriminant analysis of v1, v2, v3, and v4 for groups defined by catvar discrim logistic v1 v2 v3 v4, group(catvar)
```

```
As above, but use prior probabilities that are proportional to group size discrim logistic v1 v2 v3 v4, group(catvar) /// priors(proportional)
```

```
As above, but suppress iteration log
discrim logistic v1 v2 v3 v4, group(catvar) ///
priors(proportional) nolog
```

#### Menu

 ${\it Statistics} > {\it Multivariate analysis} > {\it Discriminant analysis} > {\it Logistic}$ 

### **Syntax**

discrim logistic varlist [if] [in] [weight], group(groupvar) [options]

options	Description	
Model		
*group(groupvar)	variable specifying the groups	
_ priors( <i>priors</i> )	group prior probabilities	
$\overline{\mathtt{tie}}$ s (ties)	how ties in classification are to be handled	
Reporting		
<u>not</u> able	suppress resubstitution classification table	
nolog	suppress the mlogit log-likelihood iteration log	
priors	Description	
equal	equal prior probabilities; the default	
 proportional	group-size-proportional prior probabilities	
matname	row or column vector containing the group prior probabilities	
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities	
ties	Description	
	Bescription	
$\underline{\mathtt{m}}$ issing	ties in group classification produce missing values; the default	
$\underline{\mathtt{r}}\mathtt{andom}$	ties in group classification are broken randomly	
<u>f</u> irst	ties in group classification are set to the first tied group	

<sup>\*</sup>group() is required.

statsby and xi are allowed; see [U] 11.1.10 Prefix commands.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

### **Options**

Model

group(groupvar) is required and specifies the name of the grouping variable. groupvar must be a numeric variable.

priors(priors) specifies the prior probabilities for group membership. The following priors are allowed:

priors(equal) specifies equal prior probabilities. This is the default.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties (ties) specifies how ties in group classification will be handled. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values. This is the default.

ties (random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

Reporting

notable suppresses the computation and display of the resubstitution classification table. nolog suppress the mlogit log-likelihood iteration log.

### Remarks and examples

Albert and Lesaffre (1986) explain that logistic discriminant analysis is a partially parametric method falling between parametric discrimination methods such as LDA and QDA (see [MV] discrim lda and [MV] discrim qda) and nonparametric discrimination methods such as kth-nearest-neighbor (KNN) discrimination (see [MV] discrim knn). Albert and Harris (1987) provide a good explanation of logistic discriminant analysis. Instead of making assumptions about the distribution of the data within each group, logistic discriminant analysis is based on the assumption that the likelihood ratios of the groups have an exponential form; see Methods and formulas. Multinomial logistic regression provides the basis for logistic discriminant analysis; see [R] mlogit. Multinomial logistic regression can handle binary and continuous regressors, and hence logistic discriminant analysis is also appropriate for binary and continuous discriminating variables.

### Example 1: A two-group logistic discriminant analysis

Morrison (2005, 443–445) provides data on 12 subjects with a senile-factor diagnosis and 37 subjects with a no-senile-factor diagnosis. The data consist of the Wechsler Adult Intelligence Scale (WAIS) subtest scores for information, similarities, arithmetic, and picture completion. Morrison (2005, 231) performs a logistic discriminant analysis on the two groups, using the similarities and picture completion scores as the discriminating variables.

```
. use http://www.stata-press.com/data/r14/senile
(Senility WAIS subtest scores)
```

. discrim logistic sim pc, group(sf) priors(proportional)

```
Iteration 0: log likelihood = -27.276352
Iteration 1: log likelihood = -19.531198
Iteration 2: log likelihood = -19.036702
Iteration 3: log likelihood = -19.018973
Iteration 4: log likelihood = -19.018928
```

Logistic discriminant analysis

Resubstitution classification summary

Key
Number Percent

True sf	Classif No-SF	ied SF	Total
No-SF	37 100.00	0.00	37 100.00
SF	6 50.00	6 50.00	12 100.00
Total	43 87.76	6 12.24	49 100.00
Priors	0.7551	0.2449	

We specified the priors (proportional) option to obtain proportional prior probabilities for our logistic classification. These results match those of Morrison (2005, 231), though he does not state that his results are based on proportional prior probabilities. If you change to equal prior probabilities you obtain different classification results.

Which observations were misclassified? estat list with the misclassified option shows the six misclassified observations and the estimated probabilities.

. estat list, misclassified varlist

	Data		Classification		Probabilities	
Obs.	sim	pc	True	Class.	No-SF	SF
38 41 44 46 48	5 7 9 7 10	8 9 8 6 3	SF SF SF SF	No-SF * No-SF * No-SF * No-SF *	0.7353 0.8677 0.8763 0.6697 0.5584	0.2647 0.1323 0.1237 0.3303 0.4416
49	12	10	SF	No-SF *	0.9690	0.0310

<sup>\*</sup> indicates misclassified observations

See example 1 of [MV] discrim logistic postestimation for more postestimation analysis with this logistic discriminant analysis.

### Example 2: A three-group logistic discriminant analysis

Example 2 of [MV] **discrim knn** introduces a head measurement dataset with six discriminating variables and three groups; see Rencher and Christensen (2012, 290–292). We now apply discrim logistic to see how well the logistic model can discriminate between the groups.

```
. use http://www.stata-press.com/data/r14/head
(Table 8.3 Head measurements, Rencher and Christensen (2012))
. discrim logistic wdim circum fbeye eyehd earhd jaw, group(group)
Iteration 0: log likelihood = -98.875106
             log likelihood = -60.790737
Iteration 1:
Iteration 2:
              log likelihood = -53.746934
              log likelihood = -51.114631
Iteration 3:
Iteration 4:
              log likelihood = -50.249426
Iteration 5:
              log\ likelihood = -50.081199
Iteration 6:
              log\ likelihood = -50.072248
Iteration 7:
              log\ likelihood = -50.072216
```

Resubstitution classification summary

Key

Logistic discriminant analysis

Key
Number
Percent

True group	Classified high school	college	nonplayer	Total
high school	27	2	1	30
	90.00	6.67	3.33	100.00
college	1	20	9	30
	3.33	66.67	30.00	100.00
nonplayer	2	8	20	30
	6.67	26.67	66.67	100.00
Total	30	30	30	90
	33.33	33.33	33.33	100.00
Priors	0.3333	0.3333	0.3333	

The counts on the diagonal of the resubstitution classification table are similar to those obtained by discrim knn (see example 2 of [MV] discrim knn) and discrim lda (see example 1 of [MV] candisc), whereas discrim qda seems to have classified the nonplayer group more accurately (see example 3 of [MV] discrim estat).

#### Stored results

discrim logistic stores the following in e():

```
Scalars
    e(N)
                          number of observations
    e(N_groups)
                          number of groups
    e(k)
                          number of discriminating variables
    e(ibaseout)
                          base outcome number
Macros
    e(cmd)
                          discrim
    e(subcmd)
                          logistic
    e(cmdline)
                          command as typed
                          name of group variable
    e(groupvar)
    e(grouplabels)
                          labels for the groups
    e(varlist)
                          discriminating variables
    e(dropped)
                          variables dropped because of collinearity
    e(wtype)
                          weight type
    e(wexp)
                          weight expression
    e(title)
                          title in estimation output
                          how ties are to be handled
    e(ties)
    e(properties)
                          b noV
                          program used to implement estat
    e(estat_cmd)
    e(predict)
                          program used to implement predict
    e(marginsnotok)
                          predictions disallowed by margins
Matrices
    e(b)
                          coefficient vector
    e(groupcounts)
                          number of observations for each group
    e(grouppriors)
                          prior probabilities for each group
    e(groupvalues)
                          numeric value for each group
Functions
    e(sample)
                          marks estimation sample
```

### Methods and formulas

Let g be the number of groups,  $n_i$  the number of observations for group i, and  $q_i$  the prior probability for group i. Let x denote an observation measured on p discriminating variables. For consistency with the discriminant analysis literature, x will be a column vector, though it corresponds to a row in your dataset. Let  $f_i(\mathbf{x})$  represent the density function for group i, and let  $P(\mathbf{x}|G_i)$  denote the probability of observing x conditional on belonging to group i. Denote the posterior probability of group i given observation x as  $P(G_i|\mathbf{x})$ . With Bayes's theorem, we have

$$P(G_i|\mathbf{x}) = \frac{q_i f_i(\mathbf{x})}{\sum_{j=1}^g q_j f_j(\mathbf{x})}$$

Substituting  $P(\mathbf{x}|G_i)$  for  $f_i(\mathbf{x})$ , we have

$$P(G_i|\mathbf{x}) = \frac{q_i P(\mathbf{x}|G_i)}{\sum_{j=1}^g q_j P(\mathbf{x}|G_j)}$$

Dividing both the numerator and denominator by  $P(\mathbf{x}|G_q)$ , we can express this as

$$P(G_i|\mathbf{x}) = \frac{q_i L_{ig}(\mathbf{x})}{\sum_{j=1}^g q_j L_{jg}(\mathbf{x})}$$

where  $L_{ig}(\mathbf{x}) = P(\mathbf{x}|G_i)/P(\mathbf{x}|G_g)$  is the likelihood ratio of  $\mathbf{x}$  for groups i and g.

This formulation of the posterior probability allows easy insertion of the Multinomial logistic model into the discriminant analysis framework. The multinomial logistic model expresses  $L_{ig}(\mathbf{x})$  in a simple exponential form

$$L_{ig}(\mathbf{x}) = \exp(a_{0i} + \mathbf{a}_i'\mathbf{x})$$

see Albert and Harris (1987, 117). Logistic discriminant analysis uses mlogit to compute the likelihood ratios,  $L_{ig}(\mathbf{x})$ , and hence the posterior probabilities  $P(G_i|\mathbf{x})$ ; see [R] mlogit. However, mlogit and predict after mlogit assume proportional prior probabilities. discrim logistic assumes equal prior probabilities unless you specify the priors(proportional) option.

#### References

Albert, A., and E. K. Harris. 1987. Multivariate Interpretation of Clinical Laboratory Data. New York: Dekker.

Albert, A., and E. Lesaffre. 1986. Multiple group logistic discrimination. *Computers and Mathematics with Applications* 12A(2): 209–224.

Morrison, D. F. 2005. Multivariate Statistical Methods. 4th ed. Belmont, CA: Duxbury.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.

### Also see

- [MV] discrim logistic postestimation Postestimation tools for discrim logistic
- [MV] **discrim** Discriminant analysis
- [R] logistic Logistic regression, reporting odds ratios
- [R] **mlogit** Multinomial (polytomous) logistic regression
- [U] 20 Estimation and postestimation commands

### **Title**

discrim logistic postestimation — Postestimation tools for discrim logistic

Postestimation commands predict Remarks and examples Reference Also see

### **Postestimation commands**

The following postestimation commands are of special interest after discrim logistic:

Description
classification table
classification error-rate estimation
group summaries
classification listing
estimation sample summary

The following standard postestimation commands are also available:

Command	Description
* estimates	cataloging estimation results
predict	group classification and posterior probabilities

<sup>\*</sup> All estimates subcommands except table and stats are available; see [R] estimates.

### predict

### **Description for predict**

predict creates a new variable containing predictions such as group classifications and probabilities.

### Menu for predict

Statistics > Postestimation

### Syntax for predict

predict [type] no	ewvar [if] [in] [, statistic options]
$\mathtt{predict}  \left[  type  \right]  \left\{ \right.$	stub*   newvarlist } [if] [in] [, statistic options]
statistic	Description
Main	
$\underline{c}$ lassification	group membership classification; the default when one variable is specified and group() is not specified
<u>p</u> r	probability of group membership; the default when group() is specified or when multiple variables are specified
options	Description
Main	
<pre>group(group)</pre>	the group for which the statistic is to be calculated
Options	
<pre>pri ors (priors)</pre>	group prior probabilities; defaults to e(grouppriors)
ties(ties)	how ties in classification are to be handled; defaults to e(ties)
priors	Description
equal	equal prior probabilities
 proportional	group-size-proportional prior probabilities
matname	row or column vector containing the group prior probabilities
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities
ties	Description
missing	ties in group classification produce missing values
<u>r</u> andom	ties in group classification are broken randomly
$\underline{ extsf{f}}$ irst	ties in group classification are set to the first tied group

You specify one new variable with classification and specify either one or e(N\_groups) new variables with pr. group() is not allowed with classification.

### **Options for predict**

Main

classification, the default, calculates the group classification. Only one new variable may be specified.

pr calculates group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.

group(group) specifies the group for which the statistic is to be calculated and can be specified
using

#1, #2, ..., where #1 means the first category of the e(groupvar) variable, #2 the second category, etc.;

the values of the e(groupvar) variable; or

the value labels of the e(groupvar) variable if they exist.

group() is not allowed with classification.

Options

priors (*priors*) specifies the prior probabilities for group membership. If priors () is not specified, e(grouppriors) is used. The following *priors* are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) is used. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values.

ties (random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

### Remarks and examples

Classifications and probabilities after discrim logistic are obtained with the predict command. The common estat subcommands after discrim are also available for producing classification tables, error-rate tables, classification listings, and group summaries; see [MV] discrim estat.

### Example 1: Error rates and predictions for logistic discriminant analysis

Continuing with our logistic discriminant analysis of the senility dataset of Morrison (2005), introduced in example 1 of [MV] **discrim logistic**, we illustrate the use of the estat errorrate postestimation command.

. use http://www.stata-press.com/data/r14/senile
(Senility WAIS subtest scores)

- . discrim logistic sim pc, group(sf) priors(proportional) notable nolog
- . estat errorrate, pp

Error rate estimated from posterior probabilities

Error Rate	sf No-SF	SF	Total
Stratified	.0305051	.5940575	.168518
Unstratified	.0305051	.5940575	.168518
Priors	.755102	. 244898	

We specified the pp option to obtain the posterior probability—based error-rate estimates. The stratified and unstratified estimates are identical because proportional priors were used. The estimates were based on proportional priors because the logistic discriminant analysis model used proportional priors and we did not specify the priors() option in our call to estat errorrate.

The error-rate estimate for the senile-factor group is much higher than for the no-senile-factor group.

What error-rate estimates would we obtain with equal group priors?

. estat errorrate, pp priors(equal)

Error rate estimated from posterior probabilities

	sf		
Error Rate	No-SF	SF	Total
Stratified	.2508207	.2069481	.2288844
Unstratified	.06308	.4289397	.2460098
Priors	.5	.5	

Stratified and unstratified estimates are now different. This happens when group sizes have a different proportion from that of the prior probabilities.

Morrison (2005, 231) shows a classification of the subjects where, if the estimated probability of belonging to the senile-factor group is less than 0.35, he classifies the subject to the no-senile-factor group; if the probability is more than 0.66, he classifies the subject to the senile-factor group; and if the probability is between those extremes, he classifies the subject to an uncertain group.

We can use predict to implement this same strategy. The pr option requests probabilities. Because the model was estimated with proportional prior probabilities, the prediction, by default, will also be based on proportional prior probabilities.

- . predict prob0 prob1, pr
- . generate newgrp = 1
- . replace newgrp = 0 if prob1 <= 0.35</pre> (38 real changes made)
- . replace newgrp = 2 if prob1 >= 0.66 (5 real changes made)
- . label define newgrp 0 "No-SF" 1 "Uncertain" 2 "SF"
- . label values newgrp newgrp
- . tabulate sf newgrp

Senile-fac tor		newgrp		
diagnosis	No-SF	Uncertain	SF	Total
No-SF	33	4	0	37
SF	5	2	5	12
Total	38	6	5	49

Six observations are placed in the uncertain group.

Reference

Morrison, D. F. 2005. Multivariate Statistical Methods. 4th ed. Belmont, CA: Duxbury.

### Also see

- [MV] discrim logistic Logistic discriminant analysis
- [MV] discrim estat Postestimation tools for discrim
- [MV] discrim Discriminant analysis
- [U] 20 Estimation and postestimation commands

#### **Title**

discrim qda — Quadratic discriminant analysis

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

## **Description**

discrim qda performs quadratic discriminant analysis. See [MV] discrim for other discrimination commands.

### **Quick start**

Quadratic discriminant analysis of v1, v2, v3, and v4 for groups defined by catvar discrim qda v1 v2 v3 v4, group(catvar)

As above, but use prior probabilities proportional to group size discrim qda v1 v2 v3 v4, group(catvar) priors(proportional)

Display the leave-one-out and the resubstitution classification tables discrim qda v1 v2 v3 v4, group(catvar) lootable

As above, but suppress the resubstitution classification table discrim qda v1 v2 v3 v4, group(catvar) lootable notable

### Menu

Statistics > Multivariate analysis > Discriminant analysis > Quadratic (QDA)

### **Syntax**

discrim qda varlist [if] [in] [weight], group(groupvar) [options]

options	Description		
Model			
group( <i>groupvar</i> )	variable specifying the groups		
priors(priors)	group prior probabilities		
ties (ties)	how ties in classification are to be handled		
Reporting			
<u>not</u> able	suppress resubstitution classification table		
<u>loo</u> table	display leave-one-out classification table		
priors	Description		
equal	equal prior probabilities; the default		
 proportional	group-size-proportional prior probabilities		
matname	row or column vector containing the group prior probabilities		
matrix_exp	matrix expression providing a row or column vector of the group prior probabilities		
ties	Description		
missing	ties in group classification produce missing values; the default		
$\underline{\mathtt{r}}\mathtt{andom}$	ties in group classification are broken randomly		
first	ties in group classification are set to the first tied group		

<sup>\*</sup>group() is required.

statsby and xi are allowed; see [U] 11.1.10 Prefix commands.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

### **Options**

Model

group(groupvar) is required and specifies the name of the grouping variable. groupvar must be a numeric variable.

priors(priors) specifies the prior probabilities for group membership. The following priors are allowed:

priors (equal) specifies equal prior probabilities. This is the default.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors(matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties (ties) specifies how ties in group classification will be handled. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values. This is the default.

ties(random) specifies that ties in group classification are broken randomly.

ties(first) specifies that ties in group classification are set to the first tied group.

Reporting

notable suppresses the computation and display of the resubstitution classification table.

lootable displays the leave-one-out classification table.

### Remarks and examples

Quadratic discriminant analysis (QDA) was introduced by Smith (1947). It is a generalization of linear discriminant analysis (LDA). Both LDA and QDA assume that the observations come from a multivariate normal distribution. LDA assumes that the groups have equal covariance matrices. QDA removes this assumption, allowing the groups to have different covariance matrices.

One of the penalties associated with QDA's added flexibility is that if any groups have fewer observations,  $n_i$ , than discriminating variables, p, the covariance matrix for that group is singular and QDA cannot be performed. Even if there are enough observations to invert the covariance matrix, if the sample size is relatively small for a group, the estimation of the covariance matrix for that group may not do a good job of representing the group's population covariance, leading to inaccuracies in classification.

### > Example 1: QDA classification tables and error rates

We illustrate QDA with a small dataset introduced in example 1 of [MV] manova. Andrews and Herzberg (1985, 357–360) present data on six apple tree rootstock groups with four measurements on eight trees from each group.

We request the display of the leave-one-out (LOO) classification table in addition to the standard resubstitution classification table produced by discrim qda.

- . use http://www.stata-press.com/data/r14/rootstock (Table 6.2 Rootstock Data, Rencher and Christensen (2012))
- . discrim qda y1 y2 y3 y4, group(rootstock) lootable

Quadratic discriminant analysis
Resubstitution classification summary

Key
Number Percent

True	Classified						
rootstock	1	2	3	4	5	6	Total
1	8 100.00	0.00	0.00	0.00	0.00	0.00	8 100.00
2	0.00	7 87.50	0.00	1 12.50	0.00	0.00	8 100.00
3	1 12.50	0.00	6 75.00	0.00	1 12.50	0.00	8 100.00
4	0.00	0.00	1 12.50	7 87.50	0.00	0.00	8 100.00
5	0.00	3 37.50	0.00	0.00	4 50.00	1 12.50	8 100.00
6	2 25.00	0.00	0.00	0.00	1 12.50	5 62.50	8 100.00
Total	11 22.92	10 20.83	7 14.58	8 16.67	6 12.50	6 12.50	48 100.00
Priors	0.1667	0.1667	0.1667	0.1667	0.1667	0.1667	

Leave-one-out classification summary

Key
Number Percent

True	Classif	ied					
rootstock	1	2	3	4	5	6	Total
1	2 25.00	0.00	0.00	3 37.50	1 12.50	2 25.00	8 100.00
2	0.00	3 37.50	0.00	2 25.00	2 25.00	1 12.50	8 100.00
3	1 12.50	2 25.00	4 50.00	0.00	1 12.50	0.00	8 100.00
4	1 12.50	1 12.50	3 37.50	2 25.00	0.00	1 12.50	8 100.00
5	0.00	4 50.00	1 12.50	0.00	2 25.00	1 12.50	8 100.00
6	3 37.50	1 12.50	0.00	0.00	2 25.00	2 25.00	8 100.00
Total	7 14.58	11 22.92	8 16.67	7 14.58	8 16.67	7 14.58	48 100.00
Priors	0.1667	0.1667	0.1667	0.1667	0.1667	0.1667	

Compare the counts on the diagonal of the resubstitution classification table with those on the LOO table. The LOO table has fewer of the observations with correct classifications. The resubstitution classification table is overly optimistic.

The estat errorrate postestimation command provides estimates of the error rates for the groups. We request the count-based estimates, first for the resubstitution classification and then for the LOO classification. We also suppress display of the prior probabilities, which will default to equal across the groups because that is how we estimated our QDA model. See [MV] discrim estat for details of the estat errorrate command.

# . estat errorrate, nopriors Error rate estimated by error count

	rootstock				
	1	2	3	4	5
Error rate	0	.125	.25	.125	.5
	rootstock 6	Total			
Error rate	.375	.2291667			

. estat errorrate, nopriors looclass

Error rate estimated by leave-one-out error count

	rootstock 1	2	3	4	5
Error rate	.75	.625	.5	.75	.75
	rootstock				
	6	Total			
Error rate	.75	.6875			

The estimated group error rates are much higher in the LOO table.

See example 2 of [MV] discrim qda postestimation for an examination of the squared Mahalanobis distances between the rootstock groups. We could also list the misclassified observations, produce group summaries, examine covariances and correlations, and generate classification and probability variables and more; see [MV] discrim qda postestimation.

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See example 3 of [MV] discrim estat and example 1 of [MV] discrim qda postestimation for other examples of the use of discrim qda.

#### Stored results

discrim qda stores the following in e():

```
Scalars
                          number of observations
    e(N)
                          number of groups
    e(N_groups)
    e(k)
                          number of discriminating variables
Macros
    e(cmd)
                          discrim
    e(subcmd)
                          ada
    e(cmdline)
                          command as typed
    e(groupvar)
                          name of group variable
    e(grouplabels)
                          labels for the groups
    e(varlist)
                          discriminating variables
    e(wtype)
                          weight type
                          weight expression
    e(wexp)
                          title in estimation output
    e(title)
    e(ties)
                          how ties are to be handled
    e(properties)
                          nob noV
    e(estat_cmd)
                          program used to implement estat
    e(predict)
                          program used to implement predict
    e(marginsnotok)
                          predictions disallowed by margins
Matrices
    e(groupcounts)
                          number of observations for each group
    e(grouppriors)
                          prior probabilities for each group
    e(groupvalues)
                          numeric value for each group
    e(means)
                          group means on discriminating variables
    e(SSCP_W#)
                          within group SSCP matrix for group #
    e(W#_eigvals)
                          eigenvalues of e(SSCP_W#)
    e(W#_eigvecs)
                          eigenvectors of e(SSCP_W#)
    e(sqrtS#inv)
                          Cholesky (square root) of the inverse covariance matrix for group #
Functions
    e(sample)
                          marks estimation sample
```

#### Methods and formulas

Let g be the number of groups,  $n_i$  the number of observations for group i, and  $q_i$  the prior probability for group i. Let  $\mathbf{x}$  denote an observation measured on p discriminating variables. For consistency with the discriminant analysis literature,  $\mathbf{x}$  will be a column vector, though it corresponds to a row in your dataset. Let  $f_i(\mathbf{x})$  represent the density function for group i, and let  $P(\mathbf{x}|G_i)$  denote the probability of observing  $\mathbf{x}$  conditional on belonging to group i. Denote the posterior probability of group i given observation  $\mathbf{x}$  as  $P(G_i|\mathbf{x})$ . With Bayes's theorem, we have

$$P(G_i|\mathbf{x}) = \frac{q_i f_i(\mathbf{x})}{\sum_{j=1}^g q_j f_j(\mathbf{x})}$$

Substituting  $P(\mathbf{x}|G_i)$  for  $f_i(\mathbf{x})$ , we have

$$P(G_i|\mathbf{x}) = \frac{q_i P(\mathbf{x}|G_i)}{\sum_{j=1}^g q_j P(\mathbf{x}|G_j)}$$

QDA assumes that the groups are multivariate normal. Let  $S_i$  denote the within-group sample covariance matrix for group i and  $\bar{x}_i$  denote the sample mean of group i. The squared Mahalanobis distance between observation x and  $\bar{x}_i$  is

$$D_i^2 = (\mathbf{x} - \mathbf{\bar{x}}_i)' \mathbf{S}_i^{-1} (\mathbf{x} - \mathbf{\bar{x}}_i)$$

Plugging these sample estimates into the multivariate normal density gives

$$P(\mathbf{x}|G_i) = (2\pi)^{-p/2} |\mathbf{S}_i|^{-1/2} e^{-D_i^2/2}$$

Substituting this into the formula for  $P(G_i|\mathbf{x})$  and simplifying gives

$$P(G_i|\mathbf{x}) = \frac{q_i|\mathbf{S}_i|^{-1/2}e^{-D_i^2/2}}{\sum_{j=1}^g q_j|\mathbf{S}_j|^{-1/2}e^{-D_j^2/2}}$$

as the QDA posterior probability of observation  ${\bf x}$  belonging to group i.

The squared Mahalanobis distance between group means is produced by estat grdistances; see [MV] discrim qda postestimation.

Classification functions can be derived from the Mahalanobis QDA; see Huberty (1994, 58). Let  $Q_i(\mathbf{x})$  denote the quadratic classification function for the *i*th group applied to observation  $\mathbf{x}$ .

$$Q_i(\mathbf{x}) = -D_i^2/2 - \ln|\mathbf{S}_i|/2 + \ln(q_i)$$

An observation can be classified based on largest posterior probability or based on largest quadratic classification function score.

### References

Andrews, D. F., and A. M. Herzberg, ed. 1985. Data: A Collection of Problems from Many Fields for the Student and Research Worker. New York: Springer.

Huberty, C. J. 1994. Applied Discriminant Analysis. New York: Wiley.

Rencher, A. C. 1998. Multivariate Statistical Inference and Applications. New York: Wiley.

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Rencher, A. C., and W. F. Christensen. 2012. *Methods of Multivariate Analysis*. 3rd ed. Hoboken, NJ: Wiley. Smith, C. A. B. 1947. Some examples of discrimination. *Annals of Eugenics* 13: 272–282.

### Also see

[MV] discrim qda postestimation — Postestimation tools for discrim qda

[MV] discrim — Discriminant analysis

[U] 20 Estimation and postestimation commands

### **Title**

discrim qda postestimation — Postestimation tools for discrim qda

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

### **Postestimation commands**

The following postestimation commands are of special interest after discrim qda:

Command	Description
estat classtable	classification table
estat correlations	group correlation matrices and p-values
estat covariance	group covariance matrices
estat errorrate	classification error-rate estimation
estat grdistances	Mahalanobis and generalized squared distances between the group means
estat grsummarize	group summaries
estat list	classification listing
estat summarize	estimation sample summary

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results
predict	group classification and posterior probabilities

<sup>\*</sup> All estimates subcommands except table and stats are available; see [R] estimates.

### predict

### **Description for predict**

predict creates a new variable containing predictions such as group classifications, probabilities, Mahalanobis squared distances, leave-one-out group classifications, leave-one-out probabilities, and leave-one-out Mahalanobis squared distances.

### Menu for predict

Statistics > Postestimation

### Syntax for predict

```
predict [type] newvar [if] [in] [, statistic options]
    predict [type] { stub* | newvarlist } [if] [in] [, statistic options]
 statistic
                            Description
Main
 classification
                            group membership classification; the default when one variable is
                              specified and group() is not specified
                           probability of group membership; the default when group() is
 pr
                              specified or when multiple variables are specified
 mahalanobis
                            Mahalanobis squared distance between observations and groups
 clscore
                            group classification function score
*looclass
                            leave-one-out group membership classification; may be used only
                              when one new variable is specified
                            leave-one-out probability of group membership
^stloopr
*loomahal
                            leave-one-out Mahalanobis squared distance between observations and
                              groups
                            Description
 options
 group(group)
                            the group for which the statistic is to be calculated
Options
 priors(priors)
                            group prior probabilities; defaults to e(grouppriors)
 ties(ties)
                            how ties in classification are to be handled; defaults to e(ties)
```

priors	Description
equal proportional matname matrix_exp	equal prior probabilities group-size-proportional prior probabilities row or column vector containing the group prior probabilities matrix expression providing a row or column vector of the group prior probabilities
ties	Description
missing random first	ties in group classification produce missing values ties in group classification are broken randomly ties in group classification are set to the first tied group

You specify one new variable with classification or looclass and specify either one or e(N\_groups) new variables with pr, loopr, mahalanobis, loomahal, or clscore.

Unstarred statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample. Starred statistics are calculated only for the estimation sample, even when if e(sample) is not specified.

group() is not allowed with classification or looclass.

### Options for predict

Main

- classification, the default, calculates the group classification. Only one new variable may be specified.
- pr calculates group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- mahalanobis calculates the squared Mahalanobis distance between the observations and group means. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- clscore produces the group classification function score. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables.
- looclass calculates the leave-one-out group classifications. Only one new variable may be specified. Leave-one-out calculations are restricted to e(sample) observations.
- loopr calculates the leave-one-out group membership posterior probabilities. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables. Leave-one-out calculations are restricted to e(sample) observations.
- loomahal calculates the leave-one-out squared Mahalanobis distance between the observations and group means. If you specify the group() option, specify one new variable. Otherwise, you must specify e(N\_groups) new variables. Leave-one-out calculations are restricted to e(sample) observations.

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group(group) specifies the group for which the statistic is to be calculated and can be specified using

#1, #2, ..., where #1 means the first category of the e(groupvar) variable, #2 the second category, etc.;

the values of the e(groupvar) variable; or

the value labels of the e(groupvar) variable if they exist.

group() is not allowed with classification or looclass.

Options

priors (*priors*) specifies the prior probabilities for group membership. If priors () is not specified, e(grouppriors) is used. The following *priors* are allowed:

priors(equal) specifies equal prior probabilities.

priors(proportional) specifies group-size-proportional prior probabilities.

priors (matname) specifies a row or column vector containing the group prior probabilities.

priors (matrix\_exp) specifies a matrix expression providing a row or column vector of the group prior probabilities.

ties(ties) specifies how ties in group classification will be handled. If ties() is not specified, e(ties) is used. The following ties are allowed:

ties(missing) specifies that ties in group classification produce missing values.

ties(random) specifies that ties in group classification are broken randomly.

 $ties(\underline{f}irst)$  specifies that ties in group classification are set to the first tied group.

#### estat

### **Description for estat**

estat correlations displays group correlation matrices. Two-tailed p-values for the correlations are also available.

estat covariance displays group covariance matrices.

estat grdistances provides Mahalanobis squared distances and generalized squared distances between the group means.

#### Menu for estat

Statistics > Postestimation

### Syntax for estat

```
Group correlation matrices and p-values
```

```
estat correlations [, correlations_options]
```

#### Group covariance matrices

```
estat covariance [, covariance_options]
```

### Mahalanobis and generalized squared distances between the group means

```
estat grdistances [, grdistances_options]
```

correlations_options	Description
Main	
p	display two-sided p-values
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g
<u>noha</u> lf	display full matrix even if symmetric
covariance_options	Description
Main	
format(%fmt)	numeric display format; default is %9.0g
<u>noha</u> lf	display full matrix even if symmetric

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grdistances_options	Description
Main	
<u>mah</u> alanobis	display Mahalanobis squared distances between group means; the default
generalized	display generalized Mahalanobis squared distances between group means
all	equivalent to mahalanobis generalized
<pre>format(%fmt)</pre>	numeric display format; default is %9.0g
Options	
priors(priors)	group prior probabilities; defaults to e(grouppriors)

### Options for estat

Options for estat are presented under the following headings:

Options for estat covariance Options for estat covariance Options for estat grdistances

### **Options for estat correlations**

\_\_\_\_\_ Main 🗎

p specifies that two-sided p-values be computed and displayed for the correlations.

format(%fmt) specifies the matrix display format. The default is format(%8.5f).

nohalf specifies that, even though the matrix is symmetric, the full matrix be printed. The default is to print only the lower triangle.

### Options for estat covariance

Main

format(%fmt) specifies the matrix display format. The default is format(%9.0g).

nohalf specifies that, even though the matrix is symmetric, the full matrix be printed. The default is to print only the lower triangle.

### Options for estat grdistances

Main

mahalanobis specifies that a table of Mahalanobis squared distances between group means be presented.

generalized specifies that a table of generalized Mahalanobis squared distances between group means be presented. generalized starts with what is produced by the mahalanobis option and adds a term for the possibly unequal covariances and a term accounting for prior probabilities. Prior probabilities are provided with the priors() option, or if priors() is not specified, by the values in e(grouppriors). By common convention, if prior probabilities are equal across the groups, the prior probability term is omitted.

all is equivalent to specifying mahalanobis and generalized.

format(% fmt) specifies the matrix display format. The default is format(%9.0g).

Options

priors (priors) specifies the group prior probabilities and affects only the output of the generalized option. By default, priors is determined from e(grouppriors). See Options for predict for the priors specification.

### Remarks and examples

The predict and estat commands after discrim qda help in exploring the QDA model. See [MV] discrim estat for details of the estat subcommands common to all discrim subcommands. Here we illustrate some of these common estat subcommands along with estat covariance, estat correlations, and estat grdistances that are specific to discrim qda.

#### Example 1: Group covariances and correlations and out-of-sample prediction

Everitt and Dunn (2001, 269) show data for male Egyptian skulls from the early and late predynastic epochs. Ten observations from each epoch are provided. Four measurements were taken of each skull: x1, maximum breadth; x2, basibregmatic height; x3, basialveolar length; and x4, nasal height. All measurements were in millimeters. Everitt and Dunn obtained the data from Manly (2005).

We perform a quadratic discriminant analysis on this dataset and demonstrate the use of estat and predict.

- . use http://www.stata-press.com/data/r14/skulls (Egyptian Skulls)
- . discrim qda x1 x2 x3 x4, group(predynastic)

Quadratic discriminant analysis Resubstitution classification summary

Key	
Number Percent	

True	Classif		
predynastic	early	late	Total
early	9	1	10
	90.00	10.00	100.00
late	3	7	10
	30.00	70.00	100.00
Total	12	8	20
	60.00	40.00	100.00
Priors	0.5000	0.5000	

What kind of covariance structure do the two groups have? If they are similar to one another, we might wish to switch to using LDA (see [MV] discrim lda) instead of QDA. estat covariance displays the covariance matrices for our two groups.

. estat covariance

Group covariance matrices

predynastic: early

	x1	x2	хЗ	x4
x1 x2		15.34444		
x3 x4	13.18889 16.1	-7.322222 8.077778	36.9 -2.144444	11.43333
predynastic: lat	e			
	x1	x2	х3	x4

43.12222 x1 x2 -4.966667 38.98889 xЗ 9.388889 6.611111 10.27778 x4 5.211111 12.74444 4.388889 9.122222

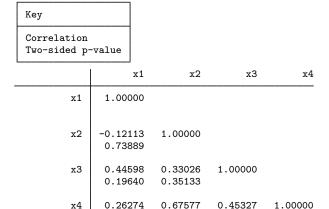
There appear to be differences, including differences in sign between some of the elements of the covariance matrices of the two groups. How substantial are these differences? The estat correlations command displays the correlation matrices for the groups. The p option requests that p-values be presented with the correlations.

. estat correlations, p Group correlation matrices predynastic: early

Key
Correlation Two-sided p-value

	x1	x2	х3	x4
x1	1.00000			
x2	0.28901 0.41800	1.00000		
x3	0.34192 0.33353	-0.30772 0.38707	1.00000	
x4	0.74984 0.01251	0.60986 0.06119	-0.10440 0.77409	1.00000

predynastic: late



0.03196

Few of the correlations in the two matrices are statistically significant. We are less sure of the apparent differences between the covariance structures for these two groups.

0.18830

Let's press forward anyway. Everitt and Dunn (2001, 269) ask for the prediction for an unknown skull. We input the unknown observation and then use predict to obtain the classification and probabilities of group membership for the observation.

- . input
- predyna~c x2 x3 x4 x1 21. . 127 129 95 51
- 22. end
- . predict grp

(option classification assumed; group classification)

0.46331

- . predict pr1 pr2, pr
- . label values grp epoch
- . list x\* grp pr1 pr2 in 21

	x1	x2	х3	x4	grp	pr1	pr2
21.	127	129	95	51	late	.3654425	.6345575

This skull is classified by our QDA model as belonging to the late predynastic epoch with probability 0.63.

estat list could also be used to obtain this same information; see [MV] discrim estat.

. estat list in 21, varlist

	Data				Classifica	tion	Probabi	lities
Obs.	x1	x2	x3	x4	True	Class.	early	late
21	127	129	95	51		late	0.3654	0.6346

We could use predict and estat to explore other aspects of this QDA model, including leaveone-out (LOO) classifications, probabilities, classification tables, and error-rate estimates.

### Example 2: Mahalanobis and generalized distances between groups

Example 1 of [MV] **discrim qda** performs a QDA on the apple tree rootstock data found in Andrews and Herzberg (1985, 357–360). We now demonstrate the use of the estat grdistances command for examining the squared Mahalanobis distances and the squared generalized distances between the rootstock groups.

- . use http://www.stata-press.com/data/r14/rootstock, clear (Table 6.2 Rootstock Data -- Rencher (2002))
- . discrim qda y1 y2 y3 y4, group(rootstock) notable
- . estat grdistances, all

Mahalanobis squared distances between groups

rootstock		rootstock 1	2	3	4	5
	1	0	18.37241	7.89988	1.622808	14.78843
	2	42.19008	0	5.489408	14.08784	1.502462
	3	36.81811	1.908369	0	6.406024	15.48121
	4	2.281963	14.77928	6.742393	0	25.72128
	5	33.70858	1.855704	4.617755	16.34139	0
	6	3.860684	17.32868	12.5828	11.24491	3.49512
		rootstock				
rootstock		6				
	1	9.152132				
	2	30.45472				
	3	72.60112				
	4	29.01146				
	5	20.50925				
	6	0				

Generalized squared distances between groups

		rootstock				
rootstock		1	2	3	4	5
	1	-17.89946	2.47128	-9.577605	-14.60611	-1.796629
	2	24.29063	-15.90113	-11.98808	-2.141072	-15.0826
	3	18.91866	-13.99276	-17.47749	-9.822891	-1.103849
	4	-15.61749	-1.121858	-10.73509	-16.22892	9.136221
	5	15.80913	-14.04543	-12.85973	.1124762	-16.58506
	6	-14.03877	1.427543	-4.894681	-4.984005	-13.08994
		rootstock				
rootstock		6				
	1	-7.241371				
	2	14.06121				
	3	56.20761				
	4	12.61796				
	5	4.115752				
	6	-16.3935				

Both tables are nonsymmetric. For QDA the Mahalanobis distance depends on the covariance of the reference group. The Mahalanobis distance for group i (the rows in the tables above) to group j (the columns in the tables above) will use the covariance matrix of group j in determining the distance. The generalized distance also factors in the prior probabilities for the groups, and so the diagonal elements are not zero and the entries can be negative. In either matrix, the smaller the number, the closer the groups.

#### Stored results

```
estat correlations stores the following in r():
Matrices
    r(Rho_#)
                  group # correlation matrix
    r(P_#)
                  two-sided p-values for group # correlations
estat covariance stores the following in r():
Matrices
    r(S_#)
                  group # covariance matrix
estat grdistances stores the following in r():
Matrices
    r(sqdist)
                  Mahalanobis squared distances between group means (mahalanobis only)
    r(gsqdist)
                  generalized squared distances between group means (generalized only)
```

### Methods and formulas

See Methods and formulas of [MV] discrim qda for background on what is produced by predict and estat grdistances. See [MV] discrim estat for more information on estat classtable, estat errorrate, estat grsummarize, and estat list.

#### References

Andrews, D. F., and A. M. Herzberg, ed. 1985. Data: A Collection of Problems from Many Fields for the Student and Research Worker. New York: Springer.

Everitt, B. S., and G. Dunn. 2001. Applied Multivariate Data Analysis. 2nd ed. London: Arnold.

Manly, B. F. J. 2005. Multivariate Statistical Methods: A Primer. 3rd ed. London: Chapman & Hall.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.

### Also see

```
[MV] discrim qda — Quadratic discriminant analysis
[MV] discrim estat — Postestimation tools for discrim
[MV] discrim — Discriminant analysis
[U] 20 Estimation and postestimation commands
```

#### Title

factor — Factor analysis

Description Quick start Menu

Syntax Options for factor and factormat Options unique to factormat Remarks and examples Stored results Options unique to factormat Methods and formulas

References Also see

### **Description**

factor and factormat perform a factor analysis of a correlation matrix. The commands produce principal factor, iterated principal factor, principal-component factor, and maximum-likelihood factor analyses. factor and factormat display the eigenvalues of the correlation matrix, the factor loadings, and the uniqueness of the variables.

factor expects data in the form of variables, allows weights, and can be run for subgroups. factormat is for use with a correlation or covariance matrix.

#### **Quick start**

Principal-factor analysis using variables v1 to v5

factor v1 v2 v3 v4 v5

As above, but retain at most 3 factors

factor v1-v5, factors(3)

Principal-component factor analysis using variables v1 to v5

factor v1-v5, pcf

Maximum-likelihood factor analysis

factor v1-v5, ml

As above, but perform 50 maximizations with different starting values

factor v1-v5, ml protect(50)

As above, but set the seed for reproducibility

factor v1-v5, ml protect(50) seed(349285)

Principal-factor analysis based on a correlation matrix cmat with a sample size of 800

factormat cmat, n(800)

As above, retain only factors with eigenvalues greater than or equal to 1

factormat cmat, n(800) mineigen(1)

#### Menu

#### factor

Statistics > Multivariate analysis > Factor and principal component analysis > Factor analysis

#### factormat

Statistics > Multivariate analysis > Factor and principal component analysis > Factor analysis of a correlation matrix

### **Syntax**

Factor analysis of data

```
factor varlist [if] [in] [weight] [, method options]
```

Factor analysis of a correlation matrix

```
factormat matname, n(#) [method options factormat_options]
```

matname is a square Stata matrix or a vector containing the rowwise upper or lower triangle of the correlation or covariance matrix. If a covariance matrix is provided, it is transformed into a correlation matrix for the factor analysis.

method	Description			
Model 2				
pf	principal factor; the default			
pcf	principal-component factor			
$\underline{\mathtt{ip}}\mathtt{f}$	iterated principal factor			
ml	maximum likelihood factor			
options	Description			
Model 2				
<pre>factors(#)</pre>	maximum number of factors to be retained			
<pre>mine igen(#)</pre>	minimum value of eigenvalues to be retained			
<pre>citerate(#)</pre>	communality reestimation iterations (ipf only)			
Reporting				
<u>bl</u> anks(#)	display loadings as blank when $ loadings  < \#$			
<u>altdiv</u> isor	use trace of correlation matrix as the divisor for reported proportions			
Maximization				
<pre>protect(#)</pre>	perform # optimizations and report the best solution (ml only)			
$\underline{\underline{r}}$ andom	use random starting values (ml only); seldom used			
seed(seed)	random-number seed (ml with protect() or random only)			
maximize_options	control the maximization process; seldom used (ml only)			
norotated	display unrotated solution, even if rotated results are available (replay only)			

norotated does not appear in the dialog box.

factormat_options	Description
Model	
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{f}}\mathtt{ull})$	matname is a square symmetric matrix; the default
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{l}}\mathtt{ower})$	matname is a vector with the rowwise lower triangle (with diagonal)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{u}}\mathtt{pper})$	matname is a vector with the rowwise upper triangle (with diagonal)
$\underline{\mathtt{nam}}\mathtt{es}(\mathit{namelist})$	variable names; required if matname is triangular
forcepsd	modifies matname to be positive semidefinite
*n(#)	number of observations
$sds(matname_2)$	vector with standard deviations of variables
$means(matname_3)$	vector with means of variables

<sup>\*</sup> n(#) is required for factormat.

bootstrap, by, jackknife, rolling, and statsby are allowed with factor; see [U] 11.1.10 Prefix commands. However, bootstrap and jackknife results should be interpreted with caution; identification of the factor parameters involves data-dependent restrictions, possibly leading to badly biased and overdispersed estimates (Milan and Whittaker 1995).

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed with factor; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

### Options for factor and factormat

Model 2

pf, pcf, ipf, and ml indicate the type of estimation to be performed. The default is pf.

pf specifies that the principal-factor method be used to analyze the correlation matrix. The factor loadings, sometimes called the factor patterns, are computed using the squared multiple correlations as estimates of the communality. pf is the default.

pcf specifies that the principal-component factor method be used to analyze the correlation matrix. The communalities are assumed to be 1.

ipf specifies that the iterated principal-factor method be used to analyze the correlation matrix. This reestimates the communalities iteratively.

ml specifies the maximum-likelihood factor method, assuming multivariate normal observations. This estimation method is equivalent to Rao's canonical-factor method and maximizes the determinant of the partial correlation matrix. Hence, this solution is also meaningful as a descriptive method for nonnormal data. ml is not available for singular correlation matrices. At least three variables must be specified with method ml.

factors(#) and mineigen(#) specify the maximum number of factors to be retained. factors()
 specifies the number directly, and mineigen() specifies it indirectly, keeping all factors with
 eigenvalues greater than the indicated value. The options can be specified individually, together,
 or not at all.

factors (#) sets the maximum number of factors to be retained for later use by the postestimation commands. factor always prints the full set of eigenvalues but prints the corresponding eigenvectors only for retained factors. Specifying a number larger than the number of variables in the *varlist* is equivalent to specifying the number of variables in the *varlist* and is the default.

- mineigen(#) sets the minimum value of eigenvalues to be retained. The default for all methods except pcf is  $5 \times 10^{-6}$  (effectively zero), meaning that factors associated with negative eigenvalues will not be printed or retained. The default for pcf is 1. Many sources recommend mineigen(1), although the justification is complex and uncertain. If # is less than  $5 \times 10^{-6}$ , it is reset to  $5 \times 10^{-6}$ .
- citerate(#) is used only with ipf and sets the number of iterations for reestimating the communalities. If citerate() is not specified, iterations continue until the change in the communalities
  is small. ipf with citerate(0) produces the same results that pf does.

Reporting

blanks (#) specifies that factor loadings smaller than # (in absolute value) be displayed as blanks.

altdivisor specifies that reported proportions and cumulative proportions be computed using the trace of the correlation matrix, trace(e(C)), as the divisor. The default is to use the sum of all eigenvalues (even those that are negative) as the divisor.

Maximization

protect(#) is used only with m1 and requests that # optimizations with random starting values
be performed along with squared multiple correlation coefficient starting values and that the best
of the solutions be reported. The output also indicates whether all starting values converged to
the same solution. When specified with a large number, such as protect(50), this provides
reasonable assurance that the solution found is global and not just a local maximum. If trace is
also specified (see [R] maximize), the parameters and likelihoods of each maximization will be
printed.

random is used only with ml and requests that random starting values be used. This option is rarely used and should be used only after protect() has shown the presence of multiple maximums.

seed(seed) is used only with ml when the random or protect() options are also specified. seed()
specifies the random-number seed; see [R] set seed. If seed() is not specified, the random-number
generator starts in whatever state it was last in.

maximize\_options: <u>iter</u>ate(#), [no]log, <u>trace</u>, <u>tol</u>erance(#), and <u>ltol</u>erance(#); see [R] maximize. These options are seldom used.

The following option is available with factor but is not shown in the dialog box:

norotated specifies that the unrotated factor solution be displayed, even if a rotated factor solution is available. norotated is for use only with replaying results.

# Options unique to factormat

Model

**shape**(*shape*) specifies the shape (storage method) for the covariance or correlation matrix *matname*. The following shapes are supported:

full specifies that the correlation or covariance structure of k variables is a symmetric  $k \times k$  matrix. This is the default.

lower specifies that the correlation or covariance structure of k variables is a vector with k(k+1)/2 elements in rowwise lower-triangular order,

$$C_{11} C_{21} C_{22} C_{31} C_{32} C_{33} \dots C_{k1} C_{k2} \dots C_{kk}$$

upper specifies that the correlation or covariance structure of k variables is a vector with k(k+1)/2elements in rowwise upper-triangular order,

$$C_{11} C_{12} C_{13} \ldots C_{1k} C_{22} C_{23} \ldots C_{2k} \ldots C_{(k-1,k-1)} C_{(k-1,k)} C_{kk}$$

names (namelist) specifies a list of k different names to be used to document output and label estimation results and as variable names by predict. names() is required if the correlation or covariance matrix is in vectorized storage mode (that is, shape(lower) or shape(upper) is specified). By default, factormat verifies that the row and column names of matname and the column or row names of matname2 and matname3 from the sds() and means() options are in agreement. Using the names() option turns off this check.

forcepsd modifies the matrix *matname* to be positive semidefinite (psd) and so be a proper covariance matrix. If matname is not positive semidefinite, it will have negative eigenvalues. By setting negative eigenvalues to 0 and reconstructing, we obtain the least-squares positive-semidefinite approximation to *matname*. This approximation is a singular covariance matrix.

n(#), a required option, specifies the number of observations on which *matname* is based.

 $sds(matname_2)$  specifies a  $k \times 1$  or  $1 \times k$  matrix with the standard deviations of the variables. The row or column names should match the variable names, unless the names() option is specified. sds() may be specified only if matname is a correlation matrix. Specify sds() if you have variables in your dataset and want to use predict after factormat. sds() does not affect the computations of factormat but provides information so that predict does not assume that the standard deviations are one.

means (matname<sub>3</sub>) specifies a  $k \times 1$  or  $1 \times k$  matrix with the means of the variables. The row or column names should match the variable names, unless the names() option is specified. Specify means() if you have variables in your dataset and want to use predict after factormat. means() does not affect the computations of factormat but provides information so that predict does not assume the means are zero.

# Remarks and examples

Remarks are presented under the following headings:

Introduction Factor analysis Factor analysis from a correlation matrix

#### Introduction

Factor analysis, in the sense of exploratory factor analysis, is a statistical technique for data reduction. It reduces the number of variables in an analysis by describing linear combinations of the variables that contain most of the information and that, we hope, admit meaningful interpretations.

Factor analysis originated with the work of Spearman (1904), and has since witnessed an explosive growth, especially in the social sciences and, interestingly, in chemometrics. For an introduction, we refer to Kim and Mueller (1978a, 1978b), van Belle, Fisher, Heagerty, and Lumley (2004, chap. 14), Hamilton (2013, chap. 11), and Afifi, May, and Clark (2012). Intermediate-level treatments include Gorsuch (1983) and Harman (1976). For mathematically more advanced discussions, see Mulaik (2010), Mardia, Kent, and Bibby (1979, chap. 9), and Fuller (1987).

Structural equation modeling provides a more general framework for performing factor analysis, including confirmatory factor analysis; see [SEM] intro 5, [SEM] example 1, and [SEM] example 3.

Also see Kolenikov (2009) for another implementation of confirmatory factor analysis.

### Factor analysis

Factor analysis finds a few common factors (say, q of them) that linearly reconstruct the p original variables

$$y_{ij} = z_{i1}b_{1j} + z_{i2}b_{2j} + \dots + z_{iq}b_{qj} + e_{ij}$$

where  $y_{ij}$  is the value of the *i*th observation on the *j*th variable,  $z_{ik}$  is the *i*th observation on the *k*th common factor,  $b_{kj}$  is the set of linear coefficients called the factor loadings, and  $e_{ij}$  is similar to a residual but is known as the *j*th variable's unique factor. Everything except the left-hand-side variable is to be estimated, so the model has an infinite number of solutions. Various constraints are introduced to make the model determinate.

"Reconstruction" is typically defined in terms of prediction of the correlation matrix of the original variables, unlike principal components (see [MV] pca), where reconstruction means minimum residual variance summed across all equations (variables).

Once the factors and their loadings have been estimated, they are interpreted—an admittedly subjective process. Interpretation typically means examining the  $b_{kj}$ 's and assigning names to each factor. Because of the indeterminacy of the factor solution, we are not limited to examining solely the  $b_{kj}$ 's. The loadings could be rotated. Rotations come in two forms—orthogonal and oblique. If we restrict to orthogonal rotations, the rotated  $b_{kj}$ s, despite appearing different, are every bit as good as (and no better than) the original loadings. Oblique rotations are often desired but do not retain some important properties of the original solution; see example 3. Because there are an infinite number of potential rotations, different rotations could lead to different interpretations of the same data. These are not to be viewed as conflicting, but instead as two different ways of looking at the same thing. See [MV] factor postestimation and [MV] rotate for more information on rotation.

## Example 1: A simple factor analysis on six questions

We wish to analyze physicians' attitudes toward cost. Six questions about cost were asked of 568 physicians in the Medical Outcomes Study from Tarlov et al. (1989). We do not have the original data, so we used corr2data to create a dataset with the same correlation matrix. Factor analysis is often used to validate a combination of questions that looks meaningful at first glance. Here we wish to create a variable that summarizes the information on each physician's attitude toward cost.

Each response is coded on a five-point scale, where 1 means "agree" and 5 means "disagree":

. use http://www.stata-press.com/data/r14/bg2
(Physician-cost data)

. describe

Contains data from http://www.stata-press.com/data/r14/bg2.dta
obs: 568 Physician-cost data
vars: 7 11 Feb 2014 21:54
size: 14,768 (\_dta has notes)

variable name	storage type	display format	value label	variable label
clinid	int	%9.0g		Physician identifier
bg2cost1	float	%9.0g		Best health care is expensive
bg2cost2	float	%9.0g		Cost is a major consideration
bg2cost3	float	%9.0g		Determine cost of tests first
bg2cost4	float	%9.0g		Monitor likely complications only
bg2cost5	float	%9.0g		Use all means regardless of cost
bg2cost6	float	%9.0g		Prefer unnecessary tests to missing tests

Sorted by: clinid

We perform the factorization on bg2cost1, bg2cost2, ..., bg2cost6.

. factor bg2cost1-bg2cost6 (obs=568)

Factor analysis/correlation Number of obs 568 Method: principal factors Retained factors = 3 Rotation: (unrotated) Number of params = 15

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	0.85389	0.31282	1.0310	1.0310
Factor2	0.54107	0.51786	0.6533	1.6844
Factor3	0.02321	0.17288	0.0280	1.7124
Factor4	-0.14967	0.03951	-0.1807	1.5317
Factor5	-0.18918	0.06197	-0.2284	1.3033
Factor6	-0.25115		-0.3033	1.0000

LR test: independent vs. saturated: chi2(15) = 269.07 Prob> chi2 = 0.0000Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Factor3	Uniqueness
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5 bg2cost6	0.2470	0.3670	-0.0446	0.8023
	-0.3374	0.3321	-0.0772	0.7699
	-0.3764	0.3756	0.0204	0.7169
	-0.3221	0.1942	0.1034	0.8479
	0.4550	0.2479	0.0641	0.7274
	0.4760	0.2364	-0.0068	0.7175

factor retained only the first three factors because the eigenvalues associated with the remaining factors are negative. According to the default mineigen(0) criterion, a factor must have an eigenvalue greater than zero to be retained. You can set this threshold higher by specifying mineigen(#). Although factor elected to retain three factors, only the first two appear to be meaningful.

The first factor seems to describe the physician's average position on cost because it affects the responses to all the questions "positively", as shown by the signs in the first column of the factor-loading table. We say "positively" because, obviously, the signs on three of the loadings are negative. When we look back at the results of describe, however, we find that the direction of the responses on bg2cost2, bg2cost3, and bg2cost4 are reversed. If the physician feels that cost should not be a major influence on medical treatment, he or she is likely to disagree with these three items and to agree with the other three.

The second factor loads positively (absolutely, not logically) on all six items and could be interpreted as describing the physician's tendency to agree with any good-sounding idea put forth. Psychologists refer to this as the "positive response set". On statistical grounds, we would probably keep this second factor, although on substantive grounds, we would be tempted to drop it.

We finally point to the column with the header "uniqueness". Uniqueness is the percentage of variance for the variable that is not explained by the common factors. The quantity "1 - uniqueness" is called communality. Uniqueness could be pure measurement error, or it could represent something that is measured reliably in that particular variable, but not by any of the others. The greater the uniqueness, the more likely that it is more than just measurement error. Values more than 0.6 are usually considered high; all the variables in this problem are even higher—more than 0.71. If the uniqueness is high, then the variable is not well explained by the factors.

## Example 2: A different divisor for proportions

The cumulative proportions of the eigenvalues exceeded 1.0 in our factor analysis because of the negative eigenvalues. By default, the proportion and cumulative proportion columns are computed using the sum of all eigenvalues as the divisor. The altdivisor option allows you to display the proportions and cumulative proportions by using the trace of the correlation matrix as the divisor. This option is allowed at estimation time or when replaying results. We demonstrate by replaying the results with this option.

### . factor, altdivisor

Factor analysis/correlation	Number of obs =	568
Method: principal factors	Retained factors =	3
Rotation: (unrotated)	Number of params =	15

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	0.85389	0.31282	0.1423	0.1423
Factor2	0.54107	0.51786	0.0902	0.2325
Factor3	0.02321	0.17288	0.0039	0.2364
Factor4	-0.14967	0.03951	-0.0249	0.2114
Factor5	-0.18918	0.06197	-0.0315	0.1799
Factor6	-0.25115		-0.0419	0.1380

LR test: independent vs. saturated: chi2(15) = 269.07 Prob>chi2 = 0.0000 Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Factor3	Uniqueness
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5 bg2cost6	0.2470 -0.3374 -0.3764 -0.3221 0.4550 0.4760	0.3670 0.3321 0.3756 0.1942 0.2479 0.2364	-0.0446 -0.0772 0.0204 0.1034 0.0641 -0.0068	0.8023 0.7699 0.7169 0.8479 0.7274

Among the sources we examined, there was not a consensus on which divisor is most appropriate. Therefore, both are available.

4

## Example 3: Principal-component factors instead of principal factors

factor provides several alternative estimation strategies for the factor model. We specified no options on the factor command when we fit our first model, so we obtained the principal-factor solution. The *communalities* (defined as 1-uniqueness) were estimated using the squared multiple correlation coefficients.

We could have instead obtained the estimates from "principal-component factors", treating the communalities as all 1—meaning that there are no unique factors—by specifying the pcf option:

factor bg2cost1-bg2cost6, pcf (obs=568)

568 Factor analysis/correlation Number of obs Method: principal-component factors Retained factors = 2 Rotation: (unrotated) Number of params = 11

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	1.70622	0.30334	0.2844	0.2844
Factor2	1.40288	0.49422	0.2338	0.5182
Factor3	0.90865	0.18567	0.1514	0.6696
Factor4	0.72298	0.05606	0.1205	0.7901
Factor5	0.66692	0.07456	0.1112	0.9013
Factor6	0.59236		0.0987	1.0000

chi2(15) = 269.07 Prob>chi2 = 0.0000LR test: independent vs. saturated:

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
bg2cost1	0.3581	0.6279	0.4775
bg2cost2	-0.4850	0.5244	0.4898
bg2cost3	-0.5326	0.5725	0.3886
bg2cost4	-0.4919	0.3254	0.6521
bg2cost5	0.6238	0.3962	0.4539
bg2cost6	0.6543	0.3780	0.4290

Here we find that the principal-component factor model is inappropriate. It is based on the assumption that the uniquenesses are 0, but we find that there is considerable uniqueness—there is considerable variability left over after our two factors. We should use some other method.

# Example 4: Iterated principal-factor analysis

We could have fit our model using iterated principal factors by specifying the ipf option. Here the initial estimates of the communalities would be the squared multiple correlation coefficients, but the solution would then be iterated to obtain different (better) estimates:

. factor bg2cost1-bg2cost6, ipf (obs=568)

Factor analysis/correlation Number of obs 568 Method: iterated principal factors Retained factors = 5 Rotation: (unrotated) Number of params = 15

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	1.08361	0.31752	0.5104	0.5104
Factor2	0.76609	0.53816	0.3608	0.8712
Factor3	0.22793	0.19469	0.1074	0.9786
Factor4	0.03324	0.02085	0.0157	0.9942
Factor5	0.01239	0.01256	0.0058	1.0001
Factor6	-0.00017		-0.0001	1.0000

chi2(15) = 269.07 Prob>chi2 = 0.0000LR test: independent vs. saturated:

1

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Factor3	Factor4	Factor5	Uniqueness
bg2cost1	0.2471	0.4059	-0.1349	-0.1303	0.0288	0.7381
bg2cost2	-0.4040	0.3959	-0.2636	0.0349	0.0040	0.6093
bg2cost3	-0.4479	0.4570	0.1290	0.0137	-0.0564	0.5705
bg2cost4	-0.3327	0.1943	0.2655	0.0091	0.0810	0.7744
bg2cost5	0.5294	0.3338	0.2161	-0.0134	-0.0331	0.5604
bg2cost6	0.5174	0.2943	-0.0801	0.1208	0.0265	0.6240

Here we retained too many factors. Unlike in principal factors or principal-component factors, we cannot simply ignore the unnecessary factors because the uniquenesses are reestimated from the data and therefore depend on the number of retained factors. We need to reestimate. We use the opportunity to demonstrate the option blanks(#) for displaying "small loadings" as blanks for easier reading:

. factor bg2cost1-bg2cost6, ipf factors(2) blanks(.30)
(obs=568)

Factor analysis/correlation Number of obs = 568
Method: iterated principal factors Retained factors = 2
Rotation: (unrotated) Number of params = 11

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	1.03954	0.30810	0.5870	0.5870
Factor2	0.73144	0.60785	0.4130	1.0000
Factor3	0.12359	0.11571	0.0698	1.0698
Factor4	0.00788	0.03656	0.0045	1.0743
Factor5	-0.02867	0.07418	-0.0162	1.0581
Factor6	-0.10285		-0.0581	1.0000

LR test: independent vs. saturated: chi2(15) = 269.07 Prob>chi2 = 0.0000 Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5	-0.3590 -0.5189 -0.3230 0.4667	0.3941 0.4935 0.3286	0.7937 0.7827 0.4872 0.8699 0.6742
bg2cost6	0.5179	0.3325	0.6212

(blanks represent abs(loading)<.3)

It is instructive to compare the reported uniquenesses for this model and the previous one, where five factors were retained. Also, compared with the results we obtained from principal factors, these results do not differ much.

# Example 5: Maximum likelihood factor analysis

Finally, we could have fit our model using the maximum likelihood method by specifying the ml option. The maximum likelihood method assumes that the data are multivariate normal distributed. If the factor model provides an adequate approximation to the data, maximum likelihood estimates have favorable properties compared with the other estimation methods. Rao (1955) has shown that his canonical factor method is equivalent to the maximum likelihood method. This method seeks to maximize canonical correlations between the manifest variables and the common factors. Thus ml may be used descriptively, even if we are unwilling to assume multivariate normality.

As with ipf, if we do not specify the number of factors, Stata retains more than two factors (it retained three), and, as with ipf, we will need to reestimate with the number of factors that we really want. To save paper, we will start by retaining two factors:

```
. factor bg2cost1-bg2cost6, ml factors(2)
(obs=568)
Iteration 0:
               log\ likelihood = -28.702162
Iteration 1:
               log\ likelihood = -7.0065234
               log likelihood = -6.8513798
Iteration 2:
Iteration 3:
               log\ likelihood = -6.8429502
               log\ likelihood = -6.8424747
Iteration 4:
               log\ likelihood = -6.8424491
Iteration 5:
Iteration 6:
               log\ likelihood = -6.8424477
```

Factor analysis/correlation
Method: maximum likelihood
Rotation: (unrotated)

Log likelihood = -6.842448

Number of obs	=	568
Retained factors	=	2
Number of params	=	11
Schwarz's BIC	=	83.4482
(Akaike's) AIC	=	35.6849

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	1.02766	0.28115	0.5792	0.5792
Factor2	0.74651		0.4208	1.0000

LR test: independent vs. saturated: chi2(15) = 269.07 Prob>chi2 = 0.0000 LR test: 2 factors vs. saturated: chi2(4) = 13.58 Prob>chi2 = 0.0087

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
bg2cost1	-0.1371	0.4235	0.8018
bg2cost2	0.4140	0.1994	0.7888
bg2cost3	0.6199	0.3692	0.4794
bg2cost4	0.3577	0.0909	0.8638
bg2cost5	-0.3752	0.4355	0.6695
bg2cost6	-0.4295	0.4395	0.6224

factor displays a likelihood-ratio test of independence against the saturated model with each estimation method. Because we are factor analyzing a correlation matrix, independence implies sphericity. Passing this test is necessary for a factor analysis to be meaningful.

In addition to the "standard" output, when you use the ml option, Stata reports a likelihood-ratio test of the number of factors in the model against the saturated model. This test is only approximately chi-squared, and we have used the correction recommended by Bartlett (1951). There are many variations on this test in use by different statistical packages.

The following comments were made by the analyst looking at these results: "There is, in my opinion, weak evidence of more than two factors. The  $\chi^2$  test for more than two factors is really a test of how well you are fitting the correlation matrix. It is not surprising that the model does not fit it perfectly. The significance of 1%, however, suggests to me that there might be a third factor. As for the loadings, they yield a similar interpretation to other factor models we fit, although there are some noteworthy differences." When we challenged the analyst on this last statement, he added that he would want to rotate the resulting factors before committing himself further.

#### □ Technical note

Stata will sometimes comment, "Note: test formally not valid because a Heywood case was encountered". The approximations used in computing the  $\chi^2$  value and degrees of freedom are mathematically justified on the assumption that an *interior* solution to the factor maximum likelihood was found. This is the case in our example above, but that will not always be so.

Boundary solutions, called Heywood solutions, often produce uniquenesses of 0, and then at least at a formal level, the test cannot be justified. Nevertheless, we believe that the reported tests are useful, even in such circumstances, provided that they are interpreted cautiously. The maximum likelihood method seems to be particularly prone to producing Heywood solutions.

This message is also printed when, in principle, there are enough free parameters to completely fit the correlation matrix, another sort of boundary solution. We say "in principle" because the correlation matrix often cannot be fit perfectly, so you will see a positive  $\chi^2$  with zero degrees of freedom. This warning note is printed because the geometric assumptions underlying the likelihood-ratio test are violated.

### □ Technical note

In a factor analysis with factors estimated with the maximum likelihood method, there may possibly be more than one local maximum, and you may want assurances that the maximum reported is the global maximum. Multiple maximums are especially likely when there is more than one group of variables, the groups are reasonably uncorrelated, and you attempt to fit a model with too few factors.

When you specify the protect(#) option, Stata performs # optimizations of the likelihood function, beginning each with random starting values, before continuing with the squared multiple correlations—initialized solution. Stata then selects the maximum of the maximums and reports it, along with a note informing you if other local maximums were found. protect(50) provides considerable assurance.

If you then wish to explore any of the nonglobal maximums, include the random option. This option, which is never specified with protect(), uses random starting values and reports the solution to which those random values converge. For multiple maximums, giving the command repeatedly will eventually report all local maximums. You are advised to set the random-number seed to ensure that your results are reproducible; see [R] set seed.

## Factor analysis from a correlation matrix

You may want to perform a factor analysis directly from a correlation matrix rather than from variables in a dataset. You may not have access to the dataset, or you may have used another method of estimating a correlation matrix—for example, as a matrix of tetrachoric correlations; see [R] **tetrachoric**. You can provide either a correlation or a covariance matrix—factormat will translate a covariance matrix into a correlation matrix.

# Example 6: Factor analysis of a correlation matrix

We illustrate with a small example with three variables on respondent's senses (visual, hearing, and taste), with a correlation matrix.

Elements within a row are separated by a comma, whereas rows are separated by a backslash, \. We now use factormat to analyze C. There are two required options here. First, the option n(979) specifies that the sample size is 979. Second, factormat has to have labels for the variables. It is possible to define row and column names for C. We did not explicitly set the names of C, so Stata has generated default row and columns names—r1 r2 r3 for the rows, and c1 c2 c3 for the columns. This will confuse factormat: why does a symmetric correlation matrix have different names for the rows and for the columns? factormat would complain about the problem and stop. We could set the row and column names of C to be the same and invoke factormat again. We can also specify the names() option with the variable names to be used.

```
. factormat C, n(979) names(visual hearing taste) fac(1) ipf (obs=979)
```

```
Factor analysis/correlation Number of obs = 979
Method: iterated principal factors Retained factors = 1
Rotation: (unrotated) Number of params = 3
```

Beware: solution is a Heywood case
(i.e., invalid or boundary values of uniqueness)

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	2.43622	2.43609	1.0000	1.0000
Factor2	0.00013	0.00028	0.0001	1.0001
Factor3	-0.00015	•	-0.0001	1.0000

LR test: independent vs. saturated: chi2(3) = 3425.87 Prob>chi2 = 0.0000 Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Uniqueness
visual	1.0961	-0.2014
hearing	0.8603	0.2599
taste	0.7034	0.5053

If we have the correlation matrix already in electronic form, this is a fine method. But if we have to enter a correlation matrix by hand, we may rather want to exploit its symmetry to enter just the upper triangle or lower triangle. This is not an issue with our small three-variable example, but what about a correlation matrix of 25 variables? However, there is an advantage to entering the correlation matrix in full symmetric form: redundancy offers some protection against making data entry errors; factormat will complain if the matrix is not symmetric.

factormat allows us to enter just one of the triangles of the correlation matrix as a vector, that is, a matrix with one row or column. We enter the upper triangle, including the diagonal,

```
. matrix Cup = (1.000, 0.943, 0.771, > 1.000, 0.605, > 1.000)
```

All elements are separated by a comma; indentation and the use of three lines are done for readability. We could have typed, all the numbers "in a row".

```
. matrix Cup = (1.000, 0.943, 0.771, 1.000, 0.605, 1.000)
```

We have to specify the option shape (upper) to inform factormat that the elements in the vector Cup are the upper triangle in rowwise order.

```
. factormat Cup, n(979) shape(upper) fac(2) names(visual hearing taste)
  (output omitted)
```

If we had entered the lower triangle of C, a vector Clow, it would have been defined as

```
. matrix Clow = (1.000, 0.943, 1.000, 0.771, 0.605, 1.000)
```

The features of factormat and factor are the same for estimation. Postestimation facilities are also the same—except that predict will not work after factormat, unless variables corresponding to the names() option exist in the dataset; see [MV] factor postestimation.

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### Stored results

factor and factormat store the following in e():

```
Scalars
    e(N)
                          number of observations
    e(f)
                          number of retained factors
    e(evsum)
                          sum of all eigenvalues
    e(df_m)
                          model degrees of freedom
    e(df_r)
                          residual degrees of freedom
    e(chi2_i)
                          likelihood-ratio test of "independence vs. saturated"
                          degrees of freedom of test of "independence vs. saturated"
    e(df_i)
    e(p_i)
                          p-value of "independence vs. saturated"
    e(11_0)
                          log likelihood of null model (ml only)
    e(11)
                          log likelihood (ml only)
    e(aic)
                          Akaike's AIC (ml only)
                          Schwarz's BIC (ml only)
    e(bic)
    e(chi2_1)
                          likelihood-ratio test of "# factors vs. saturated" (ml only)
    e(df_1)
                          degrees of freedom of test of "# factors vs. saturated" (ml only)
Macros
    e(cmd)
                          factor
    e(cmdline)
                          command as typed
    e(method)
                          pf, pcf, ipf, or ml
    e(wtype)
                          weight type (factor only)
    e(wexp)
                          weight expression (factor only)
                          Factor analysis
    e(title)
    e(mtitle)
                          description of method (e.g., principal factors)
    e(hevwood)
                          Heywood case (when encountered)
    e(matrixname)
                          input matrix (factormat only)
    e(mineigen)
                          specified mineigen() option
    e(factors)
                          specified factors() option
    e(rngstate)
                          random-number state used (seed() option only)
    e(properties)
                          nob noV eigen
    e(rotate_cmd)
                          factor_rotate
    e(estat_cmd)
                          factor_estat
                          factor_p
    e(predict)
    e(marginsnotok)
                          predictions disallowed by margins
Matrices
    e(sds)
                          standard deviations of analyzed variables
    e(means)
                          means of analyzed variables
    e(C)
                          analyzed correlation matrix
                          variance matrix common factors
    e(Phi)
    e(L)
                          factor loadings
                          uniqueness (variance of specific factors)
    e(Psi)
    e(Ev)
                          eigenvalues
Functions
    e(sample)
                          marks estimation sample (factor only)
```

rotate after factor and factormat stores items in e() along with the estimation command. See Stored results of [MV] factor postestimation and [MV] rotate for details.

Before Stata version 9, factor returned results in r(). This behavior is retained under version control.

## Methods and formulas

This section describes the statistical factor model. Suppose that there are p variables and q factors. Let  $\Psi$  represent the  $p \times p$  diagonal matrix of uniquenesses, and let  $\Lambda$  represent the  $p \times q$  factor loading matrix. Let f be a  $1 \times q$  matrix of factors. The standardized (mean 0, variance 1) vector of observed variables  $\mathbf{x}$  (1  $\times$  p) is given by the system of regression equations

$$\mathbf{x} = \mathbf{f} \mathbf{\Lambda}' + \mathbf{e}$$

where e is a  $1 \times p$  vector of errors with diagonal covariance equal to the uniqueness matrix  $\Psi$ . The common factors  $\mathbf{f}$  and the specific factors  $\mathbf{e}$  are assumed to be uncorrelated.

Under the factor model, the correlation matrix of x, called  $\Sigma$ , is decomposed by factor analysis as

$$\Sigma = \Lambda \Phi \Lambda' + \Psi$$

There is an obvious freedom in reexpressing a given decomposition of  $\Sigma$ . The default and unrotated form assumes uncorrelated common factors,  $\Phi = I$ . Stata performs this decomposition by an eigenvector calculation. First, an estimate is found for the uniqueness  $\Psi$ , and then the columns of  $\Lambda$  are computed as the q leading eigenvectors, scaled by the square root of the appropriate eigenvalue.

See Harman (1976); Mardia, Kent, and Bibby (1979); Rencher (1998, chap. 10); and Rencher and Christensen (2012, chap. 13) for discussions of estimation methods in factor analysis. Basilevsky (1994) places factor analysis in a wider statistical context and details many interesting examples and links to other methods. For details about maximum likelihood estimation, see also Lawley and Maxwell (1971) and Clarke (1970).

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### Also see

[MV] **factor postestimation** — Postestimation tools for factor and factormat

[MV] alpha — Compute interitem correlations (covariances) and Cronbach's alpha

[MV] canon — Canonical correlations

[MV] **pca** — Principal component analysis

[SEM] **intro 5** — Tour of models

[SEM] example 1 — Single-factor measurement model

[SEM] example 3 — Two-factor measurement model

[U] 20 Estimation and postestimation commands

### **Title**

factor postestimation — Postestimation tools for factor and factormat

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

## Postestimation commands

The following postestimation commands are of special interest after factor and factormat:

Command	Description
estat anti	anti-image correlation and covariance matrices
estat common	correlation matrix of the common factors
estat factors	AIC and BIC model-selection criteria for different numbers of factors
estat kmo	Kaiser-Meyer-Olkin measure of sampling adequacy
estat residuals	matrix of correlation residuals
estat rotatecompare	compare rotated and unrotated loadings
estat smc	squared multiple correlations between each variable and the rest
estat structure	correlations between variables and common factors
*estat summarize	estimation sample summary
loadingplot	plot factor loadings
rotate	rotate factor loadings
scoreplot	plot score variables
screeplot	plot eigenvalues

<sup>\*</sup> estat summarize is not available after factormat.

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results; see [R] estimates
†predict	predict regression or Bartlett scores

estimates table is not allowed, and estimates stats is allowed only with the ml factor method.

<sup>†</sup> predict after factormat works only if you have variables in memory that match the names specified in factormat. predict assumes mean zero and standard deviation one unless the means() and sds() options of factormat were provided.

# predict

### **Description for predict**

predict creates new variables containing predictions such as factors scored by the regression method or by the Bartlett method.

### Menu for predict

Statistics > Postestimation

## Syntax for predict

<pre>predict [type</pre>	[ if ] [in] [, statistic options]
statistic	Description
Main regression bartlett	regression scoring method; the default Bartlett scoring method
options	Description
Main norotated notable format(%fmt)	use unrotated results, even when rotated results are available suppress table of scoring coefficients format for displaying the scoring coefficients

## Options for predict

regression produces factors scored by the regression method. This is the default.

bartlett produces factors scored by the method suggested by Bartlett (1937, 1938). This method produces unbiased factors, but they may be less accurate than those produced by the default regression method suggested by Thomson (1951). Regression-scored factors have the smallest mean squared error from the true factors but may be biased.

norotated specifies that unrotated factors be scored even when you have previously issued a rotate command. The default is to use rotated factors if they are available and unrotated factors otherwise.

notable suppresses the table of scoring coefficients.

format(% fmt) specifies the display format for scoring coefficients.

## estat

## **Description for estat**

estat anti displays the anti-image correlation and anti-image covariance matrices. These are minus the partial covariance and minus the partial correlation matrices of all pairs of variables, holding all other variables constant.

estat common displays the correlation matrix of the common factors. For orthogonal factor loadings, the common factors are uncorrelated, and hence an identity matrix is shown. estat common is of more interest after oblique rotations.

estat factors displays model-selection criteria (AIC and BIC) for models with 1, 2, ..., # factors. Each model is estimated using maximum likelihood (that is, using the ml option of factor).

estat kmo specifies that the Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy be displayed. KMO takes values between 0 and 1, with small values meaning that overall the variables have too little in common to warrant a factor analysis. Historically, the following labels are given to values of KMO (Kaiser 1974):

0.00 to 0.49	unacceptable
0.50 to 0.59	miserable
0.60 to 0.69	mediocre
0.70 to 0.79	middling
0.80 to 0.89	meritorious
0.90 to 1.00	marvelous

estat residuals displays the raw or standardized residuals of the observed correlations with respect to the fitted (reproduced) correlation matrix.

estat rotatecompare displays the unrotated factor loadings and the most recent rotated factor loadings.

estat smc displays the squared multiple correlations between each variable and all other variables. SMC is a theoretical lower bound for communality, so it is an upper bound for uniqueness. The pf factor method estimates the communalities by smc.

estat structure displays the factor structure, that is, the correlations between the variables and the common factors.

estat summarize displays summary statistics of the variables in the factor analysis over the estimation sample. This subcommand is, of course, not available after factormat.

#### Menu for estat

Statistics > Postestimation

### Syntax for estat

```
Anti-image correlation/covariance matrices
  estat anti [, nocorr nocov <u>for</u>mat(%fmt)]
Correlation of common factors
  estat common [, norotated format(%fmt)]
Model-selection criteria
  estat factors [, factors(#) detail]
Sample adequacy measures
  estat kmo [, novar format(%fmt)]
Residuals of correlation matrix
  estat \underline{res}iduals [, \underline{f}itted \underline{o}bs \underline{sr}esiduals \underline{for}mat(fmt)
Comparison of rotated and unrotated loadings
  estat rotatecompare [, format(%fmt)]
Squared multiple correlations
  estat smc [, format(%fmt)]
Correlations between variables and common factors
  estat <u>structure</u> [, <u>norotated format(%fmt)</u>]
Summarize variables for estimation sample
  estat <u>summarize</u> [, <u>lab</u>els <u>nohea</u>der <u>noweig</u>hts]
```

# Options for estat

rotation (orthogonal or oblique).

nocorr, an option used with estat anti, suppresses the display of the anti-image correlation matrix. nocov, an option used with estat anti, suppresses the display of the anti-image covariance matrix. format(%fmt) specifies the display format. The defaults differ between the subcommands. norotated, an option used with estat common and estat structure, requests that the displayed

and returned results be based on the unrotated original factor solution rather than on the last

- factors (#), an option used with estat factors, specifies the maximum number of factors to include in the summary table.
- detail, an option used with estat factors, presents the output from each run of factor (or factormat) used in the computations of the AIC and BIC values.
- novar, an option used with estat kmo, suppresses the KMO measures of sampling adequacy for the variables in the factor analysis, displaying the overall KMO measure only.
- fitted, an option used with estat residuals, displays the fitted (reconstructed) correlation matrix on the basis of the retained factors.
- obs, an option used with estat residuals, displays the observed correlation matrix.
- sresiduals, an option used with estat residuals, displays the matrix of standardized residuals of the correlations. Be careful when interpreting these residuals; see Jöreskog and Sörbom (1988).
- labels, noheader, and noweights are the same as for the generic estat summarize command; see [R] estat summarize.

# Remarks and examples

Remarks are presented under the following headings:

Postestimation statistics Plots of eigenvalues, factor loadings, and scores Rotating the factor loadings Factor scores

### Postestimation statistics

Many postestimation statistics are available after factor and factormat.

## Example 1: Squared multiple correlations

After factor and factormat there are several "classical" methods for assessing whether the variables have enough in common to have warranted the use of a factor model. One method is to examine the squared multiple correlations of each variable with all other variables—this is usually an upper bound to communality and thus a lower bound to 1 - uniqueness (= communality) of the variables.

- . use http://www.stata-press.com/data/r14/bg2 (Physician-cost data)
- . quietly factor bg2cost1-bg2cost6, factors(2) ml
- . estat smc

Squared multiple correlations of variables with all other variables

Variable	smc
bg2cost1	0.1054
bg2cost2 bg2cost3	0.1370 0.1637
bg2cost4	0.0866
bg2cost5 bg2cost6	0.1671 0.1683
	L

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Other diagnostic tools, such as examining the anti-image correlation and anti-image covariance matrices (estat anti) and the Kaiser-Meyer-Olkin measure of sampling adequacy (estat kmo), are also available. See [MV] pca postestimation for an illustration of their use.

## Example 2: Model-selection criteria

Another set of postestimation tools help in determining the number of factors that should be retained. Later we will show the use of screeplot for producing a scree plot—a plot of the explained variance by the common factors. This is often used as a visual guide for selecting the number of factors to retain.

Some authors advocate the standard model information criteria AIC and BIC for determining the number of factors (Schwarz 1978; Akaike 1987). This presupposes that the factors are extracted by maximum likelihood. estat factors provides these measures.

. estat factors

Factor analysis with different numbers of factors (maximum likelihood)

#factors	loglik	df_m	df_r	AIC	BIC
1	-60.53727	6	9	133.0745	159.1273
2	-6.842448	11	4	35.6849	83.44823
3	-3.34e-12	15	0	30	95.13182

no Heywood cases encountered

The table shows the AIC and BIC statistics for the models with 1, 2, and 3 factors. The three-factor model is saturated, with 0 degrees of freedom. In this trivial case, and excluding the saturated case, both criteria select the two-factor model.

# ➤ Example 3: Structure matrix and observed correlations

Two estat subcommands display statistics that help in interpreting the model and the results—in particular after an oblique rotation. estat structure displays the *structure* matrix containing the correlations between the (manifest) variables and the common factors.

. estat structure

Structure matrix: correlations between variables and common factors

Factor1	Factor2
-0.1371 0.4140 0.6199 0.3577 -0.3752	0.4235 0.1994 0.3692 0.0909 0.4355
-0.4295	0.4395
	-0.1371 0.4140 0.6199 0.3577 -0.3752

This matrix of correlations coincides with the pattern matrix, that is, the matrix with factor loadings. This holds true for the unrotated factor solution as well as after an orthogonal rotation, such as a varimax rotation. It does not hold true after an oblique rotation. After an oblique rotation, the common factors are correlated. This correlation between the common factors also influences the correlation between the common factors and the manifest variables. The correlation matrix of the common factors is displayed by the common subcommand of estat. Because we have not yet rotated, we would see only an identity matrix. Later we show estat common output after an oblique rotation.

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To assess the quality of a factor model, we may compare the observed correlation matrix C with the fitted ("reconstructed") matrix  $\widehat{\Sigma} = \widehat{\Lambda} \widehat{\Phi} \widehat{\Lambda}' + \widehat{\Psi}$  by examining the raw residuals  $C - \widehat{\Sigma}$ .

. estat residuals, obs fit

Observed correlations

Variable	bg2co~1	bg2co~2	bg2co~3	bg2co~4	bg2co~5	bg2co~6
bg2cost1	1.0000					
bg2cost2	0.0920	1.0000				
bg2cost3	0.0540	0.3282	1.0000			
bg2cost4	-0.0380	0.1420	0.2676	1.0000		
bg2cost5	0.2380	-0.1394	-0.0550	-0.0567	1.0000	
bg2cost6	0.2431	-0.0671	-0.1075	-0.1329	0.3524	1.0000

Fitted ("reconstructed") values for correlations

Variable	bg2co~1	bg2co~2	bg2co~3	bg2co~4	bg2co~5	bg2co~6
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5 bg2cost6	1.0000 0.0277 0.0714 -0.0106 0.2359 0.2450	1.0000 0.3303 0.1662 -0.0685 -0.0902	0.9999 0.2553 -0.0718 -0.1040	1.0000 -0.0946 -0.1137	1.0000 0.3525	1.0000

Raw residuals of correlations (observed-fitted)

Variable	bg2co~1	bg2co~2	bg2co~3	bg2co~4	bg2co~5	bg2co~6
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5 bg2cost6	-0.0000 0.0643 -0.0174 -0.0274 0.0021 -0.0019	-0.0000 -0.0021 -0.0242 -0.0709 0.0231	0.0001 0.0124 0.0168 -0.0035	-0.0000 0.0379 -0.0193	0.0000	-0.0000

To gauge the size of the residuals, estat residuals can also display the standardized residuals.

. estat residuals, sres

Standardized residuals of correlations

Variable	bg2co~1	bg2co~2	bg2co~3	bg2co~4	bg2co~5	bg2co~6
bg2cost1 bg2cost2 bg2cost3 bg2cost4 bg2cost5 bg2cost6	-0.0001 1.5324 -0.4140 -0.6538 0.0484 -0.0434	-0.0003 -0.0480 -0.5693 -1.6848 0.5480	0.0011 0.2859 0.3993 -0.0836	-0.0000 0.9003 -0.4560	0.0001 -0.0037	-0.0000

Be careful when interpreting these standardized residuals, as they tend to be smaller than normalized residuals; that is, these residuals tend to have a smaller variance than 1 if the model is true (see Bollen [1989]).

### Plots of eigenvalues, factor loadings, and scores

Scree plots, factor loading plots, and score plots are easily obtained after factor and factormat.

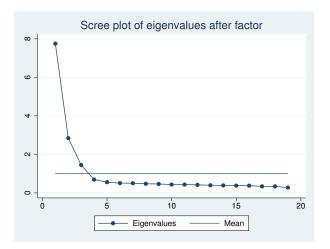
### Example 4: The scree plot

The scree plot is a popular tool for determining the number of factors to be retained. A scree plot is a plot of the eigenvalues shown in decreasing order (Cattell 1966). We fit a factor model, extracting factors with the principal factor method.

- . use http://www.stata-press.com/data/r14/sp2
- . factor ghp31-ghp05, pcf
   (output omitted)

How many factors should we retain? We issue the screeplot command with the mean option, specifying that a horizontal line be plotted at the mean of the eigenvalues (a height of 1 because we are dealing with the eigenvalues of a correlation matrix).

. screeplot, mean



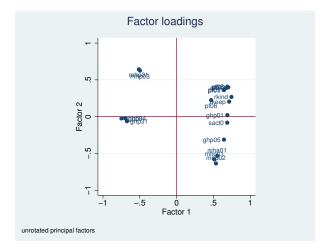
The plot suggests that we retain three factors, both because of the shape of the scree plot and because of Kaiser's well-known criterion suggesting that we retain factors with eigenvalue larger than 1. We may specify the option mineigen(1) during estimation to enforce this criterion. Here there is no need—mineigen(1) is the default with pcf.

### 4

## Example 5: Factor loadings plot

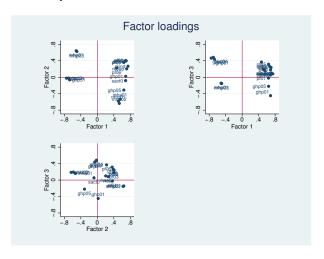
A second plot that is sometimes useful is the factor loadings plot. We display the plot with the loadings of the leading two factors.

. loadingplot, xline(0) yline(0) aspect(1) note(unrotated principal factors)



The plot makes it relatively easy to identify clusters of variables with similar loadings. With more than two factors, we can choose to see the multiple plots in a matrix style or a combined-graph style. The default is matrix style, but the combined style allows better control over various graph options—for instance, the addition of xline(0) and yline(0). Here is a combined style graph.

- . loadingplot, factors(3) combined xline(0) yline(0) aspect(1)
- > xlabel(-0.8(0.4)0.8) ylabel(-0.8(0.4)0.8)

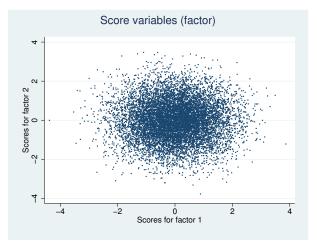


## Example 6: Score variables plot

Common factor scores can also be plotted for the observations by using the scoreplot command. (See the discussion of predict to see how you can produce score variables.)

1

. scoreplot, msymbol(smcircle) msize(tiny)



With so many observations, the plot's main purpose is to identify extreme cases. With smaller datasets with meaningful descriptions of the observations (for example, country names, brands), the score plot is good for visually clustering observations with similar loadings.

See [MV] scoreplot for more examples of loadingplot and scoreplot.

### □ Technical note

The loading plots and score plots we have shown were for the original unrotated factor solution. After rotating (which we will discuss next), these plots display the most recent rotated solution. Specify option norotated to refer to the unrotated result. To display the plots of rotated and unrotated results at the same time, you may use either of the following two approaches. First, you may display them in different Graph windows.

- . plotcmd, norotated name(name1)
- . plotcmd, name(name2)

Alternatively, you may save the plots and create a combined graph

- . plotcmd, norotated saving(name1)
- . plotcmd, saving(name2)
- . graph combine name1.gph name2.gph

See [G-2] **graph combine** for details.

# Rotating the factor loadings

Rotation is an attempt to describe the information in several factors by reexpressing them so that loadings on a few variables are as large as possible, and loadings on the rest of the variables are as small as possible. We have this freedom to reexpress because of the indeterminant nature of the factor model. For example, if you find that  $\mathbf{z}_1$  and  $\mathbf{z}_2$  are two factors, then  $\mathbf{z}_1 + \mathbf{z}_2$  and  $\mathbf{z}_1 - \mathbf{z}_2$  are equally valid solutions.

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### □ Technical note

Said more technically: we are trying to find a set of f factor variables such that the observed variables can be best explained by regressing them on the f factor variables. Usually, f is a small number such as 1 or 2. If  $f \ge 2$ , there is an inherent indeterminacy in the construction of the factors because any linear combination of the calculated factors serves equally well as a set of regressors. Rotation capitalizes on this indeterminacy to create a set of variables that looks as much like the original variables as possible.

The rotate command modifies the results of the last factor or factormat command to create a set of loadings that are more interpretable than those produced by factor or factormat. You may perform one factor analysis followed by several rotate commands, thus experimenting with different types of rotation. If you retain too few factors, the variables for several distinct concepts may be merged, as in our example below. If you retain too many factors, several factors may attempt to measure the same concept, causing the factors to get in each other's way, suggesting too many distinct concepts after rotation.

#### □ Technical note

It is possible to restrict rotation to a number of leading factors. For instance, if you extracted three factors, you may specify the option factors(2) to rotate to exclude the third factor from being rotated. The new two leading factors are combinations of the initial two leading factors and are not affected by the fixed factor.

### Example 7: Orthogonal varimax rotation

We return to our physician-cost example in [MV] factor and perform a factor analysis using the principal-component factor method, retaining two factors. We then tell rotate to apply the default orthogonal varimax rotation (Kaiser 1958).

- . use http://www.stata-press.com/data/r14/bg2, clear
  (Physician-cost data)
- . quietly factor bg2cost1-bg2cost6, pcf factors(2)
- . rotate

Factor analysis/correlation Number of obs = 568
Method: principal-component factors Retained factors = 2
Rotation: orthogonal varimax (Kaiser off) Number of params = 11

Factor	Variance	Difference	Proportion	Cumulative
Factor1	1.57170	0.03430	0.2619	0.2619
Factor2	1.53740		0.2562	0.5182

LR test: independent vs. saturated: chi2(15) = 269.07 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
bg2cost1	0.6853	0.2300	0.4775
bg2cost2	-0.0126	0.7142	0.4898
bg2cost3	-0.0161	0.7818	0.3886
bg2cost4	-0.1502	0.5703	0.6521
bg2cost5	0.7292	-0.1198	0.4539
bg2cost6	0.7398	-0.1537	0.4290

Factor rotation matrix

	Factor1	Factor2
Factor1	0.7460	-0.6659
Factor2	0.6659	0.7460

Here the factors are rotated so that the three "negative" items are grouped together and the three "positive" items are grouped.

Look at the uniqueness column. *Uniqueness* is the percentage of variance for the variable that is not explained by the common factors; we may also think of it as the variances of the specific factors for the variables. We stress that rotation involves the "common factors", so the *uniqueness* is not affected by the rotation. As we noted in [MV] **factor**, the uniqueness is relatively high in this example, placing doubt on the usefulness of the factor model here.

## 4

# Example 8: More orthogonal varimax rotation

Here we examine 19 variables describing various aspects of health. These variables were collected from a random selection of 9,999 visitors to doctors' offices by Tarlov et al. (1989). Factor analysis yields three clear factors. We then examine several rotations of these three factors.

- . use http://www.stata-press.com/data/r14/sp2
- . describe

Contains data from http://www.stata-press.com/data/r14/sp2.dta

obs: 9,999

vars: 20 26 Jan 2014 09:26 size: 779,922 (\_dta has notes)

variable name	storage type	display format	value label	variable label
patid	int	%9.0g		Case ID
ghp31	float	%9.0g		<pre>Health excellent, very good,    good, fair, poor</pre>
pf01	float	%9.0g		How long limit vigorous activity
pf02	float	%9.0g		How long limit moderate activity
pf03	float	%9.0g		How long limit walk/climb
pf04	float	%9.0g		How long limit bend/stoop
pf05	float	%9.0g		How long limit walk 1 block
pf06	float	%9.0g		How long limit eat/dress/bath
rkeep	float	%9.0g		Does health keep work-job-hse
rkind	float	%9.0g		Can't do kind/amount of work
sact0	float	%9.0g		Last month limit activities
mha01	float	%9.0g		Last month very nervous
mhp03	float	%9.0g		Last month calm/peaceful
mhd02	float	%9.0g		Last month downhearted/blue
mhp01	float	%9.0g		Last month a happy person
mhc01	float	%9.0g		Last month down in the dumps
ghp01	float	%9.0g		Somewhat ill
ghp04	float	%9.0g		Healthy as anybody I know
ghp02	float	%9.0g		Health is excellent
ghp05	float	%9.0g		Feel bad lately

Sorted by: patid

We now perform our factorization, requesting that three factors be retained.

. factor ghp31-ghp05, factors(3) (obs=9,999)

Factor analysis/correlation Number of obs = 9,999 Method: principal factors Retained factors = 3 Rotation: (unrotated) Number of params = 54

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	7.27086	4.90563	0.7534	0.7534
Factor2	2.36523	1.38826	0.2451	0.9985
Factor3	0.97697	1.00351	0.1012	1.0997
Factor4	-0.02654	0.00538	-0.0027	1.0970
Factor5	-0.03191	0.00378	-0.0033	1.0937
Factor6	-0.03569	0.00353	-0.0037	1.0900
Factor7	-0.03922	0.00271	-0.0041	1.0859
Factor8	-0.04193	0.00662	-0.0043	1.0815
Factor9	-0.04855	0.01015	-0.0050	1.0765
Factor10	-0.05870	0.00250	-0.0061	1.0704
Factor11	-0.06120	0.00224	-0.0063	1.0641
Factor12	-0.06344	0.00376	-0.0066	1.0575
Factor13	-0.06720	0.00345	-0.0070	1.0506
Factor14	-0.07065	0.00185	-0.0073	1.0432
Factor15	-0.07250	0.00033	-0.0075	1.0357
Factor16	-0.07283	0.00772	-0.0075	1.0282
Factor17	-0.08055	0.01190	-0.0083	1.0198
Factor18	-0.09245	0.00649	-0.0096	1.0103
Factor19	-0.09894		-0.0103	1.0000

LR test: independent vs. saturated: chi2(171) = 1.0e+05 Prob>chi2 = 0.0000

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Factor3	Uniqueness
ghp31	-0.6519	-0.0562	0.3440	0.4535
pf01	0.6150	0.3226	-0.0072	0.5177
pf02	0.6867	0.3737	0.2175	0.3415
pf03	0.6712	0.3774	0.1621	0.3807
pf04	0.6540	0.3588	0.2268	0.3921
pf05	0.6209	0.3258	0.2631	0.4392
pf06	0.4370	0.1803	0.2241	0.7263
rkeep	0.6868	0.1820	0.0870	0.4876
rkind	0.7244	0.2464	0.0780	0.4085
sact0	0.6556	-0.0719	0.0461	0.5628
mha01	0.5297	-0.4773	0.1268	0.4755
mhp03	-0.4810	0.5691	-0.1238	0.4294
mhd02	0.5208	-0.5949	0.1623	0.3485
mhp01	-0.4980	0.5955	-0.1225	0.3824
mhc01	0.4927	-0.5215	0.1531	0.4618
ghp01	0.6686	0.0194	-0.3621	0.4215
ghp04	-0.6833	-0.0195	0.4089	0.3656
ghp02	-0.7398	-0.0227	0.4212	0.2748
ghp05	0.6163	-0.2760	-0.1626	0.5175
	•			

The first factor is a general health factor. (To understand that claim, compare the factor loadings with the description of the variables as shown by describe above. Also, just as with the physician-cost data, the sense of some of the coded responses is reversed.) The second factor loads most highly on the five "mental health" items. The third factor loads most highly on "general health perception" items—those with names having the letters ghp in them. The other items describe "physical health".

These designations are based primarily on the wording of the questions, which is summarized in the variable labels.

#### . rotate, varimax

Factor analysis/correlation	Number of obs =	9,999
Method: principal factors	Retained factors =	3
Rotation: orthogonal varimax (Kaiser off)	Number of params =	54

Factor	Variance	Difference	Proportion	Cumulative
Factor1	4.20556	0.83302	0.4358	0.4358
Factor2	3.37253	0.33756	0.3495	0.7852
Factor3	3.03497	•	0.3145	1.0997

LR test: independent vs. saturated: chi2(171) = 1.0e+05 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Factor3	Uniqueness
ghp31	-0.2968	-0.1647	-0.6567	0.4535
pf01	0.5872	0.0263	0.3699	0.5177
pf02	0.7740	0.0848	0.2287	0.3415
pf03	0.7386	0.0580	0.2654	0.3807
pf04	0.7484	0.0842	0.2018	0.3921
pf05	0.7256	0.1063	0.1518	0.4392
pf06	0.5023	0.1268	0.0730	0.7263
rkeep	0.6023	0.2048	0.3282	0.4876
rkind	0.6590	0.1669	0.3597	0.4085
sact0	0.4187	0.3875	0.3342	0.5628
mha01	0.1467	0.6859	0.1803	0.4755
mhp03	-0.0613	-0.7375	-0.1514	0.4294
mhd02	0.0921	0.7893	0.1416	0.3485
mhp01	-0.0570	-0.7671	-0.1612	0.3824
mhc01	0.1102	0.7124	0.1359	0.4618
ghp01	0.2783	0.1977	0.6797	0.4215
ghp04	-0.2652	-0.1908	-0.7264	0.3656
ghp02	-0.2986	-0.2116	-0.7690	0.2748
ghp05	0.1755	0.4756	0.4748	0.5175

#### Factor rotation matrix

	Factor1	Factor2	Factor3
Factor1	0.6658	0.4796	0.5715
Factor2	0.5620	-0.8263	0.0387
Factor3	0.4908	0.2954	-0.8197

With rotation, the structure of the data becomes much clearer. The first rotated factor is physical health, the second is mental health, and the third is general health perception. The a priori designation of the items is confirmed.

After rotation, physical health is the first factor. rotate has ordered the factors by explained variance. Still, we warn that the importance of any factor must be gauged against the number of variables that purportedly measure it. Here we included nine variables that measured physical health, five that measured mental health, and five that measured general health perception. Had we started with only one mental health item, it would have had a high uniqueness, but we would not want to conclude that it was, therefore, largely noise.

#### □ Technical note

Some people prefer specifying the option normalize to apply a Kaiser normalization (Horst 1965), which places equal weight on all rows of the matrix to be rotated.

## > Example 9: Oblique oblimin rotation

The literature suggests that physical health and mental health are related. Also, general health perception may be largely a combination of the two. For these reasons, an oblique rotation of a two-factor solution is worth trying. We try the oblique oblimin rotation (Harman 1976).

. factor ghp31-ghp05, factors(2)
(obs=9,999)

Factor analysis/correlation Number of obs = 9,999
Method: principal factors Retained factors = 2
Rotation: (unrotated) Number of params = 37

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	7.27086	4.90563	0.7534	0.7534
Factor2	2.36523	1.38826	0.2451	0.9985
Factor3	0.97697	1.00351	0.1012	1.0997
Factor4	-0.02654	0.00538	-0.0027	1.0970
Factor5	-0.03191	0.00378	-0.0033	1.0937
Factor6	-0.03569	0.00353	-0.0037	1.0900
Factor7	-0.03922	0.00271	-0.0041	1.0859
Factor8	-0.04193	0.00662	-0.0043	1.0815
Factor9	-0.04855	0.01015	-0.0050	1.0765
Factor10	-0.05870	0.00250	-0.0061	1.0704
Factor11	-0.06120	0.00224	-0.0063	1.0641
Factor12	-0.06344	0.00376	-0.0066	1.0575
Factor13	-0.06720	0.00345	-0.0070	1.0506
Factor14	-0.07065	0.00185	-0.0073	1.0432
Factor15	-0.07250	0.00033	-0.0075	1.0357
Factor16	-0.07283	0.00772	-0.0075	1.0282
Factor17	-0.08055	0.01190	-0.0083	1.0198
Factor18	-0.09245	0.00649	-0.0096	1.0103
Factor19	-0.09894	•	-0.0103	1.0000

LR test: independent vs. saturated: chi2(171) = 1.0e+05 Prob>chi2 = 0.0000

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
ghp31	-0.6519	-0.0562	0.5718
pf01	0.6150	0.3226	0.5178
pf02	0.6867	0.3737	0.3888
pf03	0.6712	0.3774	0.4070
pf04	0.6540	0.3588	0.4435
pf05	0.6209	0.3258	0.5084
pf06	0.4370	0.1803	0.7765
rkeep	0.6868	0.1820	0.4952
rkind	0.7244	0.2464	0.4145
sact0	0.6556	-0.0719	0.5650
mha01	0.5297	-0.4773	0.4916
mhp03	-0.4810	0.5691	0.4448
mhd02	0.5208	-0.5949	0.3748
mhp01	-0.4980	0.5955	0.3974
mhc01	0.4927	-0.5215	0.4853
ghp01	0.6686	0.0194	0.5526
ghp04	-0.6833	-0.0195	0.5327
ghp02	-0.7398	-0.0227	0.4522
ghp05	0.6163	-0.2760	0.5439

. rotate, oblimin oblique

Factor analysis/correlation Method: principal factors

Rotation: oblique oblimin (Kaiser off)

Number of obs 9,999 Retained factors = 2 Number of params = 37

Factor	Variance	Proportion	Rotated factors are correlated
Factor1	6.58719	0.6826	
Factor2	4.65444	0.4823	

LR test: independent vs. saturated: chi2(171) = 1.0e+05 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
ghp31	-0.5517	-0.2051	0.5718
pf01	0.7179	-0.0747	0.5178
pf02	0.8115	-0.0968	0.3888
pf03	0.8022	-0.1068	0.4070
pf04	0.7750	-0.0951	0.4435
pf05	0.7249	-0.0756	0.5084
pf06	0.4743	-0.0044	0.7765
rkeep	0.6712	0.0939	0.4952
rkind	0.7478	0.0449	0.4145
sact0	0.4608	0.3340	0.5650
mha01	0.0652	0.6869	0.4916
mhp03	0.0401	-0.7587	0.4448
mhd02	-0.0280	0.8003	0.3748
mhp01	0.0462	-0.7918	0.3974
mhc01	0.0039	0.7160	0.4853
ghp01	0.5378	0.2484	0.5526
ghp04	-0.5494	-0.2541	0.5327
ghp02	-0.5960	-0.2736	0.4522
ghp05	0.2805	0.5213	0.5439

#### Factor rotation matrix

	Factor1	Factor2
Factor1	0.9277	0.6831
Factor2	0.3733	-0.7303

The first factor is defined predominantly by physical health and the second by mental health. General health perception loads on both, but more on physical health than mental health. To compare the rotated and unrotated solution, looking at both in parallel form is often useful.

### . estat rotatecompare

Rotation matrix — oblique oblimin (Kaiser off)

Variable	Factor1	Factor2
Factor1	0.9277	0.6831
Factor2	0.3733	-0.7303

#### Factor loadings

	Rotated		Unrot	ated
Variable	Factor1	Factor2	Factor1	Factor2
ghp31	-0.5517	-0.2051	-0.6519	-0.0562
pf01	0.7179	-0.0747	0.6150	0.3226
pf02	0.8115	-0.0968	0.6867	0.3737
pf03	0.8022	-0.1068	0.6712	0.3774
pf04	0.7750	-0.0951	0.6540	0.3588
pf05	0.7249	-0.0756	0.6209	0.3258
pf06	0.4743	-0.0044	0.4370	0.1803
rkeep	0.6712	0.0939	0.6868	0.1820
rkind	0.7478	0.0449	0.7244	0.2464
sact0	0.4608	0.3340	0.6556	-0.0719
mha01	0.0652	0.6869	0.5297	-0.4773
mhp03	0.0401	-0.7587	-0.4810	0.5691
mhd02	-0.0280	0.8003	0.5208	-0.5949
mhp01	0.0462	-0.7918	-0.4980	0.5955
mhc01	0.0039	0.7160	0.4927	-0.5215
ghp01	0.5378	0.2484	0.6686	0.0194
ghp04	-0.5494	-0.2541	-0.6833	-0.0195
ghp02	-0.5960	-0.2736	-0.7398	-0.0227
ghp05	0.2805	0.5213	0.6163	-0.2760

Look again at the factor output. The variances of the first and second factor of the unrotated solution are 7.27 and 2.37, respectively. After an orthogonal rotation, the explained variance of 7.27 + 2.37 is distributed differently over the two factors. For instance, after an orthogonal varimax rotation, the first factor has variance 5.75, and the second factor has 3.88—within rounding error 7.27 + 2.37 = 5.75 + 3.88. The situation after an oblique rotation is different. The variances of the first and second factors are 6.59 and 4.65, which add up to more than in the orthogonal case. In the oblique case, the common factors are correlated and thus "partly explain the same variance". Therefore, the cumulative proportion of variance explained by the factors is not displayed here.

Most researchers would not be willing to accept a solution in which the common factors are highly correlated.

. estat common

Correlation matrix of the oblimin(0) rotated common factors

Factors	Factor1	Factor2
Factor1 Factor2	1 .3611	1

The correlation of .36 seems acceptable, so we think that the oblique rotation was a success here.

4

## **Factor scores**

The predict command creates a set of new variables that are estimates of the first k common factors produced by factor, factormat, or rotate. Two types of scoring are available: regression or Thomson scoring and Bartlett scoring.

The number of variables may be less than the number of factors. If so, the first such factors will be used. If the number of variables is greater than the number of factors created or rotated, the unused factors will be filled with missing values.

### Example 10: Predicting scores

Using our automobile data, we wish to develop an index of roominess on the basis of a car's headroom, rear-seat leg room, and trunk space. We begin by extracting the factors of the three variables:

- . use http://www.stata-press.com/data/r14/autofull (Automobile Models)
- . factor headroom rear\_seat trunk
  (obs=74)

Factor analysis/correlation
Method: principal factors
Rotation: (unrotated)

Number of obs	=	74
Retained factors	=	1
Number of params	=	3

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1 Factor2 Factor3	1.71426 -0.07901 -0.18231	1.79327 0.10329	1.1799 -0.0544 -0.1255	1.1799 1.1255 1.0000

LR test: independent vs. saturated: chi2(3) = 82.93 Prob>chi2 = 0.0000

Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Uniqueness
headroom	0.7280	0.4700
rear_seat	0.7144	0.4897
trunk	0.8209	0.3261

All the factor loadings are positive, so we have indeed obtained a "roominess" factor. The predict command will now create the one retained factor, which we will call f1:

. predict f1
(regression scoring assumed)
Scoring coefficients (method = regression)

Variable	Factor1
headroom	0.28323
rear_seat	0.26820
trunk	0.45964

The table with scoring coefficients informs us that the factor is obtained as a weighted sum of standardized versions of headroom, rear\_seat, and trunk with weights 0.28, 0.27, and 0.46.

If factor had retained more than one factor, typing predict f1 would still have added only the first factor to our data. Typing predict f1 f2, however, would have added the first two factors to our data. f1 is now our "roominess" index, so we might compare the roominess of domestic and foreign cars:

. table foreign, c(mean f1 sd f1) row

Foreign	mean(f1)	sd(f1)
Domestic Foreign	.2022442 4780318	.9031404
Total	4.51e-09	.8804116

We find that domestic cars are, on average, roomier than foreign cars, at least in our data.

#### □ Technical note

Are common factors not supposed to be normalized to have mean 0 and standard deviation 1? In our example above, the mean is  $4.5 \times 10^{-9}$  and the standard deviation is 0.88. Why is that?

For the mean, the deviation from zero is due to numerical roundoff, which would diminish dramatically if we had typed predict double f1 instead. The explanation for the standard deviation of 0.88, on the other hand, is not numerical roundoff. At a theoretical level, the factor is supposed to have standard deviation 1, but the estimation method almost never yields that result unless an exact solution to the factor model is found. This happens for the same reason that, when you regress y on x, you do not get the same equation as if you regress x on y, unless y and y are perfectly collinear.

By the way, if you had two factors, you would expect the correlation between the two factors to be zero because that is how they are theoretically defined. The matrix algebra, however, does not usually work out that way. It is somewhat analogous to the fact that if you regress y on x and the regression assumption that the errors are uncorrelated with the dependent variable is satisfied, then it automatically cannot be satisfied if you regress x on y.

The covariance matrix of the estimated factors is

$$E(\widehat{\mathbf{f}}\widehat{\mathbf{f}}') = \mathbf{I} - (\mathbf{I} + \mathbf{\Gamma})^{-1}$$

where

$$\Gamma = \mathbf{\Lambda}' \mathbf{\Psi}^{-1} \mathbf{\Lambda}$$

ı

The columns of  $\Lambda$  are orthogonal to each other, but the inclusion of  $\Psi$  in the middle of the equation destroys that relationship unless all the elements of  $\Psi$  are equal.

1

## Example 11: Rescaling the scores

Let's pretend that we work for the K. E. Watt Company, a fictional industry group that generates statistics on automobiles. Our "roominess" index has mean 0 and standard deviation 0.88, but indexes we present to the public generally have mean 100 and standard deviation 10. First, we wish to rescale our index:

- . generate roomidx = (f1/.88041161)\*10 + 100
- . table foreign, c(mean roomidx sd roomidx freq) row format(%9.2f)

Foreign	mean(roomidx)	sd(roomidx)	Freq.
Domestic Foreign	102.30 94.57	10.26 6.94	52.00 22.00
Total	100.00	10.00	74.00

Now when we release our results, we can write, "The K. E. Watt index of roominess shows that domestic cars are, on average, roomier, with an index of 102 versus only 95 for foreign cars."

Now let's find the "roomiest" car in our data:

- . sort roomidx
- . list fullname roomidx in 1

We can also write, "K. E. Watt finds that the Mercury Marquis is the roomiest automobile among those surveyed, with a roominess index of 117 versus an average of 100."

#### □ Technical note

predict provides two methods of scoring: the default regression scoring, which we have used above, and the optional Bartlett method. An artificial example will best illustrate the use and meaning of the methods. We begin by creating a known-to-be-correct factor model in which the true loadings are 0.4, 0.6, and 0.8. The variances of the unique factors are  $1-0.4^2=0.84$ ,  $1-0.6^2=0.64$ , and  $1-0.8^2=0.36$ , respectively. We make the sample size large enough so that random fluctuations are not important.

- . drop \_all
- . set seed 12345
- . set obs 10000

number of observations (\_N) was 0, now 10,000

- . generate ftrue = rnormal()
- . generate x1 = .4\*ftrue + sqrt(.84)\*rnormal()

- . generate x2 = .6\*ftrue + sqrt(.64)\*rnormal()
- . generate x3 = .8\*ftrue + sqrt(.36)\*rnormal()
- . summarize x1 x2 x3

Variable	Obs	Mean	Std. Dev.	Min	Max
x1	10,000	.0195519	1.011165	-3.778123	4.267452
x2	10,000	.0127835	1.001259	-3.828994	4.102375
x3	10,000	.0058335	1.002475	-3.595906	3.89754

Because we concocted our data, the iterated principal-factor method reproduces the true loadings most faithfully:

. factor x1 x2 x3, ipf factors(1) (obs=10,000)

Factor analysis/correlation Number of obs = 10,000 Method: iterated principal factors Retained factors = Rotation: (unrotated) Number of params = 3

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	1.16678	1.16662	1.0000	1.0000
Factor2	0.00016	0.00036	0.0001	1.0002
Factor3	-0.00020	•	-0.0002	1.0000

LR test: independent vs. saturated: chi2(3) = 3887.29 Prob>chi2 = 0.0000 Factor loadings (pattern matrix) and unique variances

Variable	Factor1	Uniqueness
x1	0.4156	0.8273
x2	0.6046	0.6345
x3	0.7928	0.3715

Let us now compare regression and Bartlett scoring:

. predict freg (regression scoring assumed)

Scoring coefficients (method = regression)

Variable	Factor1
x1 x2 x3	0.14449 0.27410 0.61377

. predict fbar, bartlett

Scoring coefficients (method = Bartlett)

Variable	Factor1
x1	0.20285
x2	0.38475
x3	0.86162

Comparing the two scoring vectors, we see that Bartlett scoring yields larger coefficients. The regression scoring method is biased insofar as E(freg|ftrue) is not ftrue, something we can reveal by regressing freg on ftrue:

. regress freg ftrue							
Source	SS	df	MS	Numb	er of obs	=	10,000
				- F(1,	9998)	=	25339.34
Model	5107.57467	1	5107.57467	' Prob	> F	=	0.0000
Residual	2015.26671	9,998	.201566984	R-sq	uared	=	0.7171
				- Adj	R-squared	=	0.7170
Total	7122.84138	9,999	.712355374	Root	MSE	=	.44896
freg	Coef.	Std. Err.	t	P> t	[95% Con	f.	Interval]
ftrue	.7169557	.004504	159.18	0.000	.708127		.7257843
_cons	0088417	.00449	-1.97	0.049	0176429		0000404

Note the coefficient on ftrue of 0.717 < 1. The Bartlett scoring method, on the other hand, is unbiased:

. regress fbar ftrue								
	Source	SS	df	MS	Number	of obs	=	10,000
_					- F(1, 9	9998)	=	25339.33
	Model	10065.1734	1	10065.1734	Prob >	F	=	0.0000
	Residual	3971.35998	9,998	.397215441	R-squa	ared	=	0.7171
_					- Adj R-	-squared	=	0.7170
	Total	14036.5334	9,999	1.40379372	Root N	ISE	=	.63025
_								
	fbar	Coef.	Std. Err.	t	P> t	[95% Conf		Interval]
	ftrue _cons	1.006458 0124119	.0063226		0.000 0.049	.9940642 024767		1.018851

The zero bias of the Bartlett method comes at the costs of less accuracy, for example, in terms of the mean squared error.

- . generate dbar = (fbar ftrue)^2
- . generate dreg = (freg ftrue)^2
- . summarize ftrue fbar freg dbar dreg

Max	Min	Std. Dev.	Mean	Obs	Variable
3.815439	-4.196032	.996866	.0123322	10,000	ftrue
4.550449	-3.78561	1.184818	2.08e-10	10,000	fbar
3.241498	-2.696714	.8440115	-6.44e-10	10,000	freg
7.656609	1.31e-09	.5654751	.3973295	10,000	dbar
4.814044	9.68e-10	.4053233	.2812835	10,000	dreg

Neither estimator follows the assumption that the scaled factor has unit variance. The regression estimator has a variance less than 1, and the Bartlett estimator has a variance greater than 1.

The difference between the two scoring methods is not as important as it might seem because the bias in the regression method is only a matter of scaling and shifting.

. correlate freg fbar ftrue (obs=10,000)

	freg	fbar	ftrue
freg		1.0000	
ftrue	e 0.8468	0.8468	1.0000

Therefore, the choice of which scoring method we apply is largely immaterial.

## Stored results

```
Let p be the number of variables and f, the number of factors.
predict, in addition to generating variables, also stores the following in r():
Macros
    r(method)
                             regression or Bartlett
Matrices
    r(scoef)
                             p \times f matrix of scoring coefficients
estat anti stores the following in r():
Matrices
    r(acov)
                             p \times p anti-image covariance matrix
                             p \times p anti-image correlation matrix
    r(acorr)
estat common stores the following in r():
Matrices
                             f \times f correlation matrix of common factors
    r(Phi)
estat factors stores the following in r():
Matrices
    r(stats)
                             k \times 5 matrix with log likelihood, degrees of freedom, AIC, and BIC
                             for models with 1 to k factors estimated via maximum likelihood
estat kmo stores the following in r():
Scalars
                             the Kaiser-Meyer-Olkin measure of sampling adequacy
    r(kmo)
Matrices
                             column vector of KMO measures for each variable
    r(kmow)
estat residuals stores the following in r():
Matrices
                             fitted matrix for the correlations, \widehat{\mathbf{C}} = \boldsymbol{\Lambda} \boldsymbol{\Phi} \boldsymbol{\Lambda} + \boldsymbol{\Psi}
    r(fit)
                             raw residual matrix \mathbf{C} - \widehat{\mathbf{C}}
    r(res)
    r(SR)
                             standardized residuals (sresiduals option only)
estat smc stores the following in r():
Matrices
                             vector of squared multiple correlations of variables with all other variables
    r(smc)
```

See [R] estat summarize for the stored results of estat summarize.

 $p \times f$  matrix of correlations between variables and common factors

estat structure stores the following in r():

Matrices r(st)

rotate after factor and factormat add to the existing e():

```
Scalars
                          number of factors in rotated solution
    e(r_f)
    e(r_fmin)
                          rotation criterion value
Macros
    e(r_class)
                          orthogonal or oblique
    e(r_criterion)
                          rotation criterion
    e(r_ctitle)
                          title for rotation
    e(r_normalization) kaiser or none
Matrices
    e(r_L)
                          rotated loadings
    e(r_T)
                          rotation
    e(r_Phi)
                          correlations between common factors
                          explained variance by common factors
    e(r_Ev)
```

The factors in the rotated solution are in decreasing order of e(r\_Ev).

#### Methods and formulas

Methods and formulas are presented under the following headings:

estat rotate predict

#### estat

See Methods and formulas of [MV] pca postestimation for the formulas for estat anti, estat kmo, and estat smc.

estat residuals computes the standardized residuals  $\tilde{r}_{ij}$  as

$$\widetilde{r}_{ij} = \frac{\sqrt{N}(r_{ij} - f_{ij})}{\sqrt{f_{ij}^2 + f_{ii}f_{jj}}}$$

suggested by Jöreskog and Sörbom (1986), where N is the number of observations,  $r_{ij}$  is the observed correlation of variables i and j, and  $f_{ij}$  is the fitted correlation of variables i and j. Also see Bollen (1989). Caution is warranted in interpretation of these residuals; see Jöreskog and Sörbom (1988).

estat structure computes the correlations of the variables and the common factors as  $\Lambda\Phi$ .

#### rotate

See Methods and formulas of [MV] rotatemat for the details of rotation.

The correlation of common factors after rotation is T'T, where T is the factor rotation matrix, satisfying  $\mathbf{L}_{\text{rotated}} = \mathbf{L}_{\text{unrotated}}(\mathbf{T}')^{-1}$ 

## predict

The formula for regression scoring (Thomson 1951) in the orthogonal case is

$$\hat{\mathbf{f}} = \mathbf{\Lambda}' \mathbf{\Sigma}^{-1} \mathbf{x}$$

where  $\Lambda$  is the unrotated or orthogonally rotated loading matrix. For oblique rotation, the regression scoring is defined as

$$\widehat{\mathbf{f}} = \mathbf{\Phi} \mathbf{\Lambda}' \mathbf{\Sigma}^{-1} \mathbf{x}$$

where  $\Phi$  is the correlation matrix of the common factors.

The formula for Bartlett scoring (Bartlett 1937, 1938) is

$$\Gamma^{-1} \Lambda' \Psi^{-1} \mathbf{x}$$

where

$$\Gamma = \Lambda' \Psi^{-1} \Lambda$$

See Harman (1976) and Lawley and Maxwell (1971).

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Thomson, G. H. 1951. The Factorial Analysis of Human Ability. London: University of London Press.

Also see References in [MV] factor.

## Also see

[MV] **factor** — Factor analysis

[MV] rotate — Orthogonal and oblique rotations after factor and pca

[MV] **scoreplot** — Score and loading plots

[MV] screeplot — Scree plot

[U] 20 Estimation and postestimation commands

#### Title

hotelling — Hotelling's T-squared generalized means test

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

hotelling performs Hotelling's T-squared test of whether a set of means is zero or, alternatively, equal between two groups.

See [MV] **mvtest means** for generalizations of Hotelling's one-sample test with more general hypotheses, two-sample tests that do not assume that the covariance matrices are the same in the two groups, and tests with more than two groups.

#### **Quick start**

Hotelling's T-squared test that the means of v1, v2, and v3 are jointly zero hotelling v1 v2 v3

As above, but suppress the table of means

hotelling v1 v2 v3, notable

Hotelling's T-squared test that the means of v1, v2, and v3 are the same in the two groups defined by catvar

hotelling v1 v2 v3, by(catvar)

#### Menu

 ${\it Statistics} > {\it Multivariate analysis} > {\it MANOVA}, \ {\it multivariate regression}, \ {\it and related} > {\it Hotelling's generalized means test}$ 

# **Syntax**

aweights and fweights are allowed; see [U] 11.1.6 weight.

Note: hotel is a synonym for hotelling.

# **Options**

Main

by (varname) specifies a variable identifying two groups; the test of equality of means between groups is performed. If by() is not specified, a test of means being jointly zero is performed.

notable suppresses printing a table of the means being compared.

# Remarks and examples

hotelling performs Hotelling's T-squared test of whether a set of means is zero or two sets of means are equal. It is a multivariate test that reduces to a standard t test if only one variable is specified.

## Example 1

You wish to test whether a new fuel additive improves gas mileage in both stop-and-go and highway situations. Taking 12 cars, you fill them with gas and run them on a highway-style track, recording their gas mileage. You then refill them and run them on a stop-and-go style track. Finally, you repeat the two runs, but this time you use fuel with the additive. Your dataset is

. use http://www.stata-press.com/data/r14/gasexp

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. describe

obs:

Contains data from http://www.stata-press.com/data/r14/gasexp.dta

vars: 5 size: 96 21 Nov 2014 12:56

variable name	storage type	display format	value label	variable label
id	byte	%9.0g		car ID
bmpg1	byte	%9.0g		track 1 before additive
ampg1	byte	%9.0g		track 1 after additive
bmpg2	byte	%9.0g		track 2 before additive
ampg2	float	%9.0g		track 2 after additive

Sorted by:

To perform the statistical test, you jointly test whether the differences in before-and-after results are zero:

- . generate diff1 = ampg1 bmpg1
- . generate diff2 = ampg2 bmpg2
- . hotelling diff1 diff2

Variable	Obs	Mean	Std. Dev.	Min	Max
diff1	12	1.75	2.70101	-3	5
diff2	12	2.083333	2.906367	-3.5	5.5

1-group Hotelling's T-squared = 9.6980676

F test statistic:  $((12-2)/(12-1)(2)) \times 9.6980676 = 4.4082126$ 

HO: Vector of means is equal to a vector of zeros F(2,10) = 4.40820.0424 Prob > F(2,10) =

The means are different at the 4.24% significance level.

☐ Technical note

We used Hotelling's T-squared test because we were testing two differences jointly. Had there been only one difference, we could have used a standard t test, which would have yielded the same results as Hotelling's test:

1

. ttest ampg1 = bmpg1

Paired t test

Variable	Obs	Mean	Std. Err.	Std. Dev.	[95% Conf.	Interval]
ampg1 bmpg1	12 12	22.75 21	.9384465 .7881701	3.250874 2.730301	20.68449 19.26525	24.81551 22.73475
diff	12	1.75	.7797144	2.70101	.0338602	3.46614

mean(diff) = mean(ampg1 - bmpg1) 2.2444 t = Ho: mean(diff) = 0degrees of freedom =

Ha: mean(diff) < 0Ha: mean(diff) != 0 Ha: mean(diff) > 0 Pr(T < t) = 0.9768Pr(|T| > |t|) = 0.0463Pr(T > t) = 0.0232

. ttest diff1 = 0

One-sample t test

Variable	Obs	Mean	Std. Err.	Std. Dev.	[95% Conf.	Interval]
diff1	12	1.75	.7797144	2.70101	.0338602	3.46614

mean = mean(diff1) 2,2444 t. =

Ho: mean = 0degrees of freedom =

Ha: mean < 0 Ha: mean != 0Ha: mean > 0Pr(T < t) = 0.9768Pr(|T| > |t|) = 0.0463Pr(T > t) = 0.0232

#### . hotelling diff1

Variable	Obs	Mean	Std. Dev.	Min	Max
diff1	12	1.75	2.70101	-3	5

1-group Hotelling's T-squared = 5.0373832

F test statistic:  $((12-1)/(12-1)(1)) \times 5.0373832 = 5.0373832$ 

HO: Vector of means is equal to a vector of zeros F(1,11) = 5.0374

F(1,11) = 0.0374Prob > F(1,11) = 0.0463

# ▶ Example 2

Now consider a variation on the experiment: rather than using 12 cars and running each car with and without the fuel additive, you run 24 cars, 12 with the additive and 12 without. You have the following dataset:

- . use http://www.stata-press.com/data/r14/gasexp2, clear
- . describe

size:

Contains data from http://www.stata-press.com/data/r14/gasexp2.dta

obs: 24 vars: 4

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variable name	storage type	display format	value label	variable label	
id mpg1 mpg2 additive	byte byte float byte	%9.0g %9.0g %9.0g %9.0g	yesno	car ID track 1 track 2 additive?	

#### Sorted by:

. tabulate additive

additive?	Freq.	Percent	Cum.
no yes	12 12	50.00 50.00	50.00 100.00
Total	24	100.00	

This is an unpaired experiment because there is no natural pairing of the cars; you want to test that the means of mpg1 are equal for the two groups specified by additive, as are the means of mpg2:

. hotelling mpg1 mpg2, by(additive)

-> additive = :	no				
Variable	Obs	Mean	Std. Dev.	Min	Max
mpg1	12	21	2.730301	17	25
mpg1 mpg2	12	19.91667	2.644319	16	24

3.316625

28

4

27.5

16.5

-> additive = yes Variable Obs Mean Std. Dev. Min Max mpg1 12 22.75 3.250874 17

22

2-group Hotelling's T-squared = 7.1347584

mpg2

F test statistic:  $((24-2-1)/(24-2)(2)) \times 7.1347584 = 3.4052256$ 

HO: Vectors of means are equal for the two groups

12

F(2,21) =3.4052 Prob > F(2,21) =0.0524

#### □ Technical note

As in the paired experiment, had there been only one test track, the t test would have yielded the same results as Hotelling's test:

. hotelling mpg1, by(additive)

-> additive =	no				
Variable	Obs	Mean	Std. Dev.	Min	Max
mpg1	12	21	2.730301	17	25
-> additive =	yes				
Variable	Obs	Mean	Std. Dev.	Min	Max
mpg1	12	22.75	3.250874	17	28

2-group Hotelling's T-squared = 2.0390921

F test statistic:  $((24-1-1)/(24-2)(1)) \times 2.0390921 = 2.0390921$ 

HO: Vectors of means are equal for the two groups

F(1,22) =2.0391 Prob > F(1,22) =0.1673

. ttest mpg1, by(additive)

Two-sample t test with equal variances

Group	Obs	Mean	Std. Err.	Std. Dev.	[95% Conf.	Interval]
no yes	12 12	21 22.75	.7881701 .9384465	2.730301 3.250874	19.26525 20.68449	22.73475 24.81551
combined	24	21.875	.6264476	3.068954	20.57909	23.17091
diff		-1.75	1.225518		-4.291568	.7915684

diff = mean(no) - mean(yes) t = -1.4280

Ho: diff = 0degrees of freedom =

Ha: diff < 0 Ha: diff != 0 Ha: diff > 0 Pr(T < t) = 0.0837Pr(|T| > |t|) = 0.1673Pr(T > t) = 0.9163

With more than one pair of means, however, there is no t test equivalent to Hotelling's test, although there are other logically (but not practically) equivalent solutions. One is the discriminant function: if the means of mpg1 and mpg2 are different, the discriminant function should separate the groups along that dimension.

. regress additive mpg1 mpg2

Source	SS	df	MS	Number of obs	=	24
Model Residual	1.46932917 4.53067083	2 21	.734664585 .21574623		= =	3.41 0.0524 0.2449 0.1730
Total	6	23	.260869565		=	.46448
additive	Coef.	Std. Err.	t	P> t  [95% C	onf.	Interval]
mpg1 mpg2 _cons	4570407 .5014605 0120115	.2416657 .2376762 .7437049	2.11	0.0729596 0.047 .00718 0.987 -1.558	59	.0455306 .9957352 1.534607

This test would declare the means different at the 5.24% level. You could also have fit this model by using logistic regression:

. logit additive mpg1 mpg2

log likelihood = -16.635532Iteration 0: Iteration 1: log likelihood = -13.395178Iteration 2:  $log\ likelihood = -13.371201$ log likelihood = -13.371143Iteration 3: Iteration 4: log likelihood = -13.371143

Logistic regression

Number of obs 24 6.53 LR chi2(2) = Prob > chi2 = 0.0382 Pseudo R2 0.1962

Log likelihood = -13.371143

additive	Coef.	Std. Err.	z	P> z	[95% Conf.	Interval]
mpg1	-2.306844	1.36139	-1.69	0.090	-4.975119	.3614307
mpg2	2.524477	1.367373	1.85	0.065	1555257	5.20448
_cons	-2.446527	3.689821	-0.66	0.507	-9.678443	4.78539

This test would have declared the means different at the 3.82% level.

Are the means different? Hotelling's T-squared and the discriminant function reject equality at the 5.24% level. The logistic regression rejects equality at the 3.82% level.

## Stored results

hotelling stores the following in r():

Scalars

r(N) number of observations r(T2) Hotelling's T-squared number of variables degrees of freedom r(k)r(df)

## Methods and formulas

See Wilks (1962, 556–561) for a general discussion. The original formulation was by Hotelling (1931) and Mahalanobis (1930, 1936).

For the test that the means of k variables are 0, let  $\overline{\mathbf{x}}$  be a  $1 \times k$  matrix of the means and  $\mathbf{S}$  be the estimated covariance matrix. Then  $T^2 = \overline{\mathbf{x}} \mathbf{S}^{-1} \overline{\mathbf{x}}'$ .

For two groups, the test of equality is  $T^2 = (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2) \mathbf{S}^{-1} (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)'$ .

Harold Hotelling (1895–1973) was an American economist and statistician who made many important contributions to mathematical economics, multivariate analysis, and statistical inference. After obtaining degrees in journalism and mathematics, he taught and researched at Stanford, Columbia, and the University of North Carolina. His work generalizing Student's t ratio and on principal components, canonical correlation, multivariate analysis of variance, and correlation continues to be widely used.

Prasanta Chandra Mahalanobis (1893–1972) studied physics and mathematics at Calcutta and Cambridge. He became interested in statistics and on his return to India worked on applications in anthropology, meteorology, hydrology, and agriculture. Mahalanobis became the leader in Indian statistics, specializing in multivariate problems (including what is now called the Mahalanobis distance), the design of large-scale sample surveys, and the contribution of statistics to national planning.

#### References

Hotelling, H. 1931. The generalization of Student's ratio. Annals of Mathematical Statistics 2: 360-378.

Mahalanobis, P. C. 1930. On tests and measures of group divergence. *Journal of the Asiatic Society of Bengal* 26: 541–588.

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Olkin, I., and A. R. Sampson. 2001. Harold Hotelling. In *Statisticians of the Centuries*, ed. C. C. Heyde and E. Seneta, 454–458. New York: Springer.

Rao, C. R. 1973. Prasantha Chandra Mahalanobis, 1893–1972. Biographical Memoirs of Fellows of The Royal Society 19: 455–492.

Wilks, S. S. 1962. Mathematical Statistics. New York: Wiley.

# Also see

[MV] manova — Multivariate analysis of variance and covariance

[MV] **mvtest means** — Multivariate tests of means

[R] **regress** — Linear regression

[R] **ttest** — t tests (mean-comparison tests)

#### **Title**

manova — Multivariate analysis of variance and covariance

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# **Description**

The manova command fits multivariate analysis-of-variance (MANOVA) and multivariate analysis-of-covariance (MANCOVA) models for balanced and unbalanced designs, including designs with missing cells, and for factorial, nested, or mixed designs, or designs involving repeated measures.

The mvreg command (see [MV] mvreg) will display the coefficients, standard errors, etc., of the multivariate regression model underlying the last run of manova.

See [R] **anova** for univariate ANOVA and ANCOVA models. See [MV] **mytest covariances** for Box's test of MANOVA's assumption that the covariance matrices of the groups are the same, and see [MV] **mytest means** for multivariate tests of means that do not make this assumption.

## **Quick start**

```
One-way MANOVA model of y1 and y2 for factor a
```

manova 
$$y1$$
  $y2 = a$ 

Two-way full-factorial MANOVA model for factors a and b

manova 
$$v1$$
  $v2$  =  $a##b$ 

Add continuous covariate x1 for a MANCOVA model

```
manova y1 y2 = a##b c.x1
```

MANOVA model with factor b nested within a

manova y1 y2 = a / b|a /

## Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > MANOVA

# **Syntax**

```
\underline{\text{mano}}va depvarlist = termlist [if] [in] [weight] [, options]
```

where *termlist* is a factor-variable list (see [U] **11.4.3 Factor variables**) with the following additional features:

- Variables are assumed to be categorical; use the c. factor-variable operator to override this.
- The | symbol (indicating nesting) may be used in place of the # symbol (indicating interaction).
- The / symbol is allowed after a term and indicates that the following term is the error term for the preceding terms.

options	Description	
Model		
<u>nocons</u> tant	suppress constant term	
$\underline{\mathtt{dropemp}}\mathtt{tycells}$	drop empty cells from the design matrix	
- • •	e, and statsby are allowed; see [U] 11.1.10 Prefix commands.	_

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

# **Options**

Model

noconstant suppresses the constant term (intercept) from the model.

dropemptycells drops empty cells from the design matrix. If c(emptycells) is set to keep (see [R] set emptycells), this option temporarily resets it to drop before running the MANOVA model. If c(emptycells) is already set to drop, this option does nothing.

# Remarks and examples

Remarks are presented under the following headings:

Introduction
One-way MANOVA
Reporting coefficients
Two-way MANOVA
N-way MANOVA
MANCOVA
MANOVA for Latin-square designs
MANOVA for mixed designs
MANOVA with repeated measures

#### Introduction

MANOVA is a generalization of ANOVA allowing multiple dependent variables. Several books discuss MANOVA, including Anderson (2003); Mardia, Kent, and Bibby (1979); Morrison (2005); Rencher (1998); Rencher and Christensen (2012); Seber (1984); and Timm (1975). Introductory articles are provided by Pillai (1985) and Morrison (1998). Pioneering work is found in Wilks (1932), Pillai (1955), Lawley (1938), Hotelling (1951), and Roy (1939).

Four multivariate statistics are commonly computed in MANOVA: Wilks's lambda, Pillai's trace, Lawley-Hotelling trace, and Roy's largest root. See *Methods and formulas* for details.

Why four statistics? Arnold (1981), Rencher (1998), Rencher and Christensen (2012), Morrison (1998), Pillai (1985), and Seber (1984) provide guidance. All four tests are admissible, unbiased, and invariant. Asymptotically, Wilks's lambda, Pillai's trace, and the Lawley–Hotelling trace are the same, but their behavior under various violations of the null hypothesis and with small samples is different. Roy's largest root is different from the other three, even asymptotically.

None of the four multivariate criteria appears to be most powerful against all alternative hypotheses. For instance, Roy's largest root is most powerful when the null hypothesis of equal mean vectors is violated in such a way that the mean vectors tend to lie in one line within p-dimensional space. For most other situations, Roy's largest root performs worse than the other three statistics. Pillai's trace tends to be more robust to nonnormality and heteroskedasticity than the other three statistics.

The # symbol indicates interaction. The | symbol indicates nesting ( $a \mid b$  is read "a is nested within b"). A / between *terms* indicates that the *term* to the right of the slash is the error term for the *terms* to the left of the slash.

## One-way MANOVA

A one-way MANOVA is obtained by specifying the dependent variables followed by an equal sign, followed by the categorical variable defining the groups.

# Example 1: One-way MANOVA with balanced data

Rencher and Christensen (2012, 183–186) presents an example of a balanced one-way MANOVA by using data from Andrews and Herzberg (1985, 357–360). The data from eight trees from each of six apple tree rootstocks are from table 6.2 of Rencher and Christensen (2012). Four dependent variables are recorded for each tree: trunk girth at 4 years (mm  $\times$  100), extension growth at 4 years (m), trunk girth at 15 years (mm  $\times$  100), and weight of tree above ground at 15 years (lb  $\times$  1000). The grouping variable is rootstock, and the four dependent variables are y1, y2, y3, and y4.

```
. use http://www.stata-press.com/data/r14/rootstock
(Table 6.2 Rootstock Data, Rencher and Christensen (2012))
```

. describe

Contains	data from http://www.	stata-press.com/data/r14/rootstock.dta
obs:	48	Table 6.2 Rootstock Data,
		Rencher and Christensen (2012)
vars:	5	30 Aug 2014 14:00
size:	816	(_dta has notes)

variable name	storage type	display format	value label	variable label
rootstock y1 y2 y3	byte float float float	%9.0g %4.2f %5.3f %4.2f		trunk girth at 4 years (mm x 100) extension growth at 4 years (m) trunk girth at 15 years (mm x 100)
y4	float	%5.3f		weight of tree above ground at 15 years (1b x 1000)

#### Sorted by:

. list in 7/10

	rootst~k	у1	у2	у3	у4
7.	1	1.11	3.211	3.98	1.209
8.	1	1.16	3.037	3.62	0.750
9.	2	1.05	2.074	4.09	1.036
10.	2	1.17	2.885	4.06	1.094

There are six rootstocks and four dependent variables. We test to see if the four-dimensional mean vectors of the six rootstocks are different. The null hypothesis is that the mean vectors are the same for the six rootstocks. To obtain one-way MANOVA results, we type

. manova y1 y2 y3 y4 = rootstock Number of obs = 48 W = Wilks' lambda L = Lawley-Hotelling trace P = Pillai's trace R = Roy's largest root Source Statistic df F(df1, df2) =F Prob>F 5 20.0 130.3 rootstock 0.1540 4.94 0.0000 a Р 1.3055 20.0 168.0 4.07 0.0000 a 2.9214 20.0 150.0 5.48 0.0000 a 42.0 1.8757 5.0 15.76 0.0000 u Residual 42 Total 47

e = exact, a = approximate, u = upper bound on F

All four multivariate tests reject the null hypothesis, indicating some kind of difference between the four-dimensional mean vectors of the six rootstocks.

Let's examine the output of manova. Above the table, it lists the number of observations used in the estimation. It also gives a key indicating that W stands for Wilks's lambda, P stands for Pillai's trace, L stands for Lawley-Hotelling trace, and R indicates Roy's largest root.

The first column of the table gives the source. Here we are testing the rootstock term (the only term in the model), and we are using residual error for the denominator of the test. Four lines of output are presented for rootstock, one line for each of the four multivariate tests, as indicated by the W, P, L, and R in the second column of the table.

The next column gives the multivariate statistics. Here Wilks's lambda is 0.1540, Pillai's trace is 1.3055, the Lawley–Hotelling trace is 2.9214, and Roy's largest root is 1.8757. Some authors report  $\lambda_1$  and others (including Rencher and Christensen) report  $\theta = \lambda_1/(1+\lambda_1)$  for Roy's largest root. Stata reports  $\lambda_1$ .

The column labeled "df" gives the hypothesis degrees of freedom, the residual degrees of freedom, and the total degrees of freedom. These are just as they would be for an ANOVA. Because there are six rootstocks, we have 5 degrees of freedom for the hypothesis. There are 42 residual degrees of freedom and 47 total degrees of freedom.

The next three columns are labeled "F(df1, df2) = F", and for each of the four multivariate tests, the degrees of freedom and F statistic are listed. The following column gives the associated p-values for the F statistics. Wilks's lambda has an F statistic of 4.94 with 20 and 130.3 degrees of freedom, which produces a p-value small enough that 0.0000 is reported. The F statistics and p-values for the other three multivariate tests follow on the three lines after Wilks's lambda.

The final column indicates whether the F statistic is exactly F distributed, is approximately F distributed, or is an upper bound. The letters e, e, and e indicate these three possibilities, as described in the footer at the bottom of the table. For this example, the F statistics (and corresponding e-values) for Wilks's lambda, Pillai's trace, and the Lawley-Hotelling trace are approximate. The e-f statistic for Roy's largest root is an upper bound, which means that the e-value is a lower bound.

Examining some of the underlying matrices and values used in the calculation of the four multivariate statistics is easy. For example, you can list the sum of squares and cross products (SSCP) matrices for error and the hypothesis that are found in the e(E) and  $e(H_m)$  returned matrices, the eigenvalues of  $E^{-1}H$  obtained from the  $e(eigvals_m)$  returned matrix, and the three auxiliary values (s, m, and n) that are returned in the  $e(aux_m)$  matrix.

```
. mat list e(E)
symmetric e(E)[4,4]
           y1
                      у2
                                  v3
                                             v4
у1
   .31998754
y2 1.6965639
                12.14279
   .55408744
               4.3636123
                          4.2908128
    .21713994 2.1102135
                          2.4816563
                                      1.7225248
. mat list e(H_m)
symmetric e(H_m)[4,4]
           y1
                      y2
                                  yЗ
                                             y4
y1
   .07356042
y2 .53738525
              4.1996621
y3 .33226448 2.3553887
                           6.1139358
   .20846994 1.6371084
                           3.7810439
. mat list e(eigvals_m)
e(eigvals_m)[1,4]
                                  с3
                                             c4
           c1
                      c2
r1 1.8756709 .79069412
                           .22904906
                                      .02595358
. mat list e(aux_m)
e(aux_m)[3,1]
   value
       4
s
       0
m
n
    18.5
```

The values s, m, and n are helpful when you do not want to rely on the approximate F tests but instead want to look up critical values for the multivariate tests. Tables of critical values can be found in many multivariate texts, including Rencher (1998) and Rencher and Christensen (2012).

See example 1 in [MV] manova postestimation for an illustration of using test for Wald tests on expressions involving the underlying coefficients of the model and lincom for displaying linear combinations along with standard errors and confidence intervals from this MANOVA example.

See examples 1–5 in [MV] discrim Ida postestimation for a descriptive linear discriminant analysis of the rootstock data. Many researchers use linear discriminant analysis as a method of exploring the differences between groups after a MANOVA model.

4

#### Example 2: One-way MANOVA with unbalanced data

Table 4.5 of Rencher (1998) presents data reported by Allison, Zappasodi, and Lurie (1962). The dependent variables y1, recording the number of bacilli inhaled per tubercle formed, and y2, recording tubercle size (in millimeters), were measured for four groups of rabbits. Group one (unvaccinated control) and group two (infected during metabolic depression) have seven observations each, whereas group three (infected during heightened metabolic activity) has 5 observations, and group four (infected during normal activity) has only 2 observations.

. use http://www.stata-press.com/data/r14/metabolic (Table 4.5 Metabolic Comparisons of Rabbits -- Rencher (1998))

. list

	group	у1	у2
1. 2. 3.	1 1 1	24 13.3 12.2	3.5 3.5 4
3. 4.	1	14.2	4
5.	1	22.2	3.6
6.	1	16.1	4.3
7.	1	27.9	5.2
8.	2	7.4	3.5
9.	2	13.2	3
10.	2	8.5	3
11.	2	10.1	3
12.	2	9.3	2
13.	2	8.5	2.5
14.	2	4.3	1.5
15.	3	16.4	3.2
16.	3	24	2.5
17.	3	53	1.5
18.	3	32.7	2.6
19.	3	42.8	2
20.	4	25.1	2.7
21.	4	5.9	2.3

The one-way MANOVA for testing the null hypothesis that the two-dimensional mean vectors for the four groups of rabbits are equal is

. manova y1 y2 = group

		Νι	umber of ol	os =	21			
		W = Wilks' lambda P = Pillai's trace			<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>			
	Source	St	atistic	df	F(df1,	df2) =	F	Prob>F
	group	W P L R	0.1596 1.2004 3.0096 1.5986	3	6.0 6.0 6.0 3.0	32.0 34.0 30.0 17.0	8.51 7.52	0.0000 0.0000 0.0001 0.0008
	Residual			17				
_	Total			20				

e = exact, a = approximate, u = upper bound on F

All four multivariate tests indicate rejection of the null hypothesis. This indicates that there are one or more differences among the two-dimensional mean vectors for the four groups. For this example, the F test for Wilks's lambda is exact because there are only two dependent variables in the model.

manovatest tests terms or linear combinations of the model's underlying design matrix. Example 2 of [MV] manova postestimation continues this example and illustrates manovatest.

#### Reporting coefficients

The mvreg command (see [MV] mvreg) is used as a coefficient displayer after manova. Simply type mvreg to view the coefficients, standard errors, t statistics, p-values, and confidence intervals of the multivariate regression model underlying the previous manova.

4

## Example 3: Reporting coefficients by using myreg

Continuing with example 2, we now use mvreg to display the coefficients underlying our MANOVA.

. mvr	reg						
Equation		Obs	Parms	RMSE	"R-sq"	F	P
y1		21	4	8.753754	0.5867	8.045716	0.0015
у2		21	4	.6314183	0.6108	8.891362	0.0009
		Coef.	Std. E	err. t	P> t	[95% Conf	f. Interval]
y1							
	group						
	2	-9.771429	4.6790	78 -2.09	0.052	-19.64342	.1005633
	3	15.25143	5.1256	73 2.98	0.008	4.437203	26.06565
	4	-3.028571	7.0186	-0.43	0.672	-17.83656	11.77942
	_cons	18.52857	3.3086	5.60	0.000	11.54802	25.50912
y2							
	group						
	2	-1.371429	.33750	73 -4.06	0.001	-2.083507	6593504
	3	-1.654286	.36972	07 -4.47	0.000	-2.434328	8742432
	4	-1.514286	.50626	09 -2.99	0.008	-2.582403	4461685
	_cons	4.014286	.23865	37 16.82	0.000	3.51077	4.517801

mvreg options allowed on replay, such as level(), vsquish, and base, may also be specified to alter what is displayed.

1

# Two-way MANOVA

You can include multiple explanatory variables with the manova command, and you can specify interactions by placing '#' between the variable names.

# Example 4: Two-way MANOVA with unbalanced data

Table 4.6 of Rencher (1998) presents unbalanced data from Woodard (1931) for a two-way MANOVA with three dependent variables (y1, y2, and y3) measured on patients with fractures of the jaw. y1 is age of patient, y2 is blood lymphocytes, and y3 is blood polymorphonuclears. The two design factors are gender (1 = male, 2 = female) and fracture (indicating the type of fracture: 1 = one compound fracture, 2 = two compound fractures, and 3 = one simple fracture). gender and fracture are numeric variables with value labels.

. use http://www.stata-press.com/data/r14/jaw

(Table 4.6 Two-Way Unbalanced Data for Fractures of the Jaw -- Rencher (1998))

. describe

Contains data from http://www.stata-press.com/data/r14/jaw.dta

Table 4.6 Two-Way Unbalanced Data for Fractures of the Jaw

-- Rencher (1998)

5 vars: size: 135 20 Apr 2014 14:53 (\_dta has notes)

variable name	storage type	display format	value label	variable label
gender fracture y1	byte byte byte	%9.0g %22.0g %9.0g	gender fractype	age
у2 у3	byte byte	%9.0g %9.0g		blood lymphocytes blood polymorphonuclears

#### Sorted by:

. list in 19/22

	gender	fracture	у1	у2	у3
19.	male	one simple fracture	55	32	60
20.	male	one simple fracture	30	34	62
21.	female	one compound fracture	22	56	43
22.	female	two compound fractures	22	29	68

The two-way factorial MANOVA for these data is

. manova y1 y2 y3 = gender fracture gender#fracture

			-					
	Nι	umber of o	bs =	27				
	W = Wilks' lambda			L = Lawley-Hotelling trace				
	P	= Pillai'	s trace	R = Roy'	s largest	root		
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
Model	W	0.2419	5	15.0	52.9	2.37	0.0109	- а
	Р	1.1018		15.0	63.0	2.44	0.0072	a
	L	1.8853		15.0	53.0	2.22	0.0170	a
	R	0.9248		5.0	21.0	3.88	0.0119	u
Residual			21					_
gender	W	0.7151	1	3.0	19.0	2.52	0.0885	- е
_	Р	0.2849		3.0	19.0	2.52	0.0885	е
	L	0.3983		3.0	19.0	2.52	0.0885	е
	R	0.3983		3.0	19.0	2.52	0.0885	е
fracture	W	0.4492	2	6.0	38.0	3.12	0.0139	- е
	P	0.6406		6.0	40.0	3.14	0.0128	a
	L	1.0260		6.0	36.0	3.08	0.0155	a
	R	0.7642		3.0	20.0	5.09	0.0088	u
gender#fracture	W	0.5126	2	6.0	38.0	2.51	0.0380	- е
	Р	0.5245		6.0	40.0	2.37	0.0472	a
	L	0.8784		6.0	36.0	2.64	0.0319	a
	R	0.7864		3.0	20.0	5.24	0.0078	u
Residual			21					_
Total			26					-

e = exact, a = approximate, u = upper bound on F

For MANOVA models with more than one term, the output of manova shows test results for the overall model, followed by results for each term in the MANOVA.

The interaction term, gender#fracture, is significant at the 0.05 level. Wilks's lambda for the interaction has an exact F that produces a p-value of 0.0380.

Example 3 of [MV] manova postestimation illustrates how the margins postestimation command can be used to examine details of this significant interaction. It also illustrates how to obtain residuals by using predict.

# N-way MANOVA

Higher-order MANOVA models are easily constructed using # to indicate the interaction terms.

# Example 5: MANOVA with interaction terms

Data on the wear of coated fabrics is provided by Box (1950) and is presented in table 6.20 of Rencher and Christensen (2012, 249). Variables y1, y2, and y3 are the wear after successive 1,000 revolutions of an abrasive wheel. Three factors are also recorded. treatment is the surface treatment and has two levels. filler is the filler type, also with two levels. proportion is the proportion of filler and has three levels (25%, 50%, and 75%).

. use http://www.stata-press.com/data/r14/fabric (Table 6.20 Wear of coated fabrics, Rencher and Christensen (2012))

. describe

Contains data from http://www.stata-press.com/data/r14/fabric.dta

Table 6.20 Wear of coated fabrics, Rencher and Christensen (2012)

vars: 6 size: 216 30 Aug 2014 14:01 (\_dta has notes)

variable name	storage type	display format	value label	variable label
treatment filler proportion y1 y2 y3	byte byte byte int int int	%9.0g %9.0g %9.0g %9.0g %9.0g %9.0g	prop	Surface treatment Filler type Proportion of filler First 1000 revolutions Second 1000 revolutions Third 1000 revolutions

#### Sorted by:

. label list prop

prop:

1 25% 2 50% 3 75%

. list

	treatm~t	filler	propor~n	у1	у2	у3
1.	0	1	25%	194	192	141
2.	0	1	50%	233	217	171
3.	0	1	75%	265	252	207
4.	0	1	25%	208	188	165
5.	0	1	50%	241	222	201
6.	0	1	75%	269	283	191
7.	0	2	25%	239	127	90
8.	0	2	50%	224	123	79
9.	0	2	75%	243	117	100
10.	0	2	25%	187	105	85
11.	0	2	50%	243	123	110
12.	0	2	75%	226	125	75
13.	1	1	25%	155	169	151
14.	1	1	50%	198	187	176
15.	1	1	75%	235	225	166
16.	1	1	25%	173	152	141
17.	1	1	50%	177	196	167
18.	1	1	75%	229	270	183
19.	1	2	25%	137	82	77
20.	1	2	50%	129	94	78
21.	1	2	75%	155	76	92
22.	1	2	25%	160	82	83
23.	1	2	50%	98	89	48
24.	1	2	75%	132	105	67

proportion is a numeric variable taking on values 1, 2, and 3, and is value-labeled with labels 25%, 50%, and 75%. treatment takes on values of 0 and 1, whereas filler is either 1 or 2.

First, we examine these data, ignoring the repeated-measures aspects of y1, y2, and y3. In example 12, we will take it into account.

. manova y1 y2 y3 = proportion##treatment##filler

	Numbe	er of o	bs =	24					
		Vilks' Pillai'	lambda s trace		Lawley-Ho Roy's lar	_		ace	
Source	Stat	istic	di	F(d	f1, df	(2) = I	7	Prob>F	7
Model	w o	.0007	1:	L 33	.0 30.	2 10	.10	0.0000	— ) а
	P 2	.3030		33	.0 36.	0 3	.60	0.0001	a
	L 74	.4794		33	.0 26.	0 19	.56	0.0000	) a
	R 59	. 1959		11	.0 12.	0 64	.58	0.0000	) u
Residual			12	2					
proportion	w o	. 1375	2	2 6	.0 20.	0 5	.65	0.0014	ŀе
	P 0	.9766		6	.0 22.	.0 3	.50	0.0139	) a
	L 5	.4405		6	.0 18.	.0 8	. 16	0.0002	2 a
	R 5	. 2834		3	.0 11.	0 19	.37	0.0001	u
treatment	W O	.0800	:	L 3	.0 10.	0 38	.34	0.0000	— ) е
	P 0	9200		3	.0 10.	.0 38	.34	0.0000	) e
	L 11	.5032		3	.0 10.	0 38	.34	0.0000	) e
	R 11	.5032		3	.0 10.	0 38	.34	0.0000	) e
proportion#	w o	.7115	2		.0 20.	0 0	.62	0.7134	ŀе
treatment	P 0	. 2951		6	.0 22.	0 0	. 63	0.7013	} a
	1	. 3962			.0 18.			0.7310	
	R O	.3712		3	.0 11.	0 1	. 36	0.3055	5 u —
filler	1	.0192	:		.0 10.			0.0000	
		. 9808			.0 10.			0.0000	
	1	. 1803			.0 10.			0.0000	
	R 51	. 1803		3	.0 10.	0 170	.60	0.0000	) е —
proportion#filler	1	. 1785	2		.0 20.			0.0046	
		.9583			.0 22.			0.0164	
	1	. 8350			.0 18.			0.0017	
	R 3	. 6235		3	.0 11.	0 13	. 29	0.0006	3 u 
treatment#filler	1	.3552	:	1 3	.0 10.	0 6	.05	0.0128	3 e
	1	. 6448			.0 10.			0.0128	
		.8150		3	.0 10.			0.0128	
	R 1	.8150		3	.0 10.	.0 6	. 05	0.0128	} е —
proportion#		.7518	2		.0 20.			0.7928	
treatment#filler		.2640			.0 22.			0.7589	
	1	. 3092			.0 18.			0.8260	
	R O	.2080		3	.0 11.	0 0	.76	0.5381	. u —
Residual			12	2					
Total			23	3					_
									_

e = exact, a = approximate, u = upper bound on F

1

The MANOVA table indicates that all the terms are significant, except for proportion#treatment and proportion#treatment#filler.

#### □ Technical note

MANOVA uses the same design matrix as ANOVA. manova saves the full variance—covariance matrix and coefficient vector. These need a dimension equal to the dimension of the design matrix times the number of variables in the *depvarlist*.

For large problems, you may need to increase matsize. With the fabric-wear data of example 5, a matsize of at least 108 ( $108 = 36 \times 3$ ) is needed because there are three dependent variables and the design matrix has 36 columns. The 36 columns comprise 1 column for the overall mean, 3 columns for proportion, 2 columns for treatment, 6 columns for proportion#treatment, 2 columns for filler, 6 columns for proportion#filler, 4 columns for treatment#filler, and 12 columns for proportion#treatment#filler.

#### **MANCOVA**

MANCOVA models are specified by including the covariates as *terms* in the manova preceded by the c. operator to indicate that they are to be treated as continuous instead of categorical variables.

## ▶ Example 6: MANCOVA

Table 4.9 of Rencher (1998) provides biochemical measurements on four weight groups. Rencher extracted the data from Brown and Beerstecher (1951) and Smith, Gnanadesikan, and Hughes (1962). Three dependent variables and two covariates are recorded for eight subjects within each of the four groups. The first two groups are underweight, and the last two groups are overweight. The dependent variables are modified creatinine coefficient (y1), pigment creatinine (y2), and phosphate in mg/mL (y3). The two covariates are volume in ml (x1) and specific gravity (x2).

- . use http://www.stata-press.com/data/r14/biochemical (Table 4.9, Rencher (1998))
- . describe

Contains data from http://www.stata-press.com/data/r14/biochemical.dta
obs: 32 Table 4.9, Rencher (1998)
vars: 6 22 Apr 2014 21:48
size: 512 (\_dta has notes)

variable name	storage type	display format	value label	variable label
group	byte	%9.0g		
y1	float	%9.0g		modified creatinine coefficient
у2	float	%9.0g		pigment creatinine
у3	float	%9.0g		<pre>phosphate (mg/ml)</pre>
x1	int	%9.0g		volume (ml)
x2	byte	%9.0g		specific gravity

Sorted by:

Rencher performs three tests on these data. The first is a test of equality of group effects adjusted for the covariates. The second is a test that the coefficients for the covariates are jointly equal to zero. The third is a test that the coefficients for the covariates are equal across groups.

. manova y	1 y2 y3 = g	rou	c.x1 c.x2						
·	0		umber of ob		32				
		W	= Wilks' 1	ambda	L = Lawl	ey-Hotell	ling tra	ace	
		P	= Pillai's	trace	R = Roy's largest root				
	Source	St	tatistic	df	F(df1,	df2) =	= F	Prob>F	
	Model	W	0.0619	5	15.0	66.7	7.73	0.0000	- а
		P	1.4836		15.0	78.0	5.09	0.0000	a
		L	6.7860		15.0	68.0	10.25	0.0000	a
		R	5.3042		5.0	26.0	27.58	0.0000	u
	Residual			26					
	group	W	0.1491	3	9.0	58.6	7.72	0.0000	- а
		P	0.9041		9.0	78.0	3.74	0.0006	a
		L	5.3532		9.0	68.0	13.48	0.0000	a
		R	5.2872		3.0	26.0	45.82	0.0000	u
	x1	W	0.6841	1	3.0	24.0	3.69	0.0257	е
		P	0.3159		3.0	24.0	3.69	0.0257	е
		L	0.4617		3.0	24.0	3.69	0.0257	е
		R	0.4617		3.0	24.0	3.69	0.0257	е
	x2	W	0.9692	1	3.0	24.0	0.25	0.8576	е
		P	0.0308		3.0	24.0	0.25	0.8576	е
		L	0.0318		3.0	24.0	0.25	0.8576	е
		R	0.0318		3.0	24.0	0.25	0.8576	e
	Residual			26					_
	To+21			21					

e = exact, a = approximate, u = upper bound on F

The test of equality of group effects adjusted for the covariates is shown in the MANCOVA table above. Rencher reports a Wilks's lambda value of 0.1491, which agrees with the value shown for the group term above. group is found to be significant.

The test that the coefficients for the covariates are jointly equal to zero is obtained using manovatest.

. manovatest c.x1 c.x2

		= Wilks' la = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>					
Source	S.	tatistic	df	F(df1,	df2) =	F	Prob>F	_	
x1 x2	W P L R	0.4470 0.5621 1.2166 1.1995	2	6.0 6.0 6.0 3.0	48.0 50.0 46.0 25.0	3.26 4.66	0.0027 0.0088 0.0009 0.0002	a a	
Residual			26					_	

e = exact, a = approximate, u = upper bound on F

Wilks's lambda of 0.4470 agrees with the value reported by Rencher. With a p-value of 0.0027, we reject the null hypothesis that the coefficients for the covariates are jointly zero.

To test that the coefficients for the covariates are equal across groups, we perform a MANCOVA that includes our covariates (x1 and x2) interacted with group. We then use manovatest to obtain the combined test of equal coefficients for x1 and x2 across groups.

. manova y1 y2 y3 = group c.x1 c.x2 group#c.x1 group#c.x2

	Number of obs	=	32						
	W = Wilks' lam P = Pillai's t		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>						
Source	Statistic	df	F(df1,	df2) =	F	Prob>F	_		
Model	W 0.0205 P 1.9571 L 10.6273 R 7.0602	11	33.0 33.0 33.0 11.0	53.7 60.0 50.0 20.0	3.41 5.37	0.0000 0.0000 0.0000 0.0000	a a		
Residual		20					_		
group	W 0.4930 P 0.5942 L 0.8554 R 0.5746	3	9.0 9.0 9.0 3.0	44.0 60.0 50.0 20.0	1.65 1.58	0.1317 0.1226 0.1458 0.0256	a a		
<b>x1</b>	W 0.7752 P 0.2248 L 0.2900 R 0.2900	1	3.0 3.0 3.0 3.0	18.0 18.0 18.0 18.0	1.74 1.74	0.1947 0.1947 0.1947 0.1947	e e		
х2	W 0.8841 P 0.1159 L 0.1311 R 0.1311	1	3.0 3.0 3.0 3.0	18.0 18.0 18.0 18.0	0.79 0.79	0.5169 0.5169 0.5169 0.5169	e e		
group#x1	W 0.4590 P 0.6378 L 0.9702 R 0.6647	3	9.0 9.0 9.0 3.0	44.0 60.0 50.0 20.0	1.80 1.80	0.0873 0.0869 0.0923 0.0152	a a		
group#x2	W 0.5275 P 0.5462 L 0.7567 R 0.4564	3	9.0 9.0 9.0 3.0	44.0 60.0 50.0 20.0	1.48 1.40	0.1899 0.1747 0.2130 0.0527	a a		
Residual		20					_		
Total		31					_		

e = exact, a = approximate, u = upper bound on F

<sup>.</sup> manovatest group#c.x1 group#c.x2

		= Wilks' l = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	St	atistic	df	F(df1,	df2) =	F	Prob>F	
group#x1 group#x2	W P L R	0.3310 0.8600 1.4629 0.8665	6	18.0 18.0 18.0 6.0	51.4 60.0 50.0 20.0	1.34 1.35	0.1896 0.1973 0.1968 0.0341	a a
Residual			20					_

e = exact, a = approximate, u = upper bound on F

Rencher reports 0.3310 for Wilks's lambda, which agrees with the results of manovatest above. Here we fail to reject the null hypothesis.

## MANOVA for Latin-square designs

## Example 7: MANOVA with Latin-square data

Exercise 5.11 from Timm (1975) presents data from a multivariate Latin-square design. Two dependent variables are measured in a  $4 \times 4$  Latin square. W is the student's score on determining distances within the solar system. B is the student's score on determining distances beyond the solar system. The three variables comprising the square are machine, ability, and treatment, each at four levels.

. use http://www.stata-press.com/data/r14/solardistance (Multivariate Latin Square, Timm (1975), Exercise 5.11 #1)

describe

variable name	storage type	display format	value label	variable label
machine ability	byte byte	%9.0g %9.0g		teaching machine ability tracks
treatment	byte	%9.0g		method of measuring astronomical distances
W B	byte byte	%9.0g %9.0g		Solar system distances (within) Solar system distances (beyond)

#### Sorted by:

. list

	machine	ability	treatm~t	W	В
1.	1	1	2	33	15
2.	1	2	1	40	4
3.	1	3	3	31	16
4.	1	4	4	37	10
5.	2	1	4	25	20
6.	2	2	3	30	18
7.	2	3	1	22	6
8.	2	4	2	25	18
9.	3	1	1	10	5
10.	3	2	4	20	16
11.	3	3	2	17	16
12.	3	4	3	12	4
13.	4	1	3	24	15
14.	4	2	2	20	13
15.	4	3	4	19	14
16.	4	4	1	29	20

4

. ma	anova	W	В	=	machine	ability	treatment
------	-------	---	---	---	---------	---------	-----------

	N	umber of c	obs =	16					
	W	I = Wilks'	lambda	I. = I.awl	ev-Hotelli	ing tr	ace		
			's trace	• •					
Source	S	Statistic	df	F(df1,	df2) =	F	Prob>F		
Model	W	0.0378	9	18.0	10.0	2.30	0.0898	- е	
	Р	1.3658		18.0	12.0	1.44	0.2645	a	
	L	14.7756		18.0	8.0	3.28	0.0455	a	
	R	14.0137		9.0	6.0	9.34	0.0066	u	
Residual			6					-	
machine	W	0.0561	3	6.0	10.0	5.37	0.0101	- е	
	Р	1.1853		6.0	12.0	2.91	0.0545	a	
	L	12.5352		6.0	8.0	8.36	0.0043	a	
	R	12.1818		3.0	6.0	24.36	0.0009	u	
ability	W	0.4657	3	6.0	10.0	0.78	0.6070	- е	
·	Р	0.5368		6.0	12.0	0.73	0.6322	a	
	L	1.1416		6.0	8.0	0.76	0.6199	a	
	R	1.1367		3.0	6.0	2.27	0.1802	u	
treatment	W	0.4697	3	6.0	10.0	0.77	0.6137	- е	
	Р	0.5444		6.0	12.0	0.75	0.6226	a	
	L	1.0988		6.0	8.0	0.73	0.6378	a	
	R	1.0706		3.0	6.0	2.14	0.1963	u	
Residual			6					_	
Total			15						

e = exact, a = approximate, u = upper bound on F

We find that machine is a significant factor in the model, whereas ability and treatment are not.

#### 1

# MANOVA for nested designs

Nested terms are specified using a vertical bar. A|B is read as A nested within B. A|B|C is read as A nested within B, which is nested within C. A|B#C is read as A nested within the interaction of B and C. A#B|C is read as the interaction of A and B, which is nested within C.

Different error terms can be specified for different parts of the model. The forward slash is used to indicate that the next term in the model is the error term for what precedes it. For instance, manova y1 y2 = A / B | A indicates that the multivariate tests for A are to be tested using the SSCP matrix from B | A in the denominator. Error terms (terms following the slash) are generally not tested unless they are themselves followed by a slash. The residual-error SSCP matrix is the default error-term matrix.

For example, consider  $T_1$  /  $T_2$  /  $T_3$ , where  $T_1$ ,  $T_2$ , and  $T_3$  may be arbitrarily complex terms. manova will report  $T_1$  tested by  $T_2$  and  $T_2$  tested by  $T_3$ . If we add one more slash on the end to form  $T_1$  /  $T_2$  /  $T_3$  /, then manova will also report  $T_3$  tested by the residual error.

When you have nested terms in your model, we recommend using the dropemptycells option of manova or setting c(emptycells) to drop; see [R] set emptycells. See the technical note at the end of the Nested designs section of [R] anova for details.

#### Example 8: MANOVA with nested data

A chain of retail stores produced two training videos for sales associates. The videos teach how to increase sales of the store's primary product. The videos also teach how to follow up a primary sale with secondary sales of the accessories that consumers often use with the primary product. The company trainers are not sure which video will provide the best training. To decide which video to distribute to all their stores to train sales associates, they selected three stores to use one of the training videos and three other stores to use the other training video. From each store, two employees (sales associates) were selected to receive the training. The baseline weekly sales for each of these employees was recorded and then the increase in sales over their baseline was recorded for 3 or 4 different weeks. The videotrainer data are described below.

. use http://www.stata-press.com/data/r14/videotrainer (video training)

. describe

Contains data from http://www.stata-press.com/data/r14/videotrainer.dta

42 obs: video training 5 9 May 2014 12:50

vars: 462 size:

variable name	storage type	display format	value label	variable label
video	byte	%9.0g		training video
store	byte	%9.0g		store (nested in video)
associate	byte	%9.0g		sales associate (nested in store)
primary	float	%9.0g		primary sales increase
extra	float	%9.0g		secondary sales increase

Sorted by: video store associate

In this fully nested design, video is a fixed factor, whereas the remaining terms are random factors.

. manova primary extra = video / store|video / associate|store|video /,
> dropemptycells

Nτ	umber of o	obs =	42				
W	= Wilks'	lambda	L = Lawl	ey-Hotelli	ng tra	ace	
P	= Pillai	's trace					
St	tatistic	df	F(df1,	df2) =	F	Prob>F	
W	0.2455	11	22.0	58.0	2.68	0.0014	- е
P	0.9320		22.0	60.0			
L	2.3507		22.0	56.0	2.99	0.0005	a
R	1.9867		11.0	30.0	5.42	0.0001	u
		30					
W	0.1610	1	2.0	3.0	7.82	0.0646	- е
P	0.8390		2.0	3.0	7.82	0.0646	е
L	5.2119		2.0	3.0	7.82	0.0646	е
R	5.2119		2.0	3.0	7.82	0.0646	е
		4					_
W	0.3515	4	8.0	10.0	0.86	0.5775	- е
Р	0.7853		8.0	12.0	0.97	0.5011	a
L	1.4558		8.0	8.0	0.73	0.6680	a
R	1.1029		4.0	6.0	1.65	0.2767	u
		6					_
W	0.5164	6	12.0	58.0	1.89	0.0543	- е
P	0.5316		12.0	60.0	1.81	0.0668	a
L	0.8433		12.0	56.0	1.97	0.0451	a
R	0.7129		6.0	30.0	3.56	0.0087	u
		30					_
		41					_
	W P L R W P L R	W = Wilks' P = Pillai Statistic W 0.2455 P 0.9320 L 2.3507 R 1.9867  W 0.1610 P 0.8390 L 5.2119 R 5.2119  W 0.3515 P 0.7853 L 1.4558 R 1.1029  W 0.5164 P 0.5316 L 0.8433	W 0.2455 11 P 0.9320 L 2.3507 R 1.9867  30 W 0.1610 1 P 0.8390 L 5.2119 R 5.2119  4 W 0.3515 4 P 0.7853 L 1.4558 R 1.1029  6 W 0.5164 6 P 0.5316 L 0.8433 R 0.7129  30	W = Wilks' lambda	W = Wilks' lambda       L = Lawley-Hotelli         P = Pillai's trace       R = Roy's largest         Statistic       df       F(df1, df2) =         W 0.2455       11       22.0 58.0         P 0.9320       22.0 60.0         L 2.3507       22.0 56.0         R 1.9867       11.0 30.0         30         W 0.1610       1 2.0 3.0         P 0.8390       2.0 3.0         L 5.2119       2.0 3.0         R 5.2119       2.0 3.0         L 1.4558       8.0 12.0         R 1.1029       4.0 6.0         6         W 0.5164       6 12.0 58.0         P 0.5316       12.0 60.0         L 0.8433       12.0 56.0         R 0.7129       6.0 30.0	W = Wilks' lambda	W = Wilks' lambda

e = exact, a = approximate, u = upper bound on F

There appears to be a difference in the videos (with significance levels just a bit above the standard 5% level). There also appears to be a sales associate effect but not a store effect.

See example 4 of [MV] manova postestimation for a continuation of this example. It illustrates how to test pooled terms against nonresidual error terms by using the manovatest postestimation command. In that example, store is pooled with associate from the original fully specified MANOVA. Another way of pooling is to refit the model, discarding the higher-level terms. Be careful in doing this to ensure that the remaining lower-level terms have a numbering scheme that will not mistakenly consider different subjects as being the same. The videotrainer dataset has associate numbered uniquely, so we can simply type

. ma

anova primary extra	a =	video /	associate	video /, d	ropemptycel	ls				
	N.	umber of	obs =	42						
	W = Wilks' lambda				L = Lawley-Hotelling trace					
	P	= Pillai	's trace	R = Roy	's largest	root				
Source	S	tatistic	df	F(df1,	df2) =	F	Prob>F			
Model	W	0.2455	11	22.0	58.0	2.68	0.0014	е		
	Р	0.9320		22.0	60.0	2.38	0.0042	a		
	L	2.3507		22.0	56.0	2.99	0.0005	a		
	R	1.9867		11.0	30.0	5.42	0.0001	u _		
Residual			30							
video	W	0.4079	1	2.0	9.0	6.53	0.0177	е		
	Р	0.5921		2.0	9.0	6.53	0.0177	е		
	L	1.4516		2.0	9.0	6.53	0.0177	е		
	R	1.4516		2.0	9.0	6.53	0.0177	е		
associate video			10					_		
associate video	W	0.3925	10	20.0	58.0	1.73	0.0546	е		
	Р	0.7160		20.0	60.0	1.67	0.0647	a		
	L	1.2711		20.0	56.0	1.78	0.0469	a		
	R	0.9924		10.0	30.0	2.98	0.0100	u		
Residual			30					_		
Total			41					_		

e = exact, a = approximate, u = upper bound on F

and get the same results that we obtained using manovatest to get a pooled test after the full MANOVA; see example 4 of [MV] manova postestimation.

With store omitted from the model, video now has a significance level below 5%. The increase from 4 to 10 denominator degrees of freedom for the test of video provides a more powerful test.

The margins command provides a predictive marginal mean increase in sales based on the two videos. We could request the marginal means for primary sales increase or for extra sales increase, or we can use the expression() option to obtain the marginal means for combined primary and secondary sales increase. By default, the predicted means are constructed taking into account the number of observations in each cell.

	Margin	Delta-method Std. Err.	z	P> z	[95% Conf.	Interval]
video 1 2	883.1395 698.0791	30.01873 30.01873	29.42 23.25	0.000	824.3039 639.2434	941.9752 756.9147

Alternatively, we can examine the adjusted marginal mean increase in sales letting each cell have equal weight (regardless of its sample size) by using the asbalanced option of the margins command.

```
. margins, within(video) expression(predict(eq(primary))+predict(eq(extra)))
```

> asbalanced

Adjusted predictions Number of obs 42

: predict(eq(primary))+predict(eq(extra)) Expression

within : video

Empty cells : reweight : 1.video at

(asbalanced) associate

2.video

associate (asbalanced)

	Margin	Delta-method Std. Err.	z	P> z	[95% Conf.	Interval]
video						
1	876.8818	30.32981	28.91	0.000	817.4365	936.3271
2	695.315	30.32981	22.93	0.000	635.8697	754.7603

Though the values are different between the two tables, the conclusion is the same. Using training video 1 leads to increased primary and secondary sales. 4

## MANOVA for mixed designs

## Example 9: Split-plot MANOVA

reading2.dta has data from an experiment involving two reading programs and three skillenhancement techniques. Ten classes of first-grade students were randomly assigned so that five classes were taught with one reading program and another five classes were taught with the other. The 30 students in each class were divided into six groups with 5 students each. Within each class, the six groups were divided randomly so that each of the three skill-enhancement techniques was taught to two of the groups within each class. At the end of the school year, a reading assessment test was administered to all the students. Two scores were recorded. The first was a reading score (score), and the second was a comprehension score (comprehension).

Example 13 of [R] anova uses reading.dta to illustrate mixed designs for ANOVA. reading2.dta is the same as reading.dta, except that the comprehension variable is added.

. use http://www.stata-press.com/data/r14/reading2 (Reading experiment data)

. describe

Contains data from http://www.stata-press.com/data/r14/reading2.dta obs: 300 Reading experiment data 24 Apr 2014 08:31 6 vars: size: 1,800 (\_dta has notes)

variable name	storage type	display format	value label	variable label
score	byte	%9.0g		reading score
comprehension	byte	%9.0g		comprehension score
program	byte	%9.0g		reading program
class	byte	%9.0g		class nested in program
skill	byte	%9.0g		skill enhancement technique
group	byte	%9.0g		group nested in class and skill

Sorted by:

In this split-plot MANOVA, the whole-plot treatment is the two reading programs, and the split-plot treatment is the three skill-enhancement techniques.

For this split-plot MANOVA, the error term for program is class nested within program. The error term for skill and the program by skill interaction is the class by skill interaction nested within program. Other terms are also involved in the model and can be seen below.

- . manova score comp = pr / cl|pr sk pr#sk / cl#sk|pr / gr|cl#sk|pr /,
- > dropemptycells

•	Nu	umber of o	os =	300				
	W	= Wilks'	lambda	L = Lawl	ley-Hotel	ling tra	ace	
	P	= Pillai'	s trace	R = Roy	's largest	t root		
Source	St	atistic	df	F(df1,	df2) =	= F	Prob>F	
Model	W	0.5234	59	118.0	478.0	1.55	0.0008	- е
	P	0.5249		118.0	480.0		0.0039	
	L	0.8181		118.0	476.0		0.0001	
	R	0.6830		59.0	240.0	2.78	0.0000	u –
Residual			240					_
program	W	0.4543	1	2.0	7.0	4.20	0.0632	е
	P	0.5457		2.0	7.0	4.20	0.0632	е
	L	1.2010		2.0	7.0		0.0632	
	R	1.2010		2.0	7.0	4.20	0.0632	е _
class program			8					_
skill	W	0.6754	2	4.0	30.0	1.63	0.1935	е
	P	0.3317		4.0	32.0	1.59	0.2008	a
	L	0.4701		4.0	28.0	1.65	0.1908	a
	R	0.4466		2.0	16.0	3.57	0.0522	u
program#skill	W	0.3955	2	4.0	30.0	4.43	0.0063	- е
	P	0.6117		4.0	32.0	3.53	0.0171	a
	L	1.5100		4.0	28.0	5.29	0.0027	a
	R	1.4978		2.0	16.0	11.98	0.0007	u
class#skill program			16					_
class#skill program	W	0.4010	16	32.0	58.0	1.05	0.4265	- е
	P	0.7324		32.0	60.0	1.08	0.3860	a
	L	1.1609		32.0	56.0	1.02	0.4688	а
	R	0.6453		16.0	30.0	1.21	0.3160	u
group class#skill  program			30					_
group class#skill	W	0.7713	30	60.0	478.0	1.10	0.2844	- е
program	Р	0.2363		60.0	480.0	1.07	0.3405	a
	L	0.2867		60.0	476.0	1.14	0.2344	a
	R	0.2469		30.0	240.0	1.98	0.0028	u
Residual			240					_
Total			299		-			_

e = exact, a = approximate, u = upper bound on F

The program#skill interaction is significant.

#### MANOVA with repeated measures

One approach to analyzing repeated measures in an ANOVA setting is to use correction factors for terms in an ANOVA that involve the repeated measures. These correction factors attempt to correct for the violated assumption of independence of observations; see [R] **anova**. In this approach, the data are in long form; see [D] **reshape**.

Another approach to repeated measures is to use MANOVA with the repeated measures appearing as dependent variables, followed by tests involving linear combinations of these repeated measures. This approach involves fewer assumptions than the repeated-measures ANOVA approach.

The simplest possible repeated-measures design has no between-subject factors and only one within-subject factor (the repeated measures).

#### Example 10: MANOVA with repeated-measures data

Here are data on five subjects, each of whom took three tests.

- . use http://www.stata-press.com/data/r14/nobetween
- . list

	subject	test1	test2	test3
1.	1	68	69	95
2.	2	50	74	69
3.	3	72	89	71
4.	4	61	64	61
5.	5	60	71	90

manova must be tricked into fitting a constant-only model. To do this, you generate a variable equal to one, use that variable as the single *term* in your manova, and then specify the noconstant option. From the resulting MANOVA, you then test the repeated measures with the ytransform() option of manovatest; see [MV] manova postestimation for syntax details.

- . generate mycons = 1
- . manova test1 test2 test3 = mycons, noconstant

Number of obs =

	Number of obb		O				
W = Wilks' lambda P = Pillai's trace				ey-Hotelli s largest	_	ace	
Source	Statistic	df	F(df1,	df2) =	F	Prob>F	
mycons	W 0.0076 P 0.9924 L 130.3722 R 130.3722	1	3.0 3.0 3.0 3.0	2.0 2.0 2.0 2.0	86.91 86.91	0.0114 0.0114 0.0114 0.0114	e e
Residual		4					
Total		5					_

e = exact, a = approximate, u = upper bound on F

- . mat c = (1,0,-1,0,1,-1)
- . manovatest mycons, ytransform(c)

Transformations of the dependent variables

- (1) test1 test3
- (2) test2 test3

W = Wilks' lambda P = Pillai's trace			<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	S	tatistic	df	F(df1,	df2) =	F	Prob>F
mycons	W P L R	0.2352 0.7648 3.2509 3.2509	1	2.0 2.0 2.0 2.0	3.0 3.0 3.0 3.0	4.88 4.88	0.1141 e 0.1141 e 0.1141 e 0.1141 e
Residual			4				

e = exact, a = approximate, u = upper bound on F

The test produced directly with manova is not interesting. It is testing the hypothesis that the three test score means are zero. The test produced by manovatest is of interest. From the contrasts in the matrix c, you produce a test that there is a difference between the test1, test2, and test3 scores. Here the test produces a p-value of 0.1141, and you fail to reject the null hypothesis of equality between the test scores.

You can compare this finding with the results obtained from a repeated-measures ANOVA,

- . reshape long test, i(subject) j(testnum)
- . anova test subject testnum, repeated(testnum)

which produced an uncorrected *p*-value of 0.1160 and corrected *p*-values of 0.1181, 0.1435, and 0.1665 by using the Huynh–Feldt, Greenhouse–Geisser, and Box's conservative correction, respectively.

# Example 11: Randomized block design with repeated measures

Milliken and Johnson (2009) demonstrate using manova to analyze repeated measures from a randomized block design used in studying the differences among varieties of sorghum. Table 27.1 of Milliken and Johnson (2009) provides the data. Four sorghum varieties were each planted in five blocks. A leaf-area index measurement was recorded for each of 5 weeks, starting 2 weeks after emergence.

The tests of interest include a test for equal variety marginal means, equal time marginal means, and a test for the interaction of variety and time. The MANOVA below does not directly provide these tests. manovatest after the manova gives the three tests of interest.

```
. use http://www.stata-press.com/data/r14/sorghum, clear (Leaf area index on 4 sorghum varieties, Milliken & Johnson (2009))
```

. manova time1 time2 time3 time4 time5 = variety block

	Number of obs	=	20				
	W = Wilks' la P = Pillai's		L = Lawley-Hotelling trace R = Roy's largest root				
Source	Statistic	df	F(df1,	df2)	= F	Prob>F	
Model	W 0.0001	7	35.0	36.1	9.50	0.0000	- а
	P 3.3890		35.0	60.0	3.61	0.0000	a
	L 126.2712		35.0	32.0	23.09	0.0000	a
	R 109.7360		7.0	12.0	188.12	0.0000	u
Residual		12					_
variety	W 0.0011	3	15.0	22.5	16.11	0.0000	- а
	P 2.5031		15.0	30.0	10.08	0.0000	a
	L 48.3550		15.0	20.0	21.49	0.0000	a
	R 40.0068		5.0	10.0	80.01	0.0000	u
block	W 0.0047	4	20.0	27.5	5.55	0.0000	- а
	P 1.7518		20.0	44.0	1.71	0.0681	a
	L 77.9162		20.0	26.0	25.32	0.0000	a
	R 76.4899		5.0	11.0	168.28	0.0000	u
Residual		12					_
Total		19					_

e = exact, a = approximate, u = upper bound on F

Two matrices are needed for transformations of the time# variables. m1 is a row vector containing five ones. m2 provides contrasts for time#. The manovatest, showorder command lists the underlying ordering of columns for constructing two more matrices used to obtain linear combinations from the design matrix. Matrix c1 provides contrasts on variety. Matrix c2 is used to collapse to the overall margin of the design matrix to obtain time marginal means.

```
. matrix m1 = J(1,5,1)
. matrix m2 = (1,-1,0,0,0 \setminus 1,0,-1,0,0 \setminus 1,0,0,-1,0 \setminus 1,0,0,0,-1)
. manovatest, showorder
Order of columns in the design matrix
     1: (variety==1)
     2: (variety==2)
     3: (variety==3)
     4: (variety==4)
     5: (block==1)
     6: (block==2)
     7: (block==3)
     8: (block==4)
     9: (block==5)
    10: _cons
. matrix c2 = (.25, .25, .25, .25, .2, .2, .2, .2, .2, .1)
```

The test for equal variety marginal means uses matrix m1 to obtain the sum of the time# variables and matrix c1 to provide the contrasts on variety. The second test uses m2 to provide contrasts on time# and matrix c2 to collapse to the appropriate margin for the test of time marginal means. The final test uses m2 for contrasts on time# and c1 for contrasts on variety to test the variety-by-time interaction.

. manovatest, test(c1) ytransform(m1)

Transformation of the dependent variables

(1) time1 + time2 + time3 + time4 + time5

Test constraints

- (1) 1.variety 2.variety = 0
- (2) 1.variety 3.variety = 0
- (3) 1.variety 4.variety = 0

		= Wilks' l = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	S	tatistic	df	F(df1,	df2) =	F	Prob>F	_
manovatest	W P L R	0.0435 0.9565 22.0133 22.0133	3	3.0 3.0 3.0 3.0	12.0 12.0 12.0 12.0	88.05 88.05	0.0000 0.0000 0.0000 0.0000	e e
Residual			12					

e = exact, a = approximate, u = upper bound on F

. manovatest, test(c2) ytransform(m2)

Transformations of the dependent variables

- (1) time1 time2
- (2) time1 time3
- (3) time1 time4
- (4) time1 time5

Test constraint

(1) .25\*1.variety + .25\*2.variety + .25\*3.variety + .25\*4.variety + .2\*1.block + .2\*2.block + .2\*3.block + .2\*4.block + .2\*5.block + \_cons = 0

	W = Wilks' la P = Pillai's		L = Lawley-Hotelling trace R = Roy's largest root				
Source	Statistic	df	F(df1,	df2)	= F	Prob>F	
manovatest	W 0.0050	1	4.0	9.0	445.62	0.0000	е
	P 0.9950		4.0	9.0	445.62	0.0000	е
	L 198.0544		4.0	9.0	445.62	0.0000	е
	R 198.0544		4.0	9.0	445.62	0.0000	е
Residual		12					

e = exact, a = approximate, u = upper bound on F

```
. manovatest, test(c1) ytransform(m2)
```

```
Transformations of the dependent variables
```

- (1) time1 time2
- (2) time1 time3
- (3) time1 time4
- (4) time1 time5

#### Test constraints

- (1) 1.variety 2.variety = 0
- (2) 1.variety 3.variety = 0
- (3) 1.variety 4.variety = 0

	• • • • • • • • • • • • • • • • • • • •	7 = Wilks' la 9 = Pillai's		L = Lawl R = Roy'	ace	ce		
Source	S	Statistic	df	F(df1,	df2) =	F	Prob>F	
manovatest	W P L	0.0143 2.1463 12.1760 8.7953	3	12.0 12.0 12.0 4.0	24.1 33.0 23.0 11.0	6.91 7.78	0.0000 0.0000 0.0000 0.0000	a a
Residual			12					_

e = exact, a = approximate, u = upper bound on F

All three tests are significant, indicating differences in variety, in time, and in the varietyby-time interaction.

### Example 12: MANOVA and dependent-variable effects

Recall the fabric-data example from Rencher and Christensen (2012, 249) that we used in example 5 to illustrate a three-way MANOVA. Rencher and Christensen have an additional exercise to test the period effect (the y1, y2, and y3 repeated-measures variables) and the interaction of period with the other factors in the model. The ytransform() option of manovatest provides a method to do this; see [MV] manova postestimation. Here are the tests of the period effect interacted with each term in the model. We create the matrix c with rows corresponding to the linear and quadratic contrasts for the three dependent variables.

```
. quietly manova y1 y2 y3 = proportion##treatment##filler
```

- . matrix c =  $(-1,0,1 \setminus -1,2,-1)$
- . manovatest proportion, ytransform(c)

Transformations of the dependent variables

- (1) y1 + y3
- (2) -y1 + 2\*y2 y3

		= Wilks' la = Pillai's		L = Lawl R = Roy'	_	ace		
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
proportion	W P L R	0.4749 0.5454 1.0631 1.0213	2	4.0 4.0 4.0 2.0	22.0 24.0 20.0 12.0	2.25 2.66	0.0736 0.0936 0.0630 0.0147	a a
Residual			12					_

e = exact, a = approximate, u = upper bound on F

4

. manovatest treatment, ytransform(c)

Transformations of the dependent variables

- (1) y1 + y3
- (2) y1 + 2\*y2 y3

		= Wilks' la = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>					
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	_	
treatment	W P	0.1419 0.8581	1	2.0 2.0	11.0 11.0		0.0000		
	L	6.0487		2.0	11.0	33.27	0.0000	е	
	R	6.0487		2.0	11.0	33.27	0.0000	е _	
Residual			12						

e = exact, a = approximate, u = upper bound on F

. manovatest proportion#treatment, ytransform(c)

Transformations of the dependent variables

- (1) y1 + y3
- (2) -y1 + 2\*y2 y3

W = Wilks' lambda L = Lawley-Hotelling trace P = Pillai's trace R = Roy's largest root Source | Statistic F(df1, df2) =F df Prob>F proportion#treatment W 0.7766 2 4.0 22.0 0.74 0.5740 e Ρ 0.2276 4.0 24.0 0.77 0.5550 a L 0.2824 4.0 20.0 0.71 0.5972 a 0.2620 1.57 0.2476 u 2.0 12.0 Residual 12

e = exact, a = approximate, u = upper bound on F

. manovatest filler, ytransform(c)

Transformations of the dependent variables

- (1) y1 + y3
- (2) y1 + 2\*y2 y3

W = Wilks' lambda L = Lawley-Hotelling trace P = Pillai's trace R = Roy's largest root Source Statistic df F(df1, df2) =F Prob>F W 0.0954 2.0 11.0 52.17 0.0000 e filler 1 Р 0.9046 2.0 11.0 52.17 0.0000 e 52.17 0.0000 e L 9.4863 2.0 11.0 52.17 0.0000 e 9.4863 2.0 11.0 Residual 12

e = exact, a = approximate, u = upper bound on F

. manovatest proportion#filler, ytransform(c)

Transformations of the dependent variables

(2) 
$$-y1 + 2*y2 - y3$$

	•••	W = Wilks' lambda P = Pillai's trace		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	St	atistic	df	F(df1,	df2) =	F	Prob>F	
proportion#filler	W P L R	0.6217 0.3870 0.5944 0.5698	2	4.0 4.0 4.0 2.0	22.0 24.0 20.0 12.0	1.44 1.49	0.2436 0.2515 0.2439 0.0668	a a
Residual			12					

e = exact, a = approximate, u = upper bound on F

. manovatest treatment#filler, ytransform(c)

Transformations of the dependent variables

$$(1) - y1 + y3$$

(2) 
$$-y1 + 2*y2 - y3$$

		= Wilks' = Pillai'			ey-Hotelli s largest	_	ace	
Source	S1	tatistic	df	F(df1,	df2) =	F	Prob>F	_
treatment#filler	W P L R	0.3867 0.6133 1.5857 1.5857	1	2.0 2.0 2.0 2.0	11.0 11.0 11.0 11.0	8.72 8.72	0.0054 0.0054 0.0054 0.0054	e e
Residual			12					_

e = exact, a = approximate, u = upper bound on F

. manovatest proportion#treatment#filler, ytransform(c)

Transformations of the dependent variables

$$(1) - v1 + v3$$

		= Wilks' : = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
proportion# treatment#filler	W P L R	0.7812 0.2290 0.2671 0.2028	2	4.0 4.0 4.0 2.0	22.0 24.0 20.0 12.0	0.78 0.67	0.5857 0.5518 0.6219 0.3303	a a
Residual			12					_

e = exact, a = approximate, u = upper bound on F

The first test, manovatest proportion, ytransform(c), provides the test of proportion interacted with the period effect. The F tests for Wilks's lambda, Pillai's trace, and the Lawley-Hotelling trace do not reject the null hypothesis with a significance level of 0.05 (p-values of 0.0736, 0.0936, and 0.0630). The F test for Roy's largest root is an upper bound, so the p-value of 0.0147 is a lower bound.

The tests of treatment interacted with the period effect, filler interacted with the period effect, and treatment#filler interacted with the period effect are significant. The remaining tests are not.

To test the period effect, we call manovatest with both the ytransform() and test() options. The showorder option guides us in constructing the matrix for the test() option.

```
. manovatest, showorder
Order of columns in the design matrix
     1: (proportion==1)
     2: (proportion==2)
     3: (proportion==3)
     4: (treatment==0)
     5: (treatment==1)
     6: (proportion==1)*(treatment==0)
     7: (proportion==1)*(treatment==1)
     8: (proportion==2)*(treatment==0)
     9: (proportion==2)*(treatment==1)
    10: (proportion==3)*(treatment==0)
    11: (proportion==3)*(treatment==1)
    12: (filler==1)
    13: (filler==2)
    14: (proportion==1)*(filler==1)
    15: (proportion==1)*(filler==2)
    16: (proportion==2)*(filler==1)
    17: (proportion==2)*(filler==2)
    18: (proportion==3)*(filler==1)
    19: (proportion==3)*(filler==2)
    20: (treatment==0)*(filler==1)
    21: (treatment==0)*(filler==2)
    22: (treatment==1)*(filler==1)
    23: (treatment==1)*(filler==2)
    24: (proportion==1)*(treatment==0)*(filler==1)
    25: (proportion==1)*(treatment==0)*(filler==2)
    26: (proportion==1)*(treatment==1)*(filler==1)
    27: (proportion==1)*(treatment==1)*(filler==2)
    28: (proportion==2)*(treatment==0)*(filler==1)
    29: (proportion==2)*(treatment==0)*(filler==2)
    30: (proportion==2)*(treatment==1)*(filler==1)
    31: (proportion==2)*(treatment==1)*(filler==2)
    32: (proportion==3)*(treatment==0)*(filler==1)
    33: (proportion==3)*(treatment==0)*(filler==2)
    34: (proportion==3)*(treatment==1)*(filler==1)
    35: (proportion==3)*(treatment==1)*(filler==2)
    36: _cons
```

We create a row vector, m, starting with 1/3 for three columns (corresponding to proportion), followed by 1/2 for two columns (corresponding to treatment), followed by 1/6 for six columns (for proportion#treatment), followed by 1/2 for two columns (for filler), followed by 1/6 for six columns (for proportion#filler), followed by four columns of 1/4 (for treatment#filler), followed by 1/12 for 12 columns (corresponding to the proportion#treatment#filler term), and finally, a 1 for the last column (corresponding to the constant in the model). The test of period effect then uses this m matrix and the c matrix previously defined as the basis of the test for the period effect.

```
. matrix m = J(1,3,1/3), J(1,2,1/2), J(1,6,1/6), J(1,2,1/2), J(1,6,1/6),
> J(1,4,1/4), J(1,12,1/12), (1)
. manovatest, test(m) ytrans(c)
 Transformations of the dependent variables
        - y1 + y3
        -y1 + 2*y2 - y3
 Test constraint
        .3333333*1.proportion + .3333333*2.proportion + .3333333*3.proportion +
        .5*0.treatment + .5*1.treatment + .1666667*1.proportion#0.treatment +
        .1666667*1.proportion#1.treatment + .1666667*2.proportion#0.treatment +
        .1666667*2.proportion#1.treatment + .1666667*3.proportion#0.treatment +
        .1666667*3.proportion#1.treatment + .5*1.filler + .5*2.filler +
        .1666667*1.proportion#1.filler + .1666667*1.proportion#2.filler +
        .1666667*2.proportion#1.filler + .1666667*2.proportion#2.filler +
        .1666667*3.proportion#1.filler + .1666667*3.proportion#2.filler +
        .25*0.treatment#1.filler + .25*0.treatment#2.filler +
        .25*1.treatment#1.filler + .25*1.treatment#2.filler +
        .0833333*1.proportion#0.treatment#1.filler +
        .0833333*1.proportion#0.treatment#2.filler +
        .0833333*1.proportion#1.treatment#1.filler +
        .0833333*1.proportion#1.treatment#2.filler +
        .0833333*2.proportion#0.treatment#1.filler +
        .0833333*2.proportion#0.treatment#2.filler +
        .0833333*2.proportion#1.treatment#1.filler +
        .0833333*2.proportion#1.treatment#2.filler +
        .0833333*3.proportion#0.treatment#1.filler +
        .0833333*3.proportion#0.treatment#2.filler +
        .0833333*3.proportion#1.treatment#1.filler +
        .0833333*3.proportion#1.treatment#2.filler + _cons = 0
                       W = Wilks' lambda
                                               L = Lawley-Hotelling trace
                       P = Pillai's trace
                                               R = Roy's largest root
                                                          df2) =
                       Statistic
                                               F(df1,
                                                                   F
                                                                       Prob>F
              Source
          manovatest
                          0.0208
                                          1
                                                 2.0
                                                         11.0
                                                                259.04 0.0000 e
                          0.9792
                                                 2.0
                                                         11.0
                                                                259.04 0.0000 e
                         47.0988
                                                 2.0
                                                         11.0
                                                                259.04 0.0000 e
                         47.0988
                                                 2.0
                                                         11.0
                                                                259.04 0.0000 e
            Residual
                                         12
```

e = exact, a = approximate, u = upper bound on F

This result agrees with the answers provided by Rencher and Christensen (2012).

In the previous three examples, one factor has been encoded within the dependent variables. We have seen that the ytransform() option of manovatest provides the method for testing this factor and its interactions with the factors that appear on the right-hand side of the MANOVA.

More than one factor could be encoded within the dependent variables. Again the ytransform() option of manovatest allows us to perform multivariate tests of interest.

### Example 13: MANOVA and multiple dependent-variable effects

(2)

Table 6.14 of Rencher and Christensen (2012) provides an example with two within-subject factors represented in the dependent variables and one between-subject factor.

1

```
. use http://www.stata-press.com/data/r14/table614 (Table 6.14, Rencher and Christensen (2012))
```

. list in 9/12, noobs compress

С	sub~t	ab11	ab12	ab13	ab21	ab22	ab23	ab31	ab32	ab33
1	9	41	32	23	37	51	39	27	28	30
1	10	39	32	24	30	35	31	26	29	32
2	1	47	36	25	31	36	29	21	24	27
2	2	53	43	32	40	48	47	46	50	54

There are 20 observations. Factors a and b are encoded in the names of the nine dependent variables. Variable name ab23, for instance, indicates factor a at level 2 and factor b at level 3. Factor c is the between-subject factor.

We first compute a MANOVA by using the dependent variables and our one between-subject term.

. manova ab11 ab12 ab13 ab21 ab22 ab23 ab31 ab32 ab33 = c

	Nτ	umber of obs	3 =	20					
		= Wilks' la = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>					
Source	S	tatistic	df	F(df1,	df2) =	F	Prob>F		
С	W P L R	0.5330 0.4670 0.8762 0.8762	1	9.0 9.0 9.0 9.0	10.0 10.0 10.0 10.0	0.97	0.5114 e 0.5114 e 0.5114 e 0.5114 e	e e	
Residual			18						
Total			19						

e = exact, a = approximate, u = upper bound on F

This approach provides the basis for computing tests on all terms of interest. We use the ytransform() and test() options of manovatest with the following matrices to obtain the tests of interest.

```
. mat a = (2,2,2,-1,-1,-1,-1,-1,-1 \setminus 0,0,0,1,1,1,-1,-1,-1)
. mat b = (2,-1,-1,2,-1,-1,2,-1,-1 \setminus 0,1,-1,0,1,-1,0,1,-1)
. forvalues i = 1/2 {
  2
              forvalues j = 1/2 {
  3.
                      mat g = nullmat(g) \ vecdiag(a['i',1...]'*b['j',1...])
  4.
  5. }
. mat list g
g[4,9]
    c1
        c2 c3
                 c4 c5
                          с6
                             с7
                                  с8
                                       c.9
        -2 -2
                 -2 1
                          1
                             -2
        2 -2
                  0 -1
r1
                           1
                               0
                                  -1
                                        1
                  2
                    -1
                          -1
r1
     0
         0
             0
                             -2
                                  1
                                        1
     0
         0
             0
                  0
                      1
                          -1
                               0
                                  -1
. mat j = J(1,9,1/9)
. \text{ mat xall} = (.5, .5, 1)
```

Matrices a and b correspond to factors a and b. Matrix g is the elementwise multiplication of each row of a with each row of b and corresponds to the a#b interaction. Matrix j is used to average the dependent variables, whereas matrix xall collapses over factor c.

Here are the tests for a, b, and a#b.

. manovatest, test(xall) ytrans(a)

Transformations of the dependent variables

- 2\*ab11 + 2\*ab12 + 2\*ab13 ab21 ab22 ab23 ab31 ab32 ab33
- ab21 + ab22 + ab23 ab31 ab32 ab33 (2)

Test constraint

(1)  $.5*1.c + .5*2.c + _cons = 0$ 

		= Wilks' l = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	_
manovatest	W P L R	0.6755 0.3245 0.4803 0.4803	1	2.0 2.0 2.0 2.0	17.0 17.0 17.0 17.0	4.08 4.08	0.0356 0.0356 0.0356 0.0356	e e
Residual			18					

e = exact, a = approximate, u = upper bound on F

. manovatest, test(xall) ytrans(b)

Transformations of the dependent variables

- (1) 2\*ab11 - ab12 - ab13 + 2\*ab21 - ab22 - ab23 + 2\*ab31 - ab32 - ab33
- ab12 ab13 + ab22 ab23 + ab32 ab33(2)

Test constraint

(1)  $.5*1.c + .5*2.c + _cons = 0$ 

> W = Wilks' lambda L = Lawley-Hotelling trace P = Pillai's trace R = Roy's largest root Source | Statistic df F(df1, df2) =F Prob>F manovatest ١W 0.3247 1 2.0 17.0 17.68 0.0001 e Þ 0.6753 2.0 17.0 17.68 0.0001 e 2.0799 2.0 17.0 17.68 0.0001 e T. 2.0799 2.0 17.0 17.68 0.0001 e Residual 18

> > e = exact, a = approximate, u = upper bound on F

L = Lawley-Hotelling trace

. manovatest, test(xall) ytrans(g)

Transformations of the dependent variables

- 4\*ab11 2\*ab12 2\*ab13 2\*ab21 + ab22 + ab23 2\*ab31 + ab32 + ab33 (1)
- (2) 2\*ab12 - 2\*ab13 - ab22 + ab23 - ab32 + ab33
- (3) 2\*ab21 - ab22 - ab23 - 2\*ab31 + ab32 + ab33

W = Wilks' lambda

ab22 - ab23 - ab32 + ab33(4)

Test constraint

(1)  $.5*1.c + .5*2.c + _cons = 0$ 

> P = Pillai's trace R = Roy's largest root Source Statistic df F(df1, df2) =F Prob>F manovatest 0.2255 1 4.0 15.0 12.88 0.0001 e Р 0.7745 4.0 15.0 12.88 0.0001 e 4.0 T. 3.4347 15.0 12.88 0.0001 e R. 3.4347 4.0 15.0 12.88 0.0001 e Residual 18

e = exact, a = approximate, u = upper bound on F

Factors a, b, and a#b are significant with p-values of 0.0356, 0.0001, and 0.0001, respectively. The multivariate statistics are equivalent to the  $T^2$  values Rencher and Christensen report using the relationship  $T^2=(n_1+n_2-2)\times(1-\Lambda)/\Lambda$  that applies in this situation. For instance, Wilks's lambda for factor a is reported as 0.6755 (and the actual value recorded in r(stat) is 0.67554286) so that  $T^2=(10+10-2)\times(1-0.67554286)/0.67554286=8.645$ , as reported by Rencher and Christensen.

We now compute the tests for c and the interactions of c with the other terms in the model.

. manovatest c, ytrans(j)

Transformation of the dependent variables

```
(1) .1111111*ab11 + .1111111*ab12 + .1111111*ab33 + .1111111*ab21 + .1111111*ab22 + .11111111*ab33 + .1111111*ab31 + .1111111*ab33
```

		= Wilks' la = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	S.	tatistic	df	F(df1,	df2) =	F	Prob>F	
С	W P L R	0.6781 0.3219 0.4747 0.4747	1	1.0 1.0 1.0	18.0 18.0 18.0 18.0	8.54 8.54	0.0091 0.0091 0.0091 0.0091	e e
Residual			18					_

e = exact, a = approximate, u = upper bound on F

L = Lawley-Hotelling trace

L = Lawley-Hotelling trace

. manovatest c, ytrans(a)

Transformations of the dependent variables

(1) 2\*ab11 + 2\*ab12 + 2\*ab13 - ab21 - ab22 - ab23 - ab31 - ab32 - ab33

W = Wilks' lambda

(2) ab21 + ab22 + ab23 - ab31 - ab32 - ab33

P = Pillai's trace R = Roy's largest root Source Statistic F(df1, df2) =Prob>F 0.9889 1 2.0 17.0 0.10 0.9097 e С Ρ 0.0111 2.0 17.0 0.10 0.9097 e L 0.0112 2.0 17.0 0.10 0.9097 e 0.0112 2.0 17.0 0.10 0.9097 e Residual 18

e = exact, a = approximate, u = upper bound on F

. manovatest c, ytrans(b)

Transformations of the dependent variables

(1) 2\*ab11 - ab12 - ab13 + 2\*ab21 - ab22 - ab23 + 2\*ab31 - ab32 - ab33

W = Wilks' lambda

(2) ab12 - ab13 + ab22 - ab23 + ab32 - ab33

P = Pillai's trace R = Roy's largest root Statistic df F(df1, df2) =F Prob>F Source С 0.9718 1 2.0 17.0 0.25 0.7845 e Р 0.0282 2.0 17.0 0.25 0.7845 e 0.25 0.7845 e 0.0290 2.0 17.0 0.25 0.7845 e R. 0.0290 2.0 17.0 Residual 18

. manovatest c, ytrans(g)

Transformations of the dependent variables

- (1) 4\*ab11 2\*ab12 2\*ab13 2\*ab21 + ab22 + ab23 2\*ab31 + ab32 + ab33
- (2) 2\*ab12 2\*ab13 ab22 + ab23 ab32 + ab33
- (3) 2\*ab21 ab22 ab23 2\*ab31 + ab32 + ab33
- (4) ab22 ab23 ab32 + ab33

		= Wilks' la = Pillai's			ey-Hotelli s largest	_	ace	
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
С	W	0.9029	1	4.0	15.0	0.40	0.8035	_ -
	P	0.0971		4.0	15.0	0.40	0.8035	е
	L	0.1075		4.0	15.0	0.40	0.8035	e
	R	0.1075		4.0	15.0	0.40	0.8035	е
Residual			18					_

e = exact, a = approximate, u = upper bound on F

The test of c is equivalent to an ANOVA using the sum or average of the dependent variables as the dependent variable. The test of c produces an F of 8.54 with a p-value of 0.0091, which agrees with the results of Rencher and Christensen (2012, 229–230).

The tests of a#c, b#c, and a#b#c produce p-values of 0.9097, 0.7845, and 0.8035, respectively.

In summary, the factors that are significant are a, b, a#b, and c.

4

### Stored results

manova stores the following in e():

```
Scalars
                           number of observations
    e(N)
    e(k)
                           number of parameters
    e(k_eq)
                           number of equations in e(b)
                           model degrees of freedom
    e(df_m)
    e(df_r)
                           residual degrees of freedom
    e(df_#)
                           degrees of freedom for term #
    e(rank)
                           rank of e(V)
Macros
    e(cmd)
                           manova
    e(cmdline)
                           command as typed
    e(depvar)
                           names of dependent variables
    e(indepvars)
                           names of the right-hand-side variables
    e(term_#)
                           term #
    e(errorterm_#)
                           error term for term # (defined for terms using nonresidual error)
    e(wtype)
                           weight type
                           weight expression
    e(wexp)
                           R^2 for each equation
    e(r2)
    e(rmse)
                           RMSE for each equation
    e(F)
                           F statistic for each equation
                           significance of F for each equation
    e(p_F)
    e(properties)
    e(estat_cmd)
                           program used to implement estat
    e(predict)
                           program used to implement predict
    e(marginsnotok)
                           predictions disallowed by margins
    e(marginsdefault)
                           default predict() specification for margins
    e(asbalanced)
                           factor variables fyset as asbalanced
    e(asobserved)
                           factor variables fyset as asobserved
Matrices
    e(b)
                           coefficient vector (a stacked version of e(B))
    e(B)
                           coefficient matrix
    e(E)
                           residual-error SSCP matrix
    e(xpxinv)
                           generalized inverse of X'X
    e(H_m)
                           hypothesis SSCP matrix for the overall model
                           multivariate statistics for the overall model
    e(stat_m)
                           eigenvalues of E^{-1}H for the overall model
    e(eigvals_m)
                           s, m, and n values for the overall model
    e(aux_m)
    e(H_#)
                           hypothesis SSCP matrix for term #
                           multivariate statistics for term # (if computed)
    e(stat_#)
                           eigenvalues of E^{-1}H for term # (if computed)
    e(eigvals_#)
    e(aux_#)
                           s, m, and n values for term # (if computed)
    e(V)
                           variance-covariance matrix of the estimators
Functions
    e(sample)
                           marks estimation sample
```

# Methods and formulas

Let Y denote the matrix of observations on the left-hand-side variables. Let X denote the design matrix based on the right-hand-side variables. The last column of X is equal to all ones (unless the noconstant option was specified). Categorical right-hand-side variables are placed in X as a set of indicator (sometimes called dummy) variables, whereas continuous variables enter as is. Columns of X corresponding to interactions are formed by multiplying the various combinations of columns for the variables involved in the interaction.

The multivariate model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

leads to multivariate hypotheses of the form

$$\mathbf{C}\beta\mathbf{A}'=\mathbf{0}$$

where  $\beta$  is a matrix of parameters, C specifies constraints on the design matrix X for a particular hypothesis, and A provides a transformation of Y. A is often the identity matrix.

An estimate of  $\beta$  is provided by

$$\mathbf{B} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Y}$$

The error sum of squares and cross products (SSCP) matrix is

$$\mathbf{E} = \mathbf{A}(\mathbf{Y}'\mathbf{Y} - \mathbf{B}'\mathbf{X}'\mathbf{X}\mathbf{B})\mathbf{A}'$$

and the SSCP matrix for the hypothesis is

$$\mathbf{H} = \mathbf{A}(\mathbf{C}\mathbf{B})'\{\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'\}^{-1}(\mathbf{C}\mathbf{B})\mathbf{A}'$$

The inclusion of weights, if specified, enters the formulas in a manner similar to that shown in *Methods and formulas* of [R] **regress**.

Let  $\lambda_1 > \lambda_2 > \dots > \lambda_s$  represent the nonzero eigenvalues of  $\mathbf{E}^{-1}\mathbf{H}$ .  $s = \min(p, \nu_h)$ , where p is the number of columns of  $\mathbf{Y}\mathbf{A}'$  (that is, the number of y variables or number of resultant transformed left-hand-side variables), and  $\nu_h$  is the hypothesis degrees of freedom.

Wilks's (1932) lambda statistic is

$$\Lambda = \prod_{i=1}^{s} \frac{1}{1 + \lambda_i} = \frac{|\mathbf{E}|}{|\mathbf{H} + \mathbf{E}|}$$

and is a likelihood-ratio test. This statistic is distributed as the Wilks's  $\Lambda$  distribution if **E** has the Wishart distribution, **H** has the Wishart distribution under the null hypothesis, and **E** and **H** are independent. The null hypothesis is rejected for small values of  $\Lambda$ .

Pillai's (1955) trace is

$$V = \sum_{i=1}^{s} \frac{\lambda_i}{1 + \lambda_i} = \operatorname{trace} \left\{ (\mathbf{E} + \mathbf{H})^{-1} \mathbf{H} \right\}$$

and the Lawley-Hotelling trace (Lawley 1938; Hotelling 1951) is

$$U = \sum_{i=1}^{s} \lambda_i = \operatorname{trace}(\mathbf{E}^{-1}\mathbf{H})$$

and is also known as Hotelling's generalized  $T^2$  statistic.

Roy's largest root is taken as  $\lambda_1$ , though some report  $\theta = \lambda_1/(1+\lambda_1)$ , which is bounded between zero and one. Roy's largest root provides a test based on the union-intersection approach to test construction introduced by Roy (1939).

Tables providing critical values for these four multivariate statistics are found in many of the books that discuss MANOVA, including Rencher (1998) and Rencher and Christensen (2012).

Let p be the number of columns of  $\mathbf{Y}\mathbf{A}'$  (that is, the number of y variables or the number of resultant transformed y variables),  $\nu_h$  be the hypothesis degrees of freedom,  $\nu_e$  be the error degrees of freedom,  $s = \min(\nu_h, p)$ ,  $m = (|\nu_h - p| - 1)/2$ , and  $n = (\nu_e - p - 1)/2$ . Transformations of these four multivariate statistics to F statistics are as follows.

For Wilks's lambda, an approximate F statistic (Rao 1951) with  $\mathrm{df}_1$  and  $\mathrm{df}_2$  degrees of freedom is

$$F = \frac{(1 - \Lambda^{1/t})\mathrm{df}_2}{(\Lambda^{1/t})\mathrm{df}_1}$$

where

$$\begin{split} \mathrm{df_1} &= p\nu_h & \mathrm{df_2} &= wt + 1 - p\nu_h/2 \\ w &= \nu_e + \nu_h - (p + \nu_h + 1)/2 \\ t &= \left(\frac{p^2\nu_h^2 - 4}{p^2 + \nu_h^2 - 5}\right)^{1/2} \end{split}$$

t is set to one if either the numerator or the denominator equals zero. This F statistic is exact when p equals 1 or 2 or when  $\nu_h$  equals 1 or 2.

An approximate F statistic for Pillai's trace (Pillai 1954, 1956b) with s(2m+s+1) and s(2n+s+1) degrees of freedom is

$$F = \frac{(2n+s+1)V}{(2m+s+1)(s-V)}$$

An approximate F statistic for the Lawley-Hotelling trace (Pillai 1954, 1956a) with s(2m+s+1) and 2sn+2 degrees of freedom is

$$F = \frac{2(sn+1)U}{s^2(2m+s+1)}$$

When p or  $\nu_h$  are 1, an exact F statistic for Roy's largest root is

$$F = \lambda_1 \frac{\nu_e - p + 1}{p}$$

with  $|\nu_h - p| + 1$  and  $\nu_e - p + 1$  degrees of freedom. In other cases, an upper bound F statistic (providing a lower bound on the p-value) for Roy's largest root is

$$F = \lambda_1 \frac{\nu_e - d + \nu_h}{d}$$

with d and  $\nu_e - d + \nu_h$  degrees of freedom, where  $d = \max(p, \nu_h)$ .

Samuel Stanley Wilks (1906–1964) was born in Texas. He gained degrees in architecture, mathematics, and statistics from North Texas Teachers' College and the universities of Texas and Iowa. After periods in Columbia and England, he moved to Princeton in 1933. Wilks published various widely used texts, was founding editor of the *Annals of Mathematical Statistics*, and made many key contributions to multivariate statistics. Wilks's lambda is named for him.

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### Also see

[MV] manova postestimation — Postestimation tools for manova

[MV] mvreg — Multivariate regression

[MV] **mvtest** — Multivariate tests

[D] **encode** — Encode string into numeric and vice versa

[D] reshape — Convert data from wide to long form and vice versa

[R] **anova** — Analysis of variance and covariance

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[U] 13.5 Accessing coefficients and standard errors

[U] 20 Estimation and postestimation commands

# **Title**

### manova postestimation — Postestimation tools for manova

Postestimation commands predict margins

manovatest test Remarks and examples

Stored results Methods and formulas Also see

# **Postestimation commands**

The following postestimation commands are of special interest after manova:

Command	Description
manovatest	multivariate tests after manova
screeplot	plot eigenvalues

The following standard postestimation commands are also available:

Command	Description
contrast	contrasts and ANOVA-style joint tests of estimates
estat summarize	summary statistics for the estimation sample
estat vce	variance-covariance matrix of the estimators (VCE)
estimates	cataloging estimation results
lincom	point estimates, standard errors, testing, and inference for linear combinations of coefficients
margins	marginal means, predictive margins, marginal effects, and average marginal effects
marginsplot	graph the results from margins (profile plots, interaction plots, etc.)
nlcom	point estimates, standard errors, testing, and inference for nonlinear combinations of coefficients
predict	predictions, residuals, and standard errors
predictnl	point estimates, standard errors, testing, and inference for generalized predictions
pwcompare	pairwise comparisons of estimates
test	Wald tests of simple and composite linear hypotheses
testnl	Wald tests of nonlinear hypotheses

# predict

## **Description for predict**

predict creates a new variable containing predictions such as fitted values, standard errors, residuals, and differences between the linear predictions.

### Menu for predict

Statistics > Postestimation

### Syntax for predict

```
 predict [type] newvar [if] [in] [, equation(eqno[, eqno]) statistic]
```

statistic	Description
Main	
хb	$\mathbf{x}_{j}\mathbf{b}$ , fitted values; the default
stdp	standard error of the fitted value
$\underline{\mathtt{r}}\mathtt{esiduals}$	residuals
$\underline{\mathtt{d}}\mathtt{ifference}$	difference between the linear predictions of two equations
<u>stdd</u> p	standard error of the fitted values for differences

These statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample.

# Options for predict

equation(eqno[, eqno]) specifies the equation to which you are referring.

equation() is filled in with one *eqno* for the xb, stdp, and residuals options. equation(#1) would mean that the calculation is to be made for the first equation (that is, for the first dependent variable), equation(#2) would mean the second, and so on. You could also refer to the equations by their names. equation(income) would refer to the equation named income and equation(hours), to the equation named hours.

If you do not specify equation(), results are the same as if you had specified equation(#1).

difference and stddp refer to between-equations concepts. To use these options, you must specify two equations, for example, equation(#1,#2) or equation(income,hours). When two equations must be specified, equation() is required. With equation(#1,#2), difference computes the prediction of equation(#1) minus the prediction of equation(#2).

xb, the default, calculates the fitted values—the prediction of  $x_i$ b for the specified equation.

stdp calculates the standard error of the prediction for the specified equation (the standard error of the estimated expected value or mean for the observation's covariate pattern). The standard error of the prediction is also referred to as the standard error of the fitted value.

residuals calculates the residuals.

difference calculates the difference between the linear predictions of two equations in the system. stddp calculates the standard error of the difference in linear predictions  $(\mathbf{x}_{1j}\mathbf{b} - \mathbf{x}_{2j}\mathbf{b})$  between equations 1 and 2.

For more information on using predict after multiple-equation estimation commands, see [R] predict.

# margins

### **Description for margins**

margins estimates margins of responses for linear predictions, fitted values, and differences between the linear predictions.

### Menu for margins

Statistics > Postestimation

### Syntax for margins

```
margins \begin{bmatrix} \textit{marginlist} \end{bmatrix}, \texttt{predict}(\textit{statistic} \dots) \begin{bmatrix} \texttt{predict}(\textit{statistic} \dots) \dots \end{bmatrix} \begin{bmatrix} \textit{options} \end{bmatrix} statistic Description

default linear predictions for each equation x_j b, fitted values difference difference between the linear predictions of two equations \texttt{residuals} not allowed with margins stdp not allowed with margins stddp not allowed with margins
```

xb defaults to the first equation.

Statistics not allowed with margins are functions of stochastic quantities other than e(b).

For the full syntax, see [R] margins.

margins [marginlist] [, options]

### manovatest

### **Description of manovatest**

manovatest provides multivariate tests involving terms or linear combinations of the underlying design matrix from the most recently fit manova. The four multivariate test statistics are Wilks's lambda, Pillai's trace, Lawley-Hotelling trace, and Roy's largest root. The format of the output is similar to that shown by manova; see [MV] manova.

#### Menu for manovatest

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Multivariate tests after MANOVA

### Syntax for manovatest

```
manovatest term [term ...] [/ term [term ...]] [, ytransform(matname)]
manovatest, test(matname) [ytransform(matname)]
manovatest, showorder
```

where term is a term from the termlist in the previously run manova.

### Options for manovatest

ytransform(matname) specifies a matrix for transforming the y variables (the depvarlist from manova) as part of the test. The multivariate tests are based on  $(\mathbf{AEA}')^{-1}(\mathbf{AHA}')$ . By default, A is the identity matrix. ytransform() is how you specify an A matrix to be used in the multivariate tests. Specifying ytransform() provides the same results as first transforming the y variables with YA', where Y is the matrix formed by binding the y variables by column and A is the matrix stored in *matname*; then performing manova on the transformed y's; and finally running manovatest without ytransform().

The number of columns of matname must equal the number of variables in the depvarlist from manova. The number of rows must be less than or equal to the number of variables in the depvarlist from manova. matname should have columns in the same order as the depvarlist from manova. The column and row names of *matname* are ignored.

When ytransform() is specified, a listing of the transformations is presented before the table containing the multivariate tests. You should examine this table to verify that you have applied the transformation you desired.

test(matname) is required with the second syntax of manovatest. The rows of matname specify linear combinations of the underlying design matrix of the MANOVA that are to be jointly tested. The columns correspond to the underlying design matrix (including the constant if it has not been suppressed). The column and row names of matname are ignored.

A listing of the constraints imposed by the test() option is presented before the table containing the multivariate tests. You should examine this table to verify that you have applied the linear combinations you desired. Typing manovatest, showorder allows you to examine the ordering of the columns for the design matrix from the MANOVA.

showorder causes manovatest to list the definition of each column in the design matrix. showorder is not allowed with any other option or when terms are specified.

#### test

### **Description for test**

In addition to the standard syntax of test (see [R] **test**), test after manova has two additionally allowed syntaxes; see below. test performs Wald tests of expressions involving the coefficients of the underlying regression model. Simple and composite linear hypotheses are possible.

#### Menu for test

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Wald test after MANOVA

### Syntax for test

In addition to the standard syntax of test (see [R] test), test after manova also allows the following.

```
\underline{\text{test}}, \ \text{test}(\textit{matname}) \ \left[ \ \underline{\text{m}} \text{test} \big[ (\textit{opt}) \big] \ \text{matvlc}(\textit{matname}) \ \right] \\ \underline{\text{test}}, \ \underline{\text{showorder}} \\ \text{syntax B}
```

syntax A test expression involving the coefficients of the underlying multivariate regression model; you provide information as a matrix

syntax B show underlying order of design matrix, which is useful when constructing the *matname* argument of the test() option

### **Options for test**

Main

test(matname) is required with syntax A of test. The rows of matname specify linear combinations of the underlying design matrix of the MANOVA that are to be jointly tested. The columns correspond to the underlying design matrix (including the constant if it has not been suppressed). The column and row names of matname are ignored.

A listing of the constraints imposed by the test() option is presented before the table containing the tests. You should examine this table to verify that you have applied the linear combinations you desired. Typing test, showorder allows you to examine the ordering of the columns for the design matrix from the MANOVA.

*matname* should have as many columns as the number of dependent variables times the number of columns in the basic design matrix. The design matrix is repeated for each dependent variable.

showorder causes test to list the definition of each column in the design matrix. showorder is not allowed with any other option.

Options

mtest[(opt)] specifies that tests be performed for each condition separately. opt specifies the method for adjusting p-values for multiple testing. Valid values for opt are

bonferroni Bonferroni's method
Holm's method
Sidak Šidák's method
noadjust no adjustment is to be made

Specifying mtest without an argument is equivalent to specifying mtest(noadjust).

The following option is available with test after manova but is not shown in the dialog box:

matvlc(matname), a programmer's option, saves the variance-covariance matrix of the linear combinations involved in the suite of tests. For the test of  $H_0$ :  $\mathbf{Lb} = \mathbf{c}$ , what is returned in matname is  $\mathbf{LVL'}$ , where  $\mathbf{V}$  is the estimated variance-covariance matrix of  $\mathbf{b}$ .

# Remarks and examples

Several postestimation tools are available after manova. We demonstrate these tools by extending examples 1, 2, 4, and 8 of [MV] manova.

### Example 1: test and lincom

Example 1 of [MV] manova presented a balanced one-way MANOVA on the rootstock data.

```
. use http://www.stata-press.com/data/r14/rootstock
(Table 6.2 Rootstock Data, Rencher and Christensen (2012))
. manova y1 y2 y3 y4 = rootstock
  (output omitted)
```

test provides Wald tests on expressions involving the underlying coefficients of the model, and lincom provides linear combinations along with standard errors and confidence intervals.

(1) - [y1]4.rootstock + [y3]4.rootstock = 0

	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
(1)	.2075001	.1443917	1.44	0.158	0838941	.4988943

If the equation portion of the expression is omitted, the first equation (first dependent variable) is assumed.

The manovatest postestimation command provides multivariate tests of *terms* or linear combinations of the underlying design matrix from the most recent MANOVA model.

# Example 2: manovatest

In example 2 of [MV] manova, a one-way MANOVA on the metabolic dataset was shown.

```
. use http://www.stata-press.com/data/r14/metabolic
(Table 4.5 Metabolic Comparisons of Rabbits -- Rencher (1998))
. manova y1 y2 = group
  (output omitted)
```

manovatest can test *terms* from the preceding manova. Here we test the group term from our one-way MANOVA:

4

. manovatest group

	W = Wilks' lambda P = Pillai's trace				ey-Hotelli s largest	_	ace
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F
group	W P L R	0.1596 1.2004 3.0096 1.5986	3	6.0 6.0 6.0 3.0	32.0 34.0 30.0 17.0	8.51 7.52	0.0000 e 0.0000 a 0.0001 a 0.0008 u
Residual			17				

e = exact, a = approximate, u = upper bound on F

Using manovatest to test model *terms* is not interesting here. It merely repeats information already presented by manova. Later we will see useful applications of *term* testing via manovatest.

manovatest can also be used to test linear combinations of the underlying design matrix of the MANOVA model. Whereas the MANOVA indicates that there are differences in the groups, it does not indicate the nature of those differences. Rencher discusses three linear contrasts of interest for this example: group one (the control) versus the rest, group four versus groups two and three, and group two versus group three. The test() option of manovatest allows us to test these hypotheses.

Because we did not use the noconstant option with our manova, the underlying parameterization of the design matrix has the last column corresponding to the constant in the model, whereas the first four columns correspond to the four groups of rabbits. The showorder option of manovatest illustrates this point. The tests on the three contrasts of interest follow.

```
. manovatest, showorder
Order of columns in the design matrix
     1: (group==1)
     2: (group==2)
     3: (group==3)
     4: (group==4)
     5: cons
. matrix c1 = (3,-1,-1,-1,0)
. manovatest, test(c1)
Test constraint
(1)
        3*1.group - 2.group - 3.group - 4.group = 0
                       W = Wilks' lambda
                                                L = Lawley-Hotelling trace
                       P = Pillai's trace
                                                R = Roy's largest root
                       Statistic
                                                F(df1.
                                                           df2) =
                                                                         Prob>F
              Source
                           0.4063
                                                  2.0
                                                                   11.69 0.0007 e
          manovatest
                      W
                                           1
                                                           16.0
                      Р
                           0.5937
                                                  2.0
                                                           16.0
                                                                   11.69 0.0007 e
                      L
                           1.4615
                                                  2.0
                                                           16.0
                                                                   11.69 0.0007 e
                           1.4615
                                                  2.0
                                                           16.0
                                                                   11.69 0.0007 e
            Residual
                                         17
```

e = exact, a = approximate, u = upper bound on F

. matrix c2 = (0,-1,-1,2,0)

. manovatest, test(c2)

Test constraint

(1) 
$$-2.group - 3.group + 2*4.group = 0$$

e = exact, a = approximate, u = upper bound on F

- . matrix c3 = (0,1,-1,0,0)
- . manovatest, test(c3)

Test constraint

2.group - 3.group = 0

W = Wilks' lambda L = Lawley-Hotelling trace P = Pillai's trace R = Roy's largest root Statistic F(df1, df2) =F Prob>F Source df manovatest 0.4161 2.0 16.0 11.23 0.0009 e Р 0.5839 2.0 16.0 11.23 0.0009 e L 1.4033 16.0 11.23 0.0009 e 2.0 R 1.4033 2.0 16.0 11.23 0.0009 e Residual 17

e = exact, a = approximate, u = upper bound on F

Because there is only 1 degree of freedom for each of the hypotheses, the F tests are exact (and identical for the four multivariate methods). The first test indicates that the mean vector for the control group is significantly different from the mean vectors for the other three groups. The second test, with a p-value of 0.7018, fails to reject the null hypothesis that group four equals groups two and three. The third test, with a p-value of 0.0009, indicates differences between the mean vectors of groups two and three.

Rencher also tests using weighted orthogonal contrasts. manovatest can do these tests as well.

- . matrix c1w = (14, -7, -5, -2, 0)
- . manovatest, test(c1w)

Test constraint

(1) 
$$14*1.group - 7*2.group - 5*3.group - 2*4.group = 0$$

L = Lawley-Hotelling trace W = Wilks' lambda P = Pillai's trace R = Roy's largest root Source Statistic df F(df1, df2) =F Prob>F 0.3866 2.0 16.0 manovatest W 1 12.70 0.0005 e Р 0.6134 16.0 12.70 0.0005 e 2.0 L 1.5869 2.0 16.0 12.70 0.0005 e R 1.5869 2.0 16.0 12.70 0.0005 e Residual 17

e = exact, a = approximate, u = upper bound on F

. matrix c2w = (0,-7,-5,12,0)

L = Lawley-Hotelling trace

4

. manovatest, test(c2w)

Residual

Test constraint

(1) 
$$-7*2.group - 5*3.group + 12*4.group = 0$$

W = Wilks' lambda

	P	= Pillai's	trace	R = Roy's largest root				
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
manovatest	W	0.9810	1	2.0	16.0	0.15	0.8580	е
	P	0.0190		2.0	16.0	0.15	0.8580	е
	L	0.0193		2.0	16.0	0.15	0.8580	е
	R	0.0193		2.0	16.0	0.15	0.8580	е

e = exact, a = approximate, u = upper bound on F

These two weighted contrasts do not lead to different conclusions compared with their unweighted counterparts.

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### □ Technical note

manovatest, test(matname) displays the linear combination (labeled "Test constraint") indicated by matname. You should examine this listing to make sure that the matrix you specify in test() provides the test you want.

The margins postestimation command provides, among other things, tables of predicted means and confidence intervals that are based on the most recently fit model.

# Example 3: Margins, contrasts, and predictions

Example 4 of [MV] manova presented a two-way MANOVA model on the jaw data.

```
. use http://www.stata-press.com/data/r14/jaw
(Table 4.6 Two-Way Unbalanced Data for Fractures of the Jaw -- Rencher (1998))
. manova y1 y2 y3 = gender fracture gender#fracture
(output omitted)
```

The interaction term, gender#fracture, was significant. margins may be used to examine the interaction; see [R] margins.

. margins gender#fracture, predict(equation(y1))

Adjusted predictions Number of obs = 27

Expression : Linear prediction, predict(equation(y1))

		Margin	Delta-method Std. Err.	t	P> t	[95% Conf.	Interval]
	gender# fracture male #						
one	compo male #	39.5	4.171386	9.47	0.000	30.82513	48.17487
two	compo male #	26.875	3.612526	7.44	0.000	19.36234	34.38766
one	simpl female #	45.16667	4.171386	10.83	0.000	36.49179	53.84154
one	compo female #	22	10.21777	2.15	0.043	.7509887	43.24901
two	compo female #	30.75	5.108884	6.02	0.000	20.12549	41.37451
one	simpl	36.5	7.225053	5.05	0.000	21.47468	51.52532

. margins gender#fracture, predict(equation(y2))

Adjusted predictions Number of obs = 27

Expression : Linear prediction, predict(equation(y2))

		Margin	Delta-method Std. Err.	t	P> t	[95% Conf	Intervall
					17101		
	gender# fracture						
	male #						
one	compo male #	35.5	2.150966	16.50	0.000	31.02682	39.97318
two	compo male #	32.375	1.862791	17.38	0.000	28.50111	36.24889
one	simpl female #	36.16667	2.150966	16.81	0.000	31.69349	40.63984
one	compo female #	56	5.268768	10.63	0.000	45.043	66.957
two	compo female #	33.25	2.634384	12.62	0.000	27.7715	38.7285
one	simpl	33	3.725582	8.86	0.000	25.25223	40.74777

. margins gender#fracture, predict(equation(y3))

Adjusted predictions Number of obs = 27

Expression : Linear prediction, predict(equation(y3))

		Margin	Delta-method Std. Err.	t	P> t	[95% Conf.	Interval]
	gender# fracture male #						
one	compo male #	61.16667	2.038648	30.00	0.000	56.92707	65.40627
two	compo male #	62.25	1.765521	35.26	0.000	58.5784	65.9216
one	simpl female #	58.16667	2.038648	28.53	0.000	53.92707	62.40627
one	compo female #	43	4.993647	8.61	0.000	32.61514	53.38486
two	compo female #	64	2.496823	25.63	0.000	58.80757	69.19243
one	simpl	63.5	3.531041	17.98	0.000	56.1568	70.8432

The first margins table shows the predicted mean (marginal mean), standard error, z statistic, p-value, and confidence interval of y1 (age of patient) for each combination of fracture and gender. The second and third margins tables provide this information for y2 (blood lymphocytes) and y3 (blood polymorphonuclears). These three tables of predictions are the same as those you would obtain from margins after running anova for each of the three dependent variables separately.

The predicted y2 value is larger than the predicted y3 value for females with one compound fracture. For the other five combinations of gender and fracture, the relationship is reversed. There is only 1 observation for the combination of female and one compound fracture.

There are nine possible contrasts if we contrast women with men for every fracture type and every dependent variable. We will use contrast to estimate all nine contrasts and apply Scheffé's adjustment for multiple comparisons.

. contrast gender@fracture#\_eqns, mcompare(scheffe)

Contrasts of marginal linear predictions

: asbalanced Margins

	df	F	P>F	Scheffe P>F
gender@fracture#_eqns				
one compound fracture 1	1	2.51	0.1278	0.9733
one compound fracture 2	1	12.98	0.0017	0.2333
one compound fracture 3	1	11.34	0.0029	0.3137
two compound fractures 1	1	0.38	0.5424	1.0000
two compound fractures 2	1	0.07	0.7889	1.0000
two compound fractures 3	1	0.33	0.5732	1.0000
one simple fracture 1	1	1.08	0.3107	0.9987
one simple fracture 2	1	0.54	0.4698	0.9999
one simple fracture 3	1	1.71	0.2050	0.9929
Joint	9	2.57	0.0361	
Denominator	21			

Note: Scheffe-adjusted p-values are reported for tests on individual contrasts only.

	Number of Comparisons
gender@fracture#_eqns	9

	Contrast	Std. Err.	Sche	ffe Interval]
gender@fracture#_eqns				
(female vs base) one compound fracture 1 (female vs base)	-17.5	11.03645	-68.42869	33.42869
one compound fracture 2  (female vs base)	20.5	5.69092	-5.76126	46.76126
one compound fracture 3 (female vs base)	-18.16667	5.393755	-43.05663	6.723297
two compound fractures 1 (female vs base)	3.875	6.257079	-24.99885	32.74885
two compound fractures 2  (female vs base)	.875	3.226449	-14.01373	15.76373
two compound fractures 3 (female vs base)	1.75	3.057972	-12.36128	15.86128
one simple fracture 1 (female vs base)	-8.666667	8.342772	-47.16513	29.8318
one simple fracture 2 (female vs base)	-3.166667	4.301931	-23.01831	16.68498
one simple fracture 3	5.333333	4.077296	-13.48171	24.14838

Women do not differ significantly from men in any of the nine comparisons.

Let's examine the residuals with the predict command:

- . predict y1res, residual equation(y1)
- . predict y2res, residual equation(y2)
- . predict y3res, residual equation(y3)
- . list gender fracture y1res y2res y3res

	gender	fracture	y1res	y2res	y3res
1.	male	one compound fracture	2.5	5	1666667
2.	male	one compound fracture	2.5	7.5	-6.166667
3.	male	one compound fracture	8.5	5	2.833333
4.	male	one compound fracture	-4.5	-2.5	3.833333
5.	male	one compound fracture	-14.5	-4.5	2.833333
6.	male	one compound fracture	5.5	.5	-3.166667
7.	male	two compound fractures	-3.875	-5.375	1.75
8.	male	two compound fractures	-4.875	375	1.75
9.	male	two compound fractures	-1.875	-2.375	1.75
10.	male	two compound fractures	1.125	6.625	-6.25
11.	male	two compound fractures	-2.875	-1.375	6.75
12.	male	two compound fractures	25.125	-4.375	-2.25
13.	male	two compound fractures	-9.875	-2.375	1.75
14.	male	two compound fractures	-2.875	9.625	-5.25
15.	male	one simple fracture	-13.16667	.8333333	-4.166667
16.	male	one simple fracture	6.833333	-2.166667	3.833333
17.	male	one simple fracture	7.833333	8.833333	-7.166667
18.	male	one simple fracture	3.833333	-1.166667	1.833333
19.	male	one simple fracture	9.833333	-4.166667	1.833333
20.	male	one simple fracture	-15.16667	-2.166667	3.833333
21.	female	one compound fracture	0	0	-2.84e-14
22.	female	two compound fractures	-8.75	-4.25	4
23.	female	two compound fractures	7.25	-8.25	9
24.	female	two compound fractures	-9.75	3.75	-5
25.	female	two compound fractures	11.25	8.75	-8
26.	female	one simple fracture	6.5	-3	3.5
27.	female	one simple fracture	-6.5	3	-3.5

The single observation for a female with one compound fracture has residuals that are within roundoff of zero. With only 1 observation for that cell of the design, this MANOVA model is forced to fit to that point. The largest residual (in absolute value) appears for observation 12, which has an age 25.125 higher than the model prediction for a male with two compound fractures.

### Example 4: manovatest

Example 8 of [MV] manova presents a nested MANOVA on the videotrainer data.

- . use http://www.stata-press.com/data/r14/videotrainer, clear (video training)
- . manova primary extra = video / store|video / associate|store|video /,
- > dropemptycells
   (output omitted)

The MANOVA indicated that store was not significant.

You decide to follow the rule of thumb that says to pool terms whose *p*-values are larger than 0.25. Wilks's lambda reports a *p*-value of 0.5775 for the test of store|video (see example 8 of [MV] manova). You decide to pool the store and associate terms in the MANOVA to gain power for the test of video. The forward-slash notation of manova is also allowed with manovatest to indicate nonresidual error terms. Here is the multivariate test of video using the pooled store and associate terms and then the multivariate test of the pooled term:

. manovatest video / store|video associate|store|video

	W = Wilks' lambda P = Pillai's trace		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>					
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	_
video	W P L R	0.4079 0.5921 1.4516 1.4516	1	2.0 2.0 2.0 2.0	9.0 9.0 9.0 9.0	6.53 6.53	0.0177 0.0177 0.0177 0.0177	e e
store video associate store  video			10					_

e = exact, a = approximate, u = upper bound on F

. manovatest store|video associate|store|video

	W = Wilks' lambda P = Pillai's trace			L = Lawley-Hotelling trace R = Roy's largest root				
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
store video	W	0.3925	10	20.0	58.0	1.73	0.0546	- е
associate store	P	0.7160		20.0	60.0	1.67	0.0647	a
video	L	1.2711		20.0	56.0	1.78	0.0469	a
	R	0.9924		10.0	30.0	2.98	0.0100	u
Residual			30					_

e = exact, a = approximate, u = upper bound on F

Pooling store with associate helps increase the power for the test of video.

You can show the univariate analysis for one of your dependent variables by using the ytransform() option of manovatest:

- . mat primonly = (1,0)
- . manovatest video / store|video associate|store|video, ytransform(primonly)

Transformation of the dependent variables

primary

	W = Wilks' la P = Pillai's		<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	Statistic	df	F(df1,	df2) =	F	Prob>F	_
video	W 0.8449 P 0.1551 L 0.1835 R 0.1835	1	1.0 1.0 1.0	10.0 10.0 10.0 10.0	1.84 1.84	0.2053 0.2053 0.2053 0.2053	e
store video associate store  video		10					_

e = exact, a = approximate, u = upper bound on F

. manovatest store|video associate|store|video, ytransform(primonly)

Transformation of the dependent variables

(1) primary

	W = Wilks' lambda P = Pillai's trace			<pre>L = Lawley-Hotelling trace R = Roy's largest root</pre>				
Source	St	tatistic	df	F(df1,	df2) =	F	Prob>F	
store video	W	0.6119	10	10.0	30.0	1.90	0.0846	- е
associate store	P	0.3881		10.0	30.0	1.90	0.0846	е
video	L	0.6344		10.0	30.0	1.90	0.0846	е
	R	0.6344		10.0	30.0	1.90	0.0846	е
Residual			30					_

e = exact, a = approximate, u = upper bound on F

See the second manova run from example 8 of [MV] manova for an alternate way of pooling the terms by refitting the MANOVA model.

4

See examples 6, 10, 11, 12, and 13 of [MV] manova for more examples of manovatest, including examples involving both the test() and the ytransform() options.

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### Stored results

```
manovatest stores the following in r():
Scalars
    r(df)
                   hypothesis degrees of freedom
    r(df_r)
                   residual degrees of freedom
Matrices
    r(H)
                   hypothesis SSCP matrix
                   residual-error SSCP matrix
    r(E)
    r(stat)
                   multivariate statistics
    r(eigvals)
                   eigenvalues of E-1H
                   s, m, and n values
    r(aux)
test after manova stores the following in r():
Scalars
    r(p)
                   two-sided p-value
    r(F)
                   F statistic
    r(df)
                   hypothesis degrees of freedom
    r(df_r)
                   residual degrees of freedom
    r(drop)
                   0 if no constraints dropped, 1 otherwise
    r(dropped_#) index of #th constraint dropped
    r(mtmethod)
                   method of adjustment for multiple testing
Matrices
    r(mtest)
                   multiple test results
```

### Methods and formulas

See [MV] manova for methods and formulas for the multivariate tests performed by manovatest.

### Also see

```
    [MV] manova — Multivariate analysis of variance and covariance
    [MV] screeplot — Scree plot
    [U] 20 Estimation and postestimation commands
```

### Title

matrix dissimilarity —	Compute	similarity or	dissimilarity	measures
------------------------	---------	---------------	---------------	----------

Description Syntax Options Remarks and examples References Also see

# **Description**

matrix dissimilarity computes a similarity, dissimilarity, or distance matrix.

# **Syntax**

$$\underline{\mathtt{mat}}$$
rix  $\underline{\mathtt{dis}}$ similarity matname =  $[varlist]$   $[if]$   $[in]$   $[in]$ 

options	Description
measure	similarity or dissimilarity measure; default is L2 (Euclidean)
<u>obs</u> ervations	compute similarities or dissimilarities between observations; the default
<u>var</u> iables	compute similarities or dissimilarities between variables
<pre>names(varname)</pre>	row/column names for matname (allowed with observations)
<u>allb</u> inary	check that all values are 0, 1, or missing
proportions	interpret values as proportions of binary values
$\overline{\mathtt{diss}}\mathtt{im}(\mathit{method})$	change similarity measure to dissimilarity measure

where method transforms similarities to dissimilarities by using

oneminus 
$$d_{ij} = 1 - s_{ij}$$
  $\underline{ exttt{st}}$  and  $d_{ij} = \sqrt{s_{ii} + s_{jj} - 2s_{ij}}$ 

# **Options**

*measure* specifies one of the similarity or dissimilarity measures allowed by Stata. The default is L2, Euclidean distance. Many similarity and dissimilarity measures are provided for continuous data and for binary data; see [MV] *measure\_option*.

observations and variables specify whether similarities or dissimilarities are computed between observations or variables. The default is observations.

names(varname) provides row and column names for matname. varname must be a string variable with a length of 32 or less. You will want to pick a varname that yields unique values for the row and column names. Uniqueness of values is not checked by matrix dissimilarity. names() is not allowed with the variables option. The default row and column names when the similarities or dissimilarities are computed between observations is obs#, where # is the observation number corresponding to that row or column.

allbinary checks that all values are 0, 1, or missing. Stata treats nonzero values as one (excluding missing values) when dealing with what are supposed to be binary data (including binary similarity measures). allbinary causes matrix dissimilarity to exit with an error message if the values are not truly binary. allbinary is not allowed with proportions or the Gower measure.

proportions is for use with binary similarity measures. It specifies that values be interpreted as proportions of binary values. The default action treats all nonzero values as one (excluding missing values). With proportions, the values are confirmed to be between zero and one, inclusive. See [MV] measure\_option for a discussion of the use of proportions with binary measures. proportions is not allowed with allbinary or the Gower *measure*.

dissim(method) specifies that similarity measures be transformed into dissimilarity measures. method may be oneminus or standard. oneminus transforms similarities to dissimilarities by using  $d_{ij}=1-s_{ij}$  (Kaufman and Rousseeuw 1990, 21). standard uses  $d_{ij}=\sqrt{s_{ii}+s_{jj}-2s_{ij}}$ (Mardia, Kent, and Bibby 1979, 402). dissim() does nothing when the measure is already a dissimilarity or distance. See [MV] *measure\_option* to see which *measures* are similarities.

# Remarks and examples

Commands such as cluster singlelinkage, cluster completelinkage, and mds (see [MV] cluster and [MV] mds) have options allowing the user to select the similarity or dissimilarity measure to use for its computation. If you are developing a command that requires a similarity or dissimilarity matrix, the matrix dissimilarity command provides a convenient way to obtain it.

The similarity or dissimilarity between each observation (or variable if the variables option is specified) and the others is placed in matname. The element in the ith row and jth column gives either the similarity or dissimilarity between the ith and jth observation (or variable). Whether you get a similarity or a dissimilarity depends upon the requested *measure*; see [MV] *measure\_option*.

If there are many observations (variables when the variables option is specified), you may need to increase the maximum matrix size; see [R] matsize. If the number of observations (or variables) is so large that storing the results in a matrix is not practical, you may wish to consider using the cluster measures command, which stores similarities or dissimilarities in variables; see [MV] cluster programming utilities.

When computing similarities or dissimilarities between observations, the default row and column names of matname are set to obs#, where # is the observation number. The names() option allows you to override this default. For similarities or dissimilarities between variables, the row and column names of *matname* are set to the appropriate variable names.

The order of the rows and columns corresponds with the order of your observations when you are computing similarities or dissimilarities between observations. Warning: If you reorder your data (for example, using sort or gsort) after running matrix dissimilarity, the row and column ordering will no longer match your data.

Another use of matrix dissimilarity is in performing a cluster analysis on variables instead of observations. The cluster command performs a cluster analysis of the observations; see [MV] cluster. If you instead wish to cluster variables, you can use the variables option of matrix dissimilarity to obtain a dissimilarity matrix that can then be used with clustermat; see [MV] clustermat and example 2 below.

# Example 1

Example 1 of [MV] cluster linkage introduces data with four chemical laboratory measurements on 50 different samples of a particular plant. Let's find the Canberra distance between the measurements performed by lab technician Bill found among the first 25 observations of the labtech dataset.

```
. use http://www.stata-press.com/data/r14/labtech
. matrix dissim D = x1 x2 x3 x4 if labtech=="Bill" in 1/25, canberra
. matrix list D
symmetric D[6.6]
            obs7
                                 obs20
                                            ohe22
                                                       obs23
                                                                   obs25
                      obs18
obs7
               0
obs18 1.3100445
obs20 1.1134916
                 .87626565
                                     0
      1.452748 1.0363077
                             1.0621064
                                                0
obs22
obs23
       1.0380665
                  1.4952796
                             .81602718
                                        1.6888123
                                                           0
obs25 1.4668898 1.5139834
                             1.4492336
                                        1.0668425
                                                  1.1252514
                                                                       0
```

By default, the row and column names of the matrix indicate the observations involved. The Canberra distance between the 23rd observation and the 18th observation is 1.4952796. See [MV] *measure\_option* for a description of the Canberra distance.

4

### Example 2

Example 2 of [MV] cluster linkage presents a dataset with 30 observations of 60 binary variables, a1, a2, ..., a30. In [MV] cluster linkage, the observations were clustered. Here we instead cluster the variables by computing the dissimilarity matrix by using matrix dissimilarity with the variables option followed by the clustermat command.

We use the matching option to obtain the simple matching similarity coefficient but then specify dissim(oneminus) to transform the similarities to dissimilarities by using the transformation  $d_{ij} = 1 - s_{ij}$ . The allbinary option checks that the variables really are binary (0/1) data.

```
. use http://www.stata-press.com/data/r14/homework
```

- . matrix dissim Avars = a\*, variables matching dissim(oneminus) allbinary
- . matrix subA = Avars[1..5,1..5]
- . matrix list subA

symmetric subA[5 5]

symmetric	SUDA	[5,5]			
	a1	a2	a3	a4	<b>a</b> 5
a1	0				
a2	.4	0			
a3	.4	.46666667	0		
a4	.3	.3	.36666667	0	
a5	.4	.4	.13333333	.3	0

We listed the first five rows and columns of the  $60 \times 60$  matrix. The matrix row and column names correspond to the variable names.

To perform an average-linkage cluster analysis on the 60 variables, we supply the Avars matrix created by matrix dissimilarity to the clustermat averagelinkage command; see [MV] cluster linkage.

```
. clustermat averagelinkage Avars, clear
number of observations (_N) was 0, now 60
cluster name: _clus_1
. cluster generate g5 = groups(5)
```

. table g5

Freq.	g5
21 9 25 4 1	1 2 3 4 5

We generated a variable, g5, indicating the five-group cluster solution and then tabulated to show how many variables were clustered into each of the five groups. Group five has only one member.

. list g5 if g5==5

The member corresponds to the 13th observation in the current dataset, which in turn corresponds to variable a13 from the original dataset. It appears that a13 is not like the other variables.

4

# Example 3

matrix dissimilarity drops observations containing missing values, except when the Gower measure is specified. The computation of the Gower dissimilarity between 2 observations is based on the variables where the 2 observations both have nonmissing values.

We illustrate using a dataset with 6 observations and 4 variables where only 2 of the observations have complete data.

- . use http://www.stata-press.com/data/r14/gower, clear
- . list

	b1	b2	<b>x1</b>	x2
1. 2. 3. 4.	0	1	.76	.75
2.				
3.	1	0	.72	.88
4.		1	.4	
5.	0		•	.14
6.	0	0	.55	

- . mat dissimilarity matL2 = b\* x\*, L2
- . matlist matL2, format(%8.3f)

	obs1	obs3
obs1	0.000	0.000

The resulting matrix is  $2 \times 2$  and provides the dissimilarity between observations 1 and 3. All other observations contained at least one missing value.

However, with the gower measure we obtain a  $6 \times 6$  matrix.

- . matrix dissimilarity matgow = b1 b2 x1 x2, gower
- . matlist matgow, format(%8.3f)

	obs1	obs2	obs3	obs4	obs5	obs6
obs1	0.000					
obs2		0.000				
obs3	0.572	•	0.000			
obs4	0.500	•	0.944	0.000		
obs5	0.412	•	1.000		0.000	
obs6	0.528		0.491	0.708	0.000	0.000

Because all the values for observation 2 are missing, the matrix contains missing values for the dissimilarity between observation 2 and the other observations. Notice the missing value in matgow for the dissimilarity between observations 4 and 5. There were no variables where observations 4 and 5 both had nonmissing values, and hence the Gower coefficient could not be computed.

4

### References

Kaufman, L., and P. J. Rousseeuw. 1990. Finding Groups in Data: An Introduction to Cluster Analysis. New York: Wiley.

Mardia, K. V., J. T. Kent, and J. M. Bibby. 1979. Multivariate Analysis. London: Academic Press.

### Also see

[MV] **cluster** — Introduction to cluster-analysis commands

[MV] **clustermat** — Introduction to clustermat commands

[MV] mdsmat — Multidimensional scaling of proximity data in a matrix

[MV] cluster programming utilities — Cluster-analysis programming utilities

[MV] measure\_option — Option for similarity and dissimilarity measures

[P] matrix — Introduction to matrix commands

### **Title**

mca — Multiple and joint correspondence analysis

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

mca performs multiple correspondence analysis (MCA) or joint correspondence analysis (JCA) on a series of categorical variables. MCA and JCA are two generalizations of correspondence analysis (CA) of a cross-tabulation of two variables (see [MV] ca) to the cross-tabulation of multiple variables.

mca performs an analysis of two or more integer-valued variables. Crossing (also called stacking) of integer-valued variables is also allowed.

### **Quick start**

Multiple and joint correspondence analysis

Correspondence analysis of the multiway cross-tabulation of catvar1, catvar2, and catvar3 mca catvar1 catvar2 catvar3

Also produce the MCA coordinate plot mca catvar1 catvar2 catvar3, plot

Use 3 dimensions instead of 2 and display the tables compactly mca catvar1 catvar2 catvar3, dimensions(3) compact

Use principal normalization instead of the default standard normalization mca catvar1 catvar2 catvar3, normalize(principal)

Joint correspondence analysis of catvar1, catvar2, and catvar3
 mca catvar1 catvar2 catvar3, method(joint)

Multiple and joint correspondence analysis with crossed (stacked) variables

Multiple correspondence analysis of the multiway tabulation of catvar1, catvar2 and the crossed variables catvar3 and catvar4 with the crossed variables called z

```
mca catvar1 catvar2 (z: catvar3 catvar4)
```

As above, but joint correspondence analysis

```
mca catvar1 catvar2 (z: catvar3 catvar4), method(joint)
```

#### Menu

Statistics > Multivariate analysis > Correspondence analysis > Multiple correspondence analysis (MCA)

## **Syntax**

```
Basic syntax for two or more categorical variables
```

```
mca varlist [if] [in] [weight] [, options]
```

Full syntax for use with two or more categorical or crossed (stacked) categorical variables

```
mca speclist [if] [in] [weight] [, options]
```

where

```
speclist = spec [spec ...]
spec = varlist \mid (newvar : varlist)
```

options

plot

maxlength(#)

#### Description

Model	
<pre>supplementary(speclist)</pre>	supplementary (passive) variables
method(burt)	use the Burt matrix approach to MCA; the default
$\underline{\mathtt{meth}}\mathtt{od}(\underline{\mathtt{i}}\mathtt{ndicator})$	use the indicator matrix approach to MCA
<pre>method(joint)</pre>	perform a joint correspondence analysis (JCA)
dimensions(#)	number of dimensions (factors, axes); default is dim(2)
<pre>normalize(standard)</pre>	display standard coordinates; the default
<pre>normalize(principal)</pre>	display principal coordinates
iterate(#)	<pre>maximum number of method(joint) iterations; default is   iterate(250)</pre>
tolerance(#)	<pre>tolerance for method(joint) convergence criterion; default is   tolerance(1e-5)</pre>
<u>miss</u> ing	treat missing values as ordinary values
$\underline{\mathtt{noadj}}\mathtt{ust}$	suppress the adjustment of eigenvalues (method(burt) only)
Codes	
$\mathtt{report}(\underline{\mathtt{v}}\mathtt{ariables})$	report coding of crossing variables
$\overline{\text{report}}(\underline{\text{c}}\text{rossed})$	report coding of crossed variables
report( <u>a</u> ll)	report coding of crossing and crossed variables
$\frac{\overline{\texttt{len}}}{\texttt{gth}}(\underline{\texttt{m}} \texttt{in})$	use minimal length unique codes of crossing variables
<pre>length(#)</pre>	use # as coding length of crossing variables
Reporting	
<pre>ddimensions(#)</pre>	display # singular values; default is ddim(.) (all)
<pre>points(varlist)</pre>	display tables for listed variables; default is all variables
compact	display statistics table in a compact format
log	display the iteration log (method(joint) only)

plot the coordinates (that is, mcaplot)

maxlength(12)

maximum number of characters for labels in plot; default is

bootstrap, by, jackknife, rolling, and statsby may be used with mca; see [U] 11.1.10 Prefix commands. However, bootstrap and jackknife results should be interpreted with caution; identification of the mca parameters involves data-dependent restrictions, possibly leading to badly biased and overdispersed estimates (Milan and Whittaker 1995).

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

## **Options**

Model )

supplementary(speclist) specifies that speclist are supplementary variables. Such variables do not affect the MCA solution, but their categories are mapped into the solution space. For method(indicator), this mapping uses the first method described by Greenacre (2006). For method(burt) and method(joint), the second and recommended method described by Greenacre (2006) is used, in which supplementary column principal coordinates are derived as a weighted average of the standard row coordinates, weighted by the supplementary profile. See the syntax diagram for the syntax of speclist.

method (method) specifies the method of MCA/JCA.

method(burt), the default, specifies MCA, a categorical variables analogue to principal component analysis (see [MV] pca). The Burt method performs a CA of the Burt matrix, a matrix of the two-way cross-tabulations of all pairs of variables.

method(indicator) specifies MCA via a CA on the indicator matrix formed from the variables.

method(joint) specifies JCA, a categorical variables analogue to factor analysis (see [MV] **factor**). This method analyzes a variant of the Burt matrix, in which the diagonal blocks are iteratively adjusted for the poor diagonal fit of MCA.

dimensions (#) specifies the number of dimensions (= factors = axes) to be extracted. The default is dimensions(2). If you specify dimensions(1), the categories are placed on one dimension. The number of dimensions is no larger than the number of categories in the active variables (regular and crossed) minus the number of active variables, and it can be less. This excludes supplementary variables. Specifying a larger number than the dimensions available results in extracting all dimensions.

MCA is a hierarchical method so that extracting more dimensions does not affect the coordinates and decomposition of inertia of dimensions already included. The percentages of inertia accounting for the dimensions are in decreasing order as indicated by the singular values. The first dimension accounts for the most inertia, followed by the second dimension, and then the third dimension, etc.

normalize(normalization) specifies the normalization method, that is, how the row and column coordinates are obtained from the singular vectors and singular values of the matrix of standardized residuals.

normalize(standard) specifies that coordinates are returned in standard normalization (singular values divided by the square root of the mass). This is the default.

normalize(principal) specifies that coordinates are returned in principal normalization. Principal coordinates are standard coordinates multiplied by the square root of the corresponding principal inertia.

iterate(#) is a technical and rarely used option specifying the maximum number of iterations. iterate() is permitted only with method(joint). The default is iterate(250).

- tolerance(#) is a technical and rarely used option specifying the tolerance for subsequent modification
   of the diagonal blocks of the Burt matrix. tolerance() is permitted only with method(joint).
   The default is tolerance(1e-5).
- missing treats missing values as ordinary values to be included in the analysis. Observations with missing values are omitted from the analysis by default.
- noadjust suppresses principal inertia adjustment and is allowed with method(burt) only. By default, the principal inertias (eigenvalues of the Burt matrix) are adjusted. The unmodified principal inertias present a pessimistic measure of fit because MCA fits the diagonal of **P** poorly (see Greenacre [1984]).

Codes

- report(opt) displays coding information for the crossing variables, crossed variables, or both. report() is ignored if you do not specify at least one crossed variable.
  - report(variables) displays the coding schemes of the crossing variables, that is, the variables used to define the crossed variables.
  - report(crossed) displays a table explaining the value labels of the crossed variables.
  - report(all) displays the codings of the crossing and crossed variables.
- length(opt) specifies the coding length of crossing variables.
  - length(min) specifies that the minimal-length unique codes of crossing variables be used.
  - length(#) specifies that the coding length # of crossing variables be used, where # must be between 4 and 32.

Reporting

- ddimensions(#) specifies the number of singular values to be displayed. If ddimensions() is greater than the number of singular values, all the singular values will be displayed. The default is ddimensions(.), meaning all singular values.
- points(varlist) indicates the variables to be included in the tables. By default, tables are displayed for all variables. Regular categorical variables, crossed variables, and supplementary variables may be specified in points().
- compact specifies that point statistics tables be displayed multiplied by 1,000, enabling the display of more columns without wrapping output. The compact tables can be displayed without wrapping for models with two dimensions at line size 79 and with three dimensions at line size 99.
- log displays an iteration log. This option is permitted with method(joint) only.
- plot displays a plot of the row and column coordinates in two dimensions. Use mcaplot directly to select different plotting points or for other graph refinements; see [MV] mca postestimation plots.
- maxlength(#) specifies the maximum number of characters for labels in plots. The default is maxlength(12). # must be less than 32.
  - Note: The reporting options may be specified during estimation or replay.

## Remarks and examples

Remarks are presented under the following headings:

Introduction Compare MCA on two variables and CA MCA on four variables CA of the indicator matrix CA of the Burt matrix Joint correspondence analysis

#### Introduction

Multiple correspondence analysis (MCA) and joint correspondence analysis (JCA) are methods for analyzing observations on categorical variables. MCA is usually viewed as an extension of simple correspondence analysis (CA) to more than two variables. CA analyzes a two-way contingency table; MCA and JCA analyze a multiway table.

MCA can be viewed as a generalization of principal component analysis where the variables to be analyzed are categorical, not continuous. MCA performs a CA on a Burt or indicator matrix; it explores the relationships within a set of variables, whereas CA has more focus on exploring relationships between two sets of variables. JCA is an extension of MCA that attempts to remedy discrepancies between CA and MCA.

For an introduction to MCA via CA, see Rencher and Christensen (2012) or Everitt and Dunn (2001). For an advanced introduction to MCA without previous discussion of CA, see Gower and Hand (1996). Greenacre (2006) approaches MCA from CA, then JCA from MCA, and gives a more advanced treatment. [MV] ca also introduces MCA concepts. Gower (1990) explores MCA history.

Three methods are implemented here. We will start with the simplest and most intuitive representation of unordered categorical data: the indicator matrix, usually denoted Z, a matrix of zeros and ones with columns for all categories of all variables and rows corresponding to observations. A value of one indicates that a category is observed; a zero indicates that it is not. MCA can be performed as a CA on the indicator matrix; an equivalent to this method is method(indicator) with mca.

Here is a manufactured indicator matrix **Z**, with 10 observations on three categorical variables, w, x, and y, each with two categories indicated by  $w_1, w_2, x_1, x_2, y_1, y_2$ :

For large datasets with many variables and observations, the indicator matrix is burdensome and can exceed memory limitations. The Burt matrix, usually denoted as B, is a cross-tabulation of all categories of all variables.  $\mathbf{B} = \mathbf{Z}'\mathbf{Z}$ . The Burt matrix is smaller than the indicator matrix  $\mathbf{Z}$ . Performing CA on the Burt matrix and performing CA on the indicator matrix are related but not the same: they give equivalent standard coordinates, but the total principal inertias from the indicator matrix approach and Burt matrix approach are different. Performing a CA of the Burt matrix without further calculation is method(burt) along with the noadjust option.

The Burt matrix, B, corresponding to matrix Z, above:

$$\mathbf{B} = \begin{pmatrix} w_1 & w_2 & x_1 & x_2 & y_1 & y_2 \\ w_1 & 7 & 0 & 4 & 3 & 3 & 4 \\ w_2 & 0 & 3 & 1 & 2 & 3 & 0 \\ 4 & 1 & 5 & 0 & 3 & 2 \\ 3 & 2 & 0 & 5 & 3 & 2 \\ y_1 & 3 & 3 & 3 & 3 & 6 & 0 \\ y_2 & 4 & 0 & 2 & 2 & 0 & 4 \end{pmatrix}$$

Applying CA to the Burt matrix or indicator matrix artificially inflates the chi-squared distances between profiles and the total inertia; see Gower (2006). This can be partially remedied after CA of the Burt matrix by scale readjustments of the MCA solution. Performing adjustments after a CA of the Burt matrix is the default, that is, if no method is specified method(burt) is assumed; unadjusted estimates may be obtained by using the option noadjust.

The third method, JCA, generalizes CA more naturally to more than two categorical variables. JCA attempts to account for the variation in the off-diagonal submatrices of the Burt matrix. It corrects the inflation of the total inertia. The solution can no longer be obtained by one application of the singular value decomposition (as in CA). JCA is obtained by specifying the option method(joint) to mca.

## Compare MCA on two variables and CA

We illustrate MCA with a dataset from the International Social Survey Program on environment (ISSP 1993). This example is used in the MCA literature; see Greenacre (2006). We will look at the questions on attitudes toward science. We use data from the West German sample only and remove all observations containing missing data; 871 observations remain. The survey questions are

How much do you agree or disagree with each of these statements?

- A. We believe too often in science, and not enough in feelings and faith.
- B. Overall, modern science does more harm than good.
- C. Any change humans cause in nature—no matter how scientific—is likely to make things worse.
- D. Modern science will solve our environmental problems with little change to our way of life.

Each question has five possible response categories:

- 1. Agree strongly
- 2. Agree
- 3. Neither agree nor disagree
- 4. Disagree
- 5. Disagree strongly

Supplementary demographic information is also available as coded categorical variables:

Sex: male, female

Age: (six groups) 16-24, 25-34, 35-44, 45-54, 55-64, 65 and older

Education: (six groups) primary incomplete, primary completed, secondary incomplete, secondary completed, tertiary incomplete, tertiary completed.

#### Example 1

Here is a summary of these data.

- . use http://www.stata-press.com/data/r14/issp93
  (Selection from ISSP (1993))
- . describe

Contains data from http://www.stata-press.com/data/r14/issp93.dta
obs: 871 Selection from ISSP (1993)
vars: 8 17 May 2014 09:36
size: 7,839 (\_dta has notes)

variable name	storage type	display format	value label	variable label
id	int	%9.0g		respondent identifier
A	byte	%26.0g	agree5	too much science, not enough feelings&faith
В	byte	%26.0g	agree5	science does more harm than good
C	byte	%26.0g	agree5	any change makes nature worse
D	byte	%26.0g	agree5	science will solve environmental problems
sex	byte	%9.0g	sex	sex
age	byte	%9.0g	age	age (6 categories)
edu	byte	%20.0g	edu	education (6 categories)

Sorted by:

We begin by comparing MCA with two variables to CA with two variables. The default MCA analysis is a CA of the Burt matrix, performed with adjustment to the principal inertias. The unadjusted results from MCA will give different principal inertias from the CA, although the standard coordinates would

be the same. With adjustment, results are nearly identical. For a detailed discussion of the output of ca and mca, see [MV] ca.

#### . mca A B

Multiple/Joint correspondence analysis Number of obs = 871
Total inertia = .23775345
Method: Burt/adjusted inertias Number of axes = 2

Dimension	principal inertia	percent	cumul percent
dim 1 dim 2 dim 3 dim 4	.1686131 .0586785 .010444 .0000178	70.92 24.68 4.39 0.01	70.92 95.60 99.99 100.00
Total	. 2377535	100.00	

Statistics for column categories in standard normalization

	overall			d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.068	1.000	0.100	1.017	0.502	0.071
agree	0.185	0.997	0.042	0.560	0.982	0.058
neither ag~e	0.117	0.930	0.062	0.248	0.083	0.007
disagree	0.102	0.922	0.123	-1.239	0.907	0.157
disagree s~y	0.028	0.954	0.174	-2.741	0.845	0.207
В						
agree stro~y	0.041	0.982	0.146	1.571	0.490	0.101
agree	0.100	0.962	0.034	0.667	0.932	0.044
neither ag~e	0.118	0.840	0.043	0.606	0.716	0.043
disagree	0.161	0.769	0.043	-0.293	0.228	0.014
disagree s~y	0.080	0.994	0.235	-1.926	0.900	0.298

	dimension_2					
Categories	coord	sqcorr	contrib			
Α						
agree stro~y	1.718	0.498	0.202			
agree	0.116	0.015	0.002			
neither ag~e	-1.344	0.847	0.212			
disagree	-0.268	0.015	0.007			
disagree s~y	1.672	0.109	0.077			
В						
agree stro~y	2.671	0.493	0.291			
agree	-0.201	0.029	0.004			
neither ag~e	-0.427	0.124	0.022			
disagree	-0.764	0.541	0.094			
disagree s~y	1.055	0.094	0.089			

With ca we use the norm(standard) option to obtain results in the same normalization as the preceding mca. [MV] ca discusses the normalize() option; mca has some of the normalize() options of ca.

The top table in the output for both ca and mca reports the principal inertias. The principal inertias reported by ca are simply the squares of the singular values. Two pieces of information reported by ca that are not reported by mca are the chi-squared value in the table and the explained inertia in the header. The chi-squared value is taken as a measure of dissimilarity between the row and column

profiles of the two-way table. Chi-squared distance makes sense for a two-way table but has less justification when applied to the rows and columns of either the indicator matrix or the Burt matrix (Greenacre 2006). The explained inertia is the value from the cumulative percent column in the top table corresponding to the number of dimensions selected; it is simply not reported in the mca header.

The coordinates reported in the second table are the same. The mass, inertia, and contributions are half as large in mca as they are in ca; in ca the row and column each sum to the principal inertia, but in mca there are only columns, which sum to the principal inertia.

. ca A B, norm(standard)

Correspondence analysis

Number of obs =
Pearson chi2(16) =
Prob > chi2 =

5 active rows 5 active columns Pearson chi2(16) = 207.08 Prob > chi2 = 0.0000 Total inertia = 0.2378 Number of dim. = 2 Expl. inertia (%) = 95.60

871

Dimension	singular value	principal inertia	chi2	percent	cumul percent
dim 1 dim 2 dim 3 dim 4	.4106252 .2422364 .1021961 .0042238	.1686131 .0586785 .010444 .0000178	146.86 51.11 9.10 0.02	70.92 24.68 4.39 0.01	70.92 95.60 99.99
total	.0042200	.2377535	207.08	100	

Statistics for row and column categories in standard normalization

	1	overall		d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.137	1.000	0.200	1.017	0.502	0.141
agree	0.370	0.997	0.084	0.560	0.982	0.116
neither ag~e	0.234	0.930	0.123	0.248	0.083	0.014
disagree	0.204	0.922	0.245	-1.239	0.907	0.314
disagree s~y	0.055	0.954	0.348	-2.741	0.845	0.414
В						
agree stro~y	0.082	0.982	0.291	1.571	0.490	0.201
agree	0.200	0.962	0.068	0.667	0.932	0.089
neither ag~e	0.235	0.840	0.086	0.606	0.716	0.087
disagree	0.323	0.769	0.086	-0.293	0.228	0.028
disagree s~y	0.161	0.994	0.470	-1.926	0.900	0.596

	dimension_2					
Categories	coord	sqcorr	contrib			
A						
agree stro~y	1.718	0.498	0.403			
agree	0.116	0.015	0.005			
neither ag~e	-1.344	0.847	0.423			
disagree	-0.268	0.015	0.015			
disagree s~y	1.672	0.109	0.154			
В						
agree stro~y	2.671	0.493	0.582			
agree	-0.201	0.029	0.008			
neither ag~e	-0.427	0.124	0.043			
disagree	-0.764	0.541	0.188			
disagree s~y	1.055	0.094	0.179			

#### MCA on four variables

Now we will take a look at MCA with more than two variables and at the different methods of performing MCA or JCA.

## Example 2

We continue to use the ISSP (1993) dataset, looking at all four questions on attitudes toward science. We use the default method of MCA, which is a CA of the Burt matrix for the data, followed by simple scale adjustments. We choose the principal normalization normalize(principal), which scales the coordinates by the principal inertias. MCA with the Burt matrix and adjustments explains at least 79.1% of the total inertia in the first two dimensions.

. mca A-D, normalize(principal)

Multiple/Joint correspondence analysis

Number of obs = 871

Total inertia = .17024552

Method: Burt/adjusted inertias

Number of axes = 2

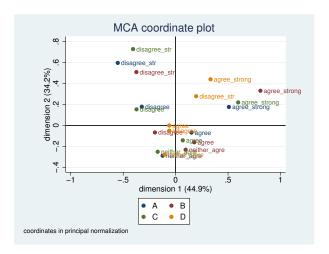
Dimension	principal inertia	percent	cumul percent
dim 1	.0764553	44.91	44.91
dim 2	.0582198	34.20	79.11
dim 3	.009197	5.40	84.51
dim 4	.0056697	3.33	87.84
dim 5	.0011719	0.69	88.53
dim 6	6.61e-06	0.00	88.53
Total	.1702455	100.00	

Statistics for column categories in principal normalization

		overall		d:	$imension_{-}$	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.034	0.963	0.060	0.508	0.860	0.115
agree	0.092	0.659	0.023	0.151	0.546	0.028
neither ag~e	0.059	0.929	0.037	-0.124	0.143	0.012
disagree	0.051	0.798	0.051	-0.322	0.612	0.069
disagree s~y	0.014	0.799	0.067	-0.552	0.369	0.055
В						
agree stro~y	0.020	0.911	0.100	0.809	0.781	0.174
agree	0.050	0.631	0.027	0.177	0.346	0.021
neither ag~e	0.059	0.806	0.027	0.096	0.117	0.007
disagree	0.081	0.620	0.033	-0.197	0.555	0.041
disagree s~y	0.040	0.810	0.116	-0.374	0.285	0.074
C						
agree stro~y	0.044	0.847	0.122	0.597	0.746	0.203
agree	0.091	0.545	0.024	0.068	0.101	0.006
neither ag~e	0.057	0.691	0.045	-0.171	0.218	0.022
disagree	0.044	0.788	0.054	-0.373	0.674	0.080
disagree s~y	0.015	0.852	0.071	-0.406	0.202	0.032
D						
agree stro~y	0.017	0.782	0.039	0.333	0.285	0.025
agree	0.067	0.126	0.012	-0.061	0.126	0.003
neither ag~e	0.058	0.688	0.044	-0.106	0.087	0.009
disagree	0.065	0.174	0.014	-0.061	0.103	0.003
disagree s~y	0.043	0.869	0.034	0.196	0.288	0.022

	dimension_2					
Categories	coord	sqcorr	contrib			
Α						
agree stro~y	0.176	0.103	0.018			
agree	-0.069	0.113	0.007			
neither ag~e	-0.289	0.786	0.084			
disagree	0.178	0.186	0.028			
disagree s~y	0.596	0.430	0.084			
В						
agree stro~y	0.331	0.131	0.038			
agree	-0.161	0.285	0.022			
neither ag~e	-0.233	0.690	0.055			
disagree	-0.068	0.065	0.006			
disagree s~y	0.509	0.526	0.179			
C						
agree stro~y	0.219	0.101	0.036			
agree	-0.143	0.444	0.032			
neither ag~e	-0.252	0.473	0.062			
disagree	0.153	0.114	0.018			
disagree s~y	0.728	0.650	0.136			
D						
agree stro~y	0.440	0.497	0.057			
agree	-0.002	0.000	0.000			
neither ag~e	-0.280	0.601	0.078			
disagree	-0.051	0.071	0.003			
disagree s~y	0.278	0.581	0.057			
D agree stro~y agree neither ag~e disagree	-0.002 -0.280 -0.051	0.000 0.601 0.071	0.000 0.078 0.003			

. mcaplot, overlay origin



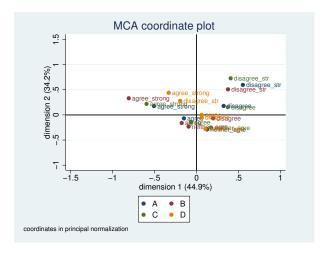
We displayed the origin axes in the plot with option origin. This plot makes it easier to see data associations. For more information on mcaplot, see [MV] mca postestimation plots.

A clear pattern is seen in the plot. Results from questions A, B, and C are clustered together, whereas question D forms a pattern of its own. Question D is formulated differently from A, B, and C, and the plot shows its incompatibility with the others.

4

Greenacre (2006, 70) produces this same plot. To obtain equivalent results, we reflect over the y axis with xnegate and adjust the scale of the graph with xlabel() and ylabel().

. mcaplot, overlay xnegate origin ylabel(-1(.5)1.5) xlabel(-1.5(.5)1)



#### □ Technical note

The percentage of inertia in the top table of the mca output does not add up to 100%, although all singular values are displayed. Why? The percentages are lower-bound estimates in the Burt method with adjustments.

#### □ Technical note

Readers who are familiar with the discussion of the normalize() option in [MV] ca might be wondering why we are doing analysis of coordinates in the principal normalization. Principal normalization in ca does not allow good associations between the row and column categories, and so the symmetric normalization is the default used for ca. Principal normalization does allow studying the row categories or column categories separately from each other in ca. In mca there are only column categories. Consequently, the principal normalization is often preferred.

#### CA of the indicator matrix

#### Example 3

We compare the previous result with that obtained using the method(indicator) option to perform an equivalent analysis to CA on the indicator matrix for these data. The first two dimensions explain only 22.2% of the total principal inertia.

. mca A-D, method(indicator)

Multiple/Joint correspondence analysis Number of obs 871 Total inertia 4 Method: Indicator matrix Number of axes 2

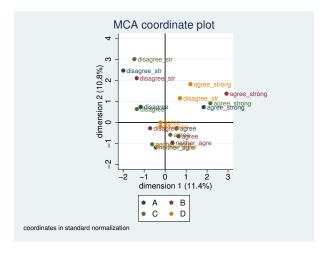
principal cumul percent Dimension inertia percent dim 1 .4573792 11.43 11.43 dim 2 .4309658 10.77 22.21 dim 3 .3219257 8.05 30.26 dim 4 .3064732 7.66 37.92 dim 5 .2756747 6.89 44.81 dim 6 6.30 51.11 .251928 dim 7 6.06 57.17 .2425591 dim 8 .2349506 5.87 63.05 dim 9 .225468 5.64 68.68 dim 10 .2206291 5.52 74.20 dim 11 .2098376 5.25 79.44 dim 12 .1971485 4.93 84.37 dim 13 .1778833 4.45 88.82 dim 14 4.23 93.05 .1691119 dim 15 .1528191 3.82 96.87 dim 16 .1252462 3.13 100.00 Total 4 100.00

Statistics for column categories in standard normalization

	overall			overall dimension_1		1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.034	0.280	0.054	1.837	0.244	0.078
agree	0.092	0.100	0.039	0.546	0.080	0.019
neither ag~e	0.059	0.218	0.048	-0.447	0.028	0.008
disagree	0.051	0.220	0.050	-1.166	0.160	0.047
disagree s~y	0.014	0.260	0.059	-1.995	0.106	0.037
В						
agree stro~y	0.020	0.419	0.057	2.924	0.347	0.118
agree	0.050	0.095	0.050	0.642	0.047	0.014
neither ag~e	0.059	0.140	0.048	0.346	0.017	0.005
disagree	0.081	0.127	0.042	-0.714	0.111	0.028
disagree s~y	0.040	0.527	0.052	-1.354	0.161	0.050
С						
agree stro~y	0.044	0.525	0.052	2.158	0.450	0.137
agree	0.091	0.102	0.040	0.247	0.016	0.004
neither ag~e	0.057	0.189	0.048	-0.619	0.051	0.015
disagree	0.044	0.216	0.051	-1.349	0.179	0.054
disagree s~y	0.015	0.312	0.059	-1.468	0.063	0.022
D						
agree stro~y	0.017	0.155	0.058	1.204	0.049	0.017
agree	0.067	0.008	0.046	-0.221	0.008	0.002
neither ag~e	0.058	0.195	0.048	-0.385	0.020	0.006
disagree	0.065	0.015	0.046	-0.222	0.008	0.002
disagree s~y	0.043	0.168	0.052	0.708	0.048	0.015

	dimension_2				
Categories	coord	sqcorr	contrib		
Α					
agree stro~y	0.727	0.036	0.012		
agree	-0.284	0.020	0.005		
neither ag~e	-1.199	0.190	0.055		
disagree	0.737	0.060	0.018		
disagree s~y	2.470	0.153	0.055		
В					
agree stro~y	1.370	0.072	0.025		
agree	-0.667	0.048	0.015		
neither ag~e	-0.964	0.123	0.036		
disagree	-0.280	0.016	0.004		
disagree s~y	2.108	0.367	0.117		
C					
agree stro~y	0.909	0.075	0.024		
agree	-0.592	0.086	0.021		
neither ag~e	-1.044	0.137	0.040		
disagree	0.635	0.037	0.012		
disagree s~y	3.017	0.249	0.089		
D					
agree stro~y	1.822	0.106	0.038		
agree	-0.007	0.000	0.000		
neither ag~e	-1.159	0.175	0.051		
disagree	-0.211	0.007	0.002		
disagree s~y	1.152	0.120	0.038		

. mcaplot, overlay origin



Even though the first two dimensions explain only 22.2% of the total inertia, and difficulties exist in justifying the full chi-squared geometry for the CA of the indicator matrix, the same clear pattern we saw in the previous plot is seen here. Variables A, B, and C are related, but variable D does not belong with the rest.

#### CA of the Burt matrix

#### Example 4

Now we will look at results with method(burt) and the noadjust option. This performs a CA on the Burt matrix without adjusting the principal inertias. This model does slightly better than the indicator matrix approach, explaining 35.0% of the principal inertia in the first two dimensions. We display column points only for variable A to reduce the output.

. mca A-D, method(burt) noadjust points(A)

Multiple/Joint correspondence analysis

Method: Burt/unadiusted inertias

Number of obs = 871 Total inertia = 1.1276841 Number of axes = 2

nethod. Durty	Numb		
	principal		cumul
Dimension	inertia	percent	percent
dim 1	.2091957	18.55	18.55
dim 2	.1857315	16.47	35.02
dim 3	.1036362	9.19	44.21
dim 4	.0939258	8.33	52.54
dim 5	.0759966	6.74	59.28
dim 6	.0634677	5.63	64.91
dim 7	.0588349	5.22	70.12
dim 8	.0552018	4.90	75.02
dim 9	.0508358	4.51	79.53
dim 10	.0486772	4.32	83.84
dim 11	.0440318	3.90	87.75
dim 12	.0388675	3.45	91.20
dim 13	.0316425	2.81	94.00
dim 14	.0285988	2.54	96.54
dim 15	.0233537	2.07	98.61
dim 16	.0156866	1.39	100.00
Total	1.127684	100.00	

Statistics for column categories in standard normalization

		overall		d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.034	0.445	0.055	1.837	0.391	0.115
agree	0.092	0.169	0.038	0.546	0.136	0.028
neither ag~e	0.059	0.344	0.047	-0.447	0.047	0.012
disagree	0.051	0.350	0.050	-1.166	0.258	0.069
disagree s~y	0.014	0.401	0.060	-1.995	0.170	0.055
				l		

	dimension_2					
Categories	coord	sqcorr	contrib			
A						
agree stro~y	0.727	0.054	0.018			
agree	-0.284	0.033	0.007			
neither ag~e	-1.199	0.298	0.084			
disagree	0.737	0.092	0.028			
disagree s~y	2.470	0.231	0.084			

We do not provide a plot for this mca example; it would be the same as the previous one. MCA via the indicator matrix or the Burt matrix produces the same standard coordinates, although they produce different principal inertias. If normalize(principal) is used, different coordinates will be produced. Principal normalization relies on the principal inertias for normalization.

For more information on normalization, see either *Methods and formulas* in mca or the discussion of normalization in [MV] ca.

## Joint correspondence analysis

## ▶ Example 5

JCA attempts to remedy inflation of the total inertia by the block diagonal submatrices of the Burt matrix and is implemented as method(joint). Results using JCA explain 90% of the principal inertia in the first two dimensions. With JCA, we must specify the dimensions we want in advance. The output contains principal inertias only for the first two dimensions (the default). For other methods, principal inertias for all dimensions are displayed. More dimensions can be requested with the dim() option. JCA is an iterative method, with repeated CAs and adjustments taking place until convergence is achieved.

We ask for coordinates in the principal normalization, norm(principal), and ask for coordinates of only variable A to be displayed.

. mca A-D, method(joint) norm(principal) points(A)

Multiple/Joint correspondence analysis

Number of obs = 871

Total inertia = .18242477

Method: Joint (JCA)

Number of axes = 2

principal cumul Dimension inertia percent percent dim 1 .099091 54.32 54.32 dim 2 .0650329 35.65 89.97 Total .1824248 100.00

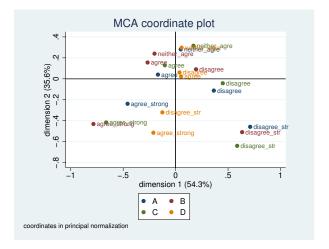
Statistics for column categories in principal normalization

		overall		d:	imension_	1
Categories	mass	quality	%inert	coord	sqcorr	contrib
A						
agree stro~y	0.034	0.964	0.052	-0.458	0.759	0.072
agree	0.092	0.774	0.020	-0.169	0.733	0.027
neither ag~e	0.059	0.884	0.030	0.048	0.025	0.001
disagree	0.051	0.887	0.046	0.364	0.810	0.068
disagree s~y	0.014	0.899	0.060	0.711	0.636	0.070
	I			I		

	dimension_2				
Categories	coord	sqcorr	contrib		
A					
agree stro~y	-0.238	0.205	0.030		
agree	0.040	0.042	0.002		
neither ag~e	0.281	0.859	0.071		
disagree	-0.112	0.077	0.010		
disagree s~y	-0.458	0.264	0.044		

4

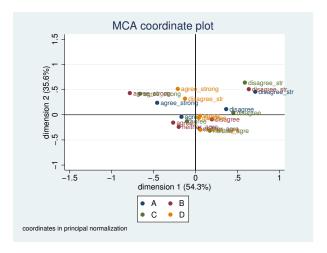
. mcaplot, overlay origin



The plot shows the same relationships among the variables that we saw in the one after the indicator matrix approach to MCA. The main difference between the plots is the change in scale, partially because of the normalization and largely because of the change of method.

These same data are analyzed and plotted in Greenacre (2006, 66). To obtain an equivalent plot, we perform a reflection on the data with ynegate, add in the origin axes with origin, and use the same scale with options xlabel() and ylabel(),

. mcaplot, overlay ynegate origin ylabel(-1(.5)1.5) xlabel(-1.5(.5)1)



Note the similarities between this plot and the one obtained through the default approach to MCA via the Burt matrix and adjustments.

#### Stored results

mca stores the following in e():

```
Scalars
                     number of observations
  e(N)
                     number of dimensions
  e(f)
  e(inertia)
                     total inertia
                     1 if all eigenvalues are distinct, 0 otherwise
  e(ev_unique)
                     1 if eigenvalues are adjusted, 0 otherwise (method(burt) only)
  e(adjust)
  e(converged)
                     1 if successful convergence, 0 otherwise (method(joint) only)
  e(iter)
                     number of iterations (method(joint) only)
  e(inertia_od)
                     proportion of off-diagonal inertia explained by extracted dimensions (method(joint) only)
Macros
  e(cmd)
                     mca
  e(cmdline)
                     command as typed
  e(names)
                     names of MCA variables (crossed or actual)
  e(supp)
                     names of supplementary variables
                     per crossed variable: crossing variables separated by "\"
  e(defs)
                     missing if missing values are treated as ordinary values
  e(missing)
                     1 if there are crossed variables, 0 otherwise
  e(crossed)
  e(wtype)
                     weight type
                     weight expression
  e(wexp)
  e(title)
                     title in output
  e(method)
                     burt, indicator, or joint
  e(norm)
                     standard or principal
  e(properties)
                     nob noV eigen
  e(estat_cmd)
                     program used to implement estat
                     program used to implement predict
  e(predict)
  e(marginsnotok) predictions disallowed by margins
Matrices
  e(Coding#)
                     row vector with coding of variable #
  e(A)
                     standard coordinates for column categories
  e(F)
                     principal coordinates for column categories
  e(cMass)
                     column mass
  e(cDist)
                     distance column to centroid
  e(cInertia)
                     column inertia
  e(cGS)
                     general statistics of column categories
                     [.,1] column mass
                     [.,2] overall quality
                     [..3] inertia/sum(inertia)
                     [..3*f+1] dim f: coordinate in e(norm) normalization
                     [.,3*f+2] dim f: contribution of the profiles to principal axes
                     [.,3*f+3] dim f: contribution of principal axes to profiles
                          (= squared correlation of profile and axes)
  e(rSCW)
                     weight matrix for row standard coordinates
  e(Ev)
                     principal inertias/eigenvalues
                     explained inertia (percent)
  e(inertia_e)
  e(Bmod)
                     modified Burt matrix of active variables (method(joint) only)
  e(inertia_sub)
                     variable-by-variable inertias (method(joint) only)
Functions
  e(sample)
                     marks estimation sample
```

#### Methods and formulas

Methods and formulas are presented under the following headings:

Notation
Using ca to compute MCA
CA of an indicator or Burt matrix
JCA
Supplementary variables
predict

#### **Notation**

We use notation that is fairly standard in the literature on correspondence analysis (for example, Greenacre [2006]). Let  $x_1, \ldots, x_q$  be categorical variables on N observations that are active in the analysis. To simplify notation, but without loss of generality, we assume that  $x_j$  is coded with consecutive integers  $1, \ldots, n_j$ . Let  $\mathbf{Z}^{(j)}$  be the  $N \times n_j$  binary indicator matrix associated with  $x_j$ ,  $\mathbf{Z}^{(j)}_{ih} = 1$  if and only if  $x_{ij} = h$ . Let

$$\mathbf{Z} = \left(\mathbf{Z}^{(1)}, \mathbf{Z}^{(2)}, \dots, \mathbf{Z}^{(q)}\right)$$

be the  $N \times J$  indicator matrix of the set of active x-variables, where  $J = n_1 + \cdots + n_q$ .

We will be consistent in letting i index observations  $1, \ldots, N$ , j index variables  $1, \ldots, q$ , and h index categories  $1, \ldots, n_j$ , or  $1, \ldots, J$ .

The  $J \times J$  Burt matrix is defined as  $\mathbf{B} = \mathbf{Z}'\mathbf{Z}$ , or  $\mathbf{B} = \mathbf{Z}'\mathbf{D}(w)\mathbf{Z}$ , where w is the weight for the analysis and  $\mathbf{D}(w)$  is a  $J \times J$  square matrix with the weights on the diagonal and 0 off diagonal. The diagonal block of  $\mathbf{B}$  associated with variable  $x_j$  is a diagonal matrix with the frequencies of  $x_j$  on the diagonal. The off-diagonal block of  $\mathbf{B}$  associated with variables  $x_j$  and  $x_k$  is the two-way cross-tabulation of  $x_j$  and  $x_k$ .

In an analogous way, we define  $\mathbf{B}^*$ , the Burt matrix with more rows containing cross-tabulation from the supplementary variables.  $\mathbf{B}^* = \mathbf{Z}^{*'}\mathbf{Z}$ , where  $\mathbf{Z}^*$  is the indicator matrix with more columns for the supplementary variables.

 $\mathbf{D}(v)$ , in general, represents a diagonal matrix with the elements of vector v on the diagonal and 0 off diagonal; 1 is a column vector of ones where length is defined by the context.

## Using ca to compute MCA

The indicator approach to MCA involves an equivalent technique to performing a standard CA on the indicator matrix  $\mathbf{Z}$ ; see Greenacre (2006). We refer to *Methods and formulas* in [MV]  $\mathbf{ca}$  for details. The indicator approach could be handled by forming  $\mathbf{Z}$  and invoking camat on  $\mathbf{Z}$ . If you had k categorical variables named v1, ..., vk, you could perform CA on the indicator matrix by taking the steps in the following code fragment:

```
tab v1, gen(V1_)
...
tab vk, gen(Vk_)
mkmat V1_* ... Vk_*, matrix(VALL)
camat VALL
```

#### CA of an indicator or Burt matrix

**Z** may be a rather large matrix: the number of rows is equal to the number of observations, and memory limitations would pose a limit for applications. Moreover, the interest in MCA is mostly on the column space, and so much computation would be wasted. Therefore, the implementation in mca exploits the close analogy between the indicator and Burt matrix approach for efficiency (see Greenacre [1984, chap. 5; 2006, app. A.3]). The consequence is that the CA results for the rows of **Z** are not computed. You may use the above scheme if you need row information.

Much literature (for example, Everitt and Dunn [2001]; Rencher and Christensen [2012]) identifies MCA with the application of CA on the Burt matrix  $\mathbf{B} = \mathbf{Z}'\mathbf{Z}$ .

This discussion is related to that of *Methods and formulas* in [MV] ca. We define

$$\mathbf{B}_{++} = \sum_{k=1}^{J} \sum_{h=1}^{J} \mathbf{B}_{kh}$$

$$\mathbf{P} = \mathbf{B}/\mathbf{B}_{++}$$

$$\mathbf{c} = \sum_{k=1}^{J} \mathbf{P}_{k*} = \mathbf{P}_{+*} = \mathbf{P}'\mathbf{1} \quad \text{here * represents all possible values}$$

$$\mathbf{S} = \mathbf{D}(\mathbf{c})^{-1/2} (\mathbf{P} - \mathbf{c}\mathbf{c}') \mathbf{D}(\mathbf{c})^{-1/2}$$

 ${\bf c}$  is called the column mass.  ${\bf D}({\bf c})$  is the diagonal matrix with diagonal  ${\bf c}$ ;  ${\bf D}({\bf c})^{-1/2}$  is therefore the diagonal matrix with elements  $1/\sqrt{c_t}$ , where  $c_t$  is an element of  ${\bf c}$ .  ${\bf B}$  and  ${\bf S}$  are symmetric. Thus the singular-value decomposition commonly associated with CA is equivalent to the spectral or eigen decomposition of  ${\bf S}$ .

$$S = V\Phi V', \qquad \phi_1 \ge \phi_2 \ge \dots$$

For identification purposes and to facilitate resampling methods, the eigenvectors of V are directed so that for h,  $V_{kh} > 0$  for the first k for which  $V_{kh} \neq 0$ . The standard column coordinates A are the same for the indicator and the Burt approach and are defined as

$$\mathbf{A} = \mathbf{D}(\mathbf{c})^{-1}\mathbf{V}$$

 $\mathbf{D}(\mathbf{c})^{-1}$  is the diagonal matrix with elements  $1/c_t$ , where  $c_t$  is an element of  $\mathbf{c}$ .

In the indicator approach to MCA, the tth principal inertia is defined as  $\lambda_t = \phi_t$ , the total inertia as  $\sum_t \lambda_t$ . The inertia of column j or variable j,  $\mathbf{In}^{(j)}$ , is computed elementwise as

$$In_h^{(j)} = \sum_{i=1}^{N} w_i \frac{(Z_{ih}^{(j)} - qc_h^{(j)})^2}{q^2 c_h^{(j)} w_+}$$

where  $Z_{ih}^{(j)}$  is the i,hth element of the indicator matrix for variable  $j,w_i$  is the weight for observation i,q is the number of active variables,  $c_h^{(j)}$  is the column mass of variable j for category h, and  $w_+$  is the sum of the weights over the observations.

In the Burt approach to MCA, the unadjusted principal inertia is defined as  $\lambda_t^{\mathrm{unadj}} = \phi_t^2$ , the total unadjusted inertia as  $\sum_t \lambda_t^{\mathrm{unadj}}$ , and the unadjusted column inertias as  $\mathbf{1'S} \odot \mathbf{S}$ , with  $\odot$  the Hadamard or elementwise matrix product. The adjusted principal inertia,  $\lambda_t^{\mathrm{adj}}$ , is defined as

$$\lambda_t^{\mathrm{adj}} = \left(\frac{q}{q-1}\right)^2 \! \left(\phi_t^2 - \frac{1}{q}\right)^2 \qquad \text{provided } q\phi_t > 1$$

The total inertia is defined as

total inertia 
$$=\left(\frac{q}{q-1}\right)\sum\phi_t^2-\frac{(J-q)}{q^2}$$

The standard coordinates are independent of the principal inertia; with or without adjustment, these are defined as before

$$\mathbf{A} = \mathbf{D}(\mathbf{c})^{-1} \mathbf{V}$$

The principal coordinates F are defined as

$$\mathbf{F} = \mathbf{A}\mathbf{D}(\mathbf{\Lambda})^{1/2}$$

where  $\Lambda$  is a vector of adjusted or unadjusted principal inertias and  $\mathbf{D}(\Lambda)^{1/2}$  is the diagonal matrix with elements  $\lambda_t^{1/2}$  on the diagonals.

#### **JCA**

The implementation of JCA uses the alternating least-squares method proposed by Greenacre (1988, 2006). This algorithm forms a modification of the Burt matrix, changing the diagonal blocks associated with the variables, keeping the off-diagonal blocks unchanged. In the first iteration,  $\mathbf{B}_0 = \mathbf{B}$ . In iteration m, the blocks are replaced by the f-dimensional MCA approximation of the adjusted Burt matrix  $\mathbf{B}_{m-1}$ . Iteration continues until the change in the elements of  $\mathbf{B}_m$  and  $\mathbf{B}_{m-1}$  falls below a convergence tolerance. The JCA coordinates and inertias are computed from the converged solution,  $\mathbf{B}_{\infty}$ , analogous to the (adjusted) Burt method. The total inertia of the modified Burt matrix is defined as the sum of the inertias of the off-diagonal blocks.

To compute the f-dimensional MCA approximation of the adjusted Burt matrix  $\mathbf{B}_{m-1}$ , we perform MCA on  $\mathbf{B}_{m-1}$  and then reconstruct the approximation of the data from the solution

$$\widehat{\mathbf{B}}_{hk} = \mathbf{B}_{++} c_h c_k \left( 1 + \sum_{t=1}^f \phi_t^2 A_{ht} A_{kt} \right)$$

where  $A_{ht}$  is an element of the standard coordinate matrix  $\mathbf{A}$ ,  $c_h$  and  $c_k$  are the column masses, and  $\phi_t$  are the eigenvalues as in the computation of the CA of the Burt matrix. We then update the main diagonal submatrices of  $\mathbf{B}_{m-1}$  with the corresponding entries of  $\hat{\mathbf{B}}$  to obtain  $\mathbf{B}_m$ .

## Supplementary variables

The coordinates of supplementary variables are computed as weighted averages of the column coordinates by using the so-called CA transition formulas. As outlined by Greenacre (2006), standard coordinates may be used for averaging, with the profiles of the indicator representation of supplementary columns as weights. Supplementary principal column coordinates are computed as weighted averages of the standard active column coordinates, and then supplementary standard coordinates are computed by division by the principal inertias.

To compute, we add the supplementary variables to the Burt matrix as more rows; if  $\bf B$  is the Burt matrix of the active variables then  $\bf B^*$  is the Burt matrix with the additional cross-tabulation from the supplementary variables. Define  $\bf P$  as above and  $\bf P^*$  analogously with the supplementary variables added. MCA is performed on  $\bf B$  as before, and information from this solution is then applied to  $\bf B^*$ . Let  $p^*$  represent the elements of  $\bf P^*$ . Let k index categories of supplementary variables, k index categories of active variables, and k index dimensions of the solution. Let  $\bf A$  be the standard coordinates of the active variables, as computed previously. Then the principal coordinate for category k and dimension k is computed as:

$$g_{kt} = \sum_{h=1}^{J} \frac{p_{hk}^*}{p_{+k}^*} A_{ht}$$

Coordinates in standard coordinates are obtained by division by the square root of the corresponding principal inertia as described above.

#### predict

predict after mca produces variables with the MCA coordinates as displayed by mca for both active and supplementary variables. Formulas are shown above. predict can also compute row coordinates also known as row scores. Row coordinates computed are always based on the indicator method. The standard row coordinate for the tth dimension for the ith observation with indicator matrix elements  $Z_{ih}$  is computed as

$$R_{it} = \sum_{h=1}^{J} \frac{Z_{ih} A_{ht}}{q \sqrt{\phi_t}}$$

where  $\bf A$  is the matrix of standard coordinates, q is the number of active variables in the analysis, and  $\phi_t$  is an eigenvalue of the CA on the Burt matrix. To get the row coordinate in principal normalization, one multiplies by the square root of the corresponding principal inertia.

#### References

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Milan, L., and J. C. Whittaker. 1995. Application of the parametric bootstrap to models that incorporate a singular value decomposition. *Applied Statistics* 44: 31–49.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.

## Also see

```
    [MV] mca postestimation — Postestimation tools for mca
    [MV] mca postestimation plots — Postestimation plots for mca
    [MV] ca — Simple correspondence analysis
    [MV] canon — Canonical correlations
    [MV] factor — Factor analysis
```

[MV] **pca** — Principal component analysis

[U] 20 Estimation and postestimation commands

## **Title**

mca postestimation — Postestimation tools for mca

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

## **Postestimation commands**

The following postestimation commands are of special interest after mca:

mcaplot plot of category coordinates mcaprojection MCA dimension projection plot estat coordinates display of category coordinates estat subinertia matrix of inertias of the active variables (after JCA only) estat summarize estimation sample summary	Command	Description
screep for piot principal ineriias (eigenvallies)	mcaprojection estat coordinates estat subinertia	MCA dimension projection plot display of category coordinates matrix of inertias of the active variables (after JCA only)

The following standard postestimation commands are also available:

Command	Description
*estimates	cataloging estimation results
predict	row and category coordinates

<sup>\*</sup>All estimates subcommands except table and stats are available; [R] estimates.

## predict

#### **Description for predict**

predict creates a new variable containing predictions such as row scores and scores (coordinates) for the MCA variable.

#### Menu for predict

Statistics > Postestimation

#### Syntax for predict

```
predict [type] newvar [if] [in] [, statistic normalize(norm) dimensions(#)]
predict [type] {stub*|newvarlist} [if] [in] [, statistic normalize(norm)
  dimensions(numlist)
```

statistic	Description
Main <u>row</u> scores <u>sc</u> ore(varname)	row scores (coordinates); the default scores (coordinates) for MCA variable <i>varname</i>
norm	Description
<u>st</u> andard <u>p</u> rincipal	use standard normalization use principal normalization

## Options for predict

rowscores specifies that row scores (row coordinates) be computed. The row scores returned are based on the indicator matrix approach to multiple correspondence analysis, even if another method was specified in the original mca estimation. The sample for which row scores are computed may exceed the estimation sample; for example, it may include supplementary rows (variables). score() and rowscores are mutually exclusive. rowscores is the default.

score(varname) specifies the name of a variable from the preceding MCA for which scores should be computed. The variable may be a regular categorical variable, a crossed variable, or a supplementary variable. score() and rowscores are mutually exclusive.

```
Options
```

normalize(norm) specifies the normalization of the scores (coordinates). normalize(standard) returns coordinates in standard normalization. normalize(principal) returns principal scores. The default is the normalization method specified with mca during estimation, or normalize(standard) if no method was specified.

dimensions (#) or dimensions (numlist) specifies the dimensions for which scores (coordinates) are computed. The number of dimensions specified should equal the number of variables in newvarlist. If dimensions () is not specified, scores for dimensions 1, ..., k are returned, where k is the number of variables in newvarlist. The number of variables in newvarlist should not exceed the number of dimensions extracted during estimation.

#### estat

#### **Description for estat**

estat coordinates displays the category coordinates, optionally with column statistics. estat subinertia displays the matrix of inertias of the active variables (after JCA only). estat summarize displays summary information of MCA variables over the estimation sample.

#### Menu for estat

Statistics > Postestimation

#### Syntax for estat

```
Display of category coordinates
```

```
estat coordinates [varlist] [, coordinates_options]
```

Matrix of inertias of the active variables (after JCA only)

```
estat subinertia
```

Estimation sample summary

```
estat summarize [, summarize_options]
```

Note: Variables in *varlist* must be from the preceding mca and may refer to either a regular categorical variable or a crossed variable. The variables in *varlist* may also be chosen from the supplementary variables.

coordinates_options	Description
<u>norm</u> alize( <u>s</u> tandard)	standard coordinates
$\underline{\mathtt{norm}}\mathtt{alize}(\underline{\mathtt{p}}\mathtt{rincipal})$	principal coordinates
<u>st</u> ats	include mass, distance, and inertia
<pre>format(%fmt)</pre>	display format; default is format(%9.4f)
summarize_options	Description
r	Description
Main	2000 puon
	summarize crossed and uncrossed variables as used
Main	·
Main <u>c</u> rossed	summarize crossed and uncrossed variables as used

#### **Options for estat**

Options for estat are presented under the following headings:

Options for estat coordinates Options for estat summarize

#### Options for estat coordinates

normalize(norm) specifies the normalization of the scores (coordinates). normalize(standard) returns coordinates in standard normalization. normalize(principal) returns principal scores. The default is the normalization method specified with mca during estimation, or normalize(standard) if no method was specified.

stats includes the column mass, the distance of the columns to the centroid, and the column inertias

format (% fmt) specifies the display format for the matrix, for example, format (%8.3f). The default is format (%9.4f).

#### Options for estat summarize

Main

crossed specifies summarizing the crossed variables if crossed variables are used in the MCA, rather than the crossing variables from which they are formed. The default is to summarize the crossing variables and single categorical variables used in the MCA.

labels displays variable labels.

noheader suppresses the header.

noweights ignores the weights, if any. The default when weights are present is to perform a weighted summarize on all variables except the weight variable itself. An unweighted summarize is performed on the weight variable.

## Remarks and examples

Remarks are presented under the following headings:

Postestimation statistics Predicting new variables

#### Postestimation statistics

We continue to examine the ISSP (1993) dataset on the environment. We perform joint correspondence analysis.

## Example 1: Category coordinates and subinertias

- . use http://www.stata-press.com/data/r14/issp93 (Selection from ISSP (1993))
- . mca A-D, method(joint)

Multiple/Joint correspondence analysis

Method: Joint (JCA)

Number of obs = 871 Total inertia = .18242477 Number of axes = 2

Dimension	principal inertia	percent	cumul percent
dim 1 dim 2	.099091 .0650329	54.32 35.65	54.32 89.97
Total	.1824248	100.00	

Statistics for column categories in standard normalization

Categories	mass	overall quality	%inert	d: coord	imension_ sqcorr	1 contrib
A						
agree stro~y	0.034	0.964	0.052	-1.456	0.759	0.072
agree	0.092	0.774	0.020	-0.536	0.733	0.027
neither ag~e	0.059	0.884	0.030	0.154	0.025	0.001
disagree	0.051	0.887	0.046	1.157	0.810	0.068
disagree s~y	0.014	0.899	0.060	2.258	0.636	0.070
В						
agree stro~y	0.020	0.957	0.093	-2.490	0.735	0.126
agree	0.050	0.851	0.031	-0.850	0.636	0.036
neither ag~e	0.059	0.953	0.033	-0.639	0.393	0.024
disagree	0.081	0.705	0.029	0.618	0.579	0.031
disagree s~y	0.040	0.977	0.149	2.014	0.594	0.163
C						
agree stro~y	0.044	0.983	0.149	-2.104	0.704	0.193
agree	0.091	0.665	0.020	-0.327	0.257	0.010
neither ag~e	0.057	0.839	0.047	0.539	0.188	0.016
disagree	0.044	0.907	0.054	1.429	0.899	0.090
disagree s~y	0.015	0.944	0.065	1.864	0.431	0.052
D						
agree stro~y	0.017	0.850	0.034	-0.674	0.124	0.008
agree	0.067	0.145	0.008	0.165	0.120	0.002
neither ag~e	0.058	0.769	0.038	0.181	0.027	0.002
disagree	0.065	0.178	0.010	0.116	0.047	0.001
disagree s~y	0.043	0.929	0.030	-0.402	0.125	0.007
	L			L		

	dimension_2		
Categories	coord	sqcorr	contrib
Α			
agree stro~y	-0.934	0.205	0.030
agree	0.158	0.042	0.002
neither ag~e	1.103	0.859	0.071
disagree	-0.440	0.077	0.010
disagree s~y	-1.796	0.264	0.044
В			
agree stro~y	-1.690	0.222	0.058
agree	0.611	0.216	0.019
neither ag~e	0.942	0.560	0.052
disagree	0.356	0.126	0.010
disagree s~y	-1.995	0.383	0.160
C			
agree stro~y	-1.634	0.279	0.116
agree	0.508	0.407	0.023
neither ag~e	1.237	0.651	0.087
disagree	-0.166	0.008	0.001
disagree s~y	-2.509	0.513	0.094
D			
agree stro~y	-2.018	0.727	0.070
agree	0.092	0.024	0.001
neither ag~e	1.166	0.741	0.079
disagree	0.239	0.131	0.004
disagree s~y	-1.256	0.804	0.068

If we wish to see the coordinates in the principal normalization, we do not need to rerun our analysis. We can use estat coordinates to display them.

. estat coordinates, norm(principal) Column principal coordinates

Categories	dim1	dim2
A		
agree_stro~y	4582629	2381115
agree	1686314	.0402091
neither_ag~e	.0484366	.2811716
disagree	.3642677	1123168
disagree_s~y	.7106647	4578886
В		
agree_stro~y	783911	4310436
agree	2674646	.1558017
neither_ag~e	2010783	.2402487
disagree	.1944504	.0906804
disagree_s~y	.6341215	5088398
С		
agree_stro~y	6623101	4166016
agree	1029922	.1295649
neither_ag~e	.169804	.3155628
disagree	.4496893	0423339
disagree_s~y	.5867913	6397215
D		
agree_stro~y	2123187	5145647
agree	.05208	.0233723
neither_ag~e	.0569168	.297262
disagree	.0365233	.0609881
disagree_s~y	1264563	3203889

We may also be interested in the contributions of each submatrix of the Burt matrix to the total inertia. This can be obtained by estat subinertia. Compare with Greenacre (2006, table A.12).

. estat subinertia

Subinertias: decomposition of total inertia

Variable	A	В	С	D
A B C D	.0074502 .0148596 .012149 .0032898	.022442 .0185838 .0053016	.0210336 .0096583	.0038148

## **Predicting new variables**

Coordinates (scores) can be predicted after mca. You can predict either the column coordinates or the row coordinates.

# Example 2: Predictions

We will calculate row scores by hand and via predict, rowscore. Row scores are calculated off the indicator method approach. This calculation would not work with JCA, because the standard coordinates and the principal inertias are different for JCA. The principal inertias are also a problem with the Burt method, with and without adjustment. We use the points(A) option to restrict the output from mca. Four variables were used in the original mca. predict without the dimensions() option predicts the first dimension.

. mca A-D, method(indicator) points(A)

Multiple/Joint correspondence analysis

Method: Indicator matrix

Number of obs = 871Total inertia = 4Number of axes = 2

Dimension	principal inertia	norcont	cumul percent
		percent	per cent
dim 1	.4573792	11.43	11.43
dim 2	.4309658	10.77	22.21
dim 3	.3219257	8.05	30.26
dim 4	.3064732	7.66	37.92
dim 5	.2756747	6.89	44.81
dim 6	.251928	6.30	51.11
dim 7	.2425591	6.06	57.17
dim 8	.2349506	5.87	63.05
dim 9	.225468	5.64	68.68
dim 10	.2206291	5.52	74.20
dim 11	.2098376	5.25	79.44
dim 12	.1971485	4.93	84.37
dim 13	.1778833	4.45	88.82
dim 14	.1691119	4.23	93.05
dim 15	.1528191	3.82	96.87
dim 16	.1252462	3.13	100.00
Total	4	100.00	

Statistics for column categories in standard normalization

Categories	mass	overall quality	%inert	d: coord	imension_ sqcorr	1 contrib
A						
agree stro~y	0.034	0.280	0.054	1.837	0.244	0.078
agree	0.092	0.100	0.039	0.546	0.080	0.019
neither ag~e	0.059	0.218	0.048	-0.447	0.028	0.008
disagree	0.051	0.220	0.050	-1.166	0.160	0.047
disagree s~y	0.014	0.260	0.059	-1.995	0.106	0.037

dimension_2		
coord	sqcorr	contrib
0.727	0.036	0.012
-0.284	0.020	0.005
-1.199	0.190	0.055
0.737	0.060	0.018
2.470	0.153	0.055
	0.727 -0.284 -1.199 0.737	0.727 0.036 -0.284 0.020 -1.199 0.190 0.737 0.060

- . predict double a1, score(A)
- . predict double b1, score(B)
- . predict double c1, score(C)

```
. predict double d1, score(D)
. predict double r1, rowscore
. mat Ev = e(Ev)
. scalar phi1 = Ev[1,1]
. generate double rc = (a1+b1+c1+d1)/(4*sqrt(phi1))
. assert reldif(rc, r1) < 1e-14</pre>
```

In the indicator method approach, we can also find Cronbach's alpha either via the alpha command (see [MV] alpha) or by hand.

```
. alpha a1 b1 c1 d1
Test scale = mean(unstandardized items)
Average interitem covariance: .2768234
Number of items in the scale: 4
Scale reliability coefficient: 0.6045
. scalar alpha = (4/(4-1))*(1-1/(4*phi1))
. display alpha
.60454338
```

4

## Stored results

```
estat summarize stores the following in r():
Matrices
    r(stats)
                       k \times 4 matrix of means, standard deviations, minimums, and maximums
estat coordinates stores the following in r():
Macros
    r(norm)
                       normalization method of the coordinates
Matrices
    r(Coord)
                       column coordinates
    r(Stats)
                       column statistics: mass, distance, and inertia (option stats only)
estat subinertia stores the following in r():
Matrices
                       variable-by-variable inertias
    r(inertia_sub)
```

## Methods and formulas

See Methods and formulas in [MV] mca.

## References

Greenacre, M. J. 2006. From simple to multiple correspondence analysis. In *Multiple Correspondence Analysis and Related Methods*, ed. M. J. Greenacre and J. Blasius. Boca Raton, FL: Chapman & Hall.

ISSP. 1993. International Social Survey Programme: Environment. http://www.issp.org.

## Also see

- [MV] mca Multiple and joint correspondence analysis
- [MV] mca postestimation plots Postestimation plots for mca
- [MV] screeplot Scree plot
- [MV] ca Simple correspondence analysis
- [MV] ca postestimation Postestimation tools for ca and camat
- [U] 20 Estimation and postestimation commands

#### **Title**

mca postestimation plots —	- Postestimation	plots for mca
----------------------------	------------------	---------------

Postestimation commands	mcaplot	mcaprojection	Remarks and examples
Methods and formulas	References	Also see	

#### Postestimation commands

The following postestimation commands are of special interest after mca:

Command	Description
mcaplot	plot of category coordinates
mcaprojection	MCA dimension projection plot

## mcaplot

## **Description for mcaplot**

mcaplot produces a scatterplot of category points of the MCA variables in two dimensions.

#### Menu for mcaplot

 ${\it Statistics} > {\it Multivariate analysis} > {\it Correspondence analysis} > {\it Postestimation after MCA or JCA} > {\it Plot of category coordinates}$ 

## Syntax for mcaplot

```
mcaplot [speclist] [, options]
where
speclist = spec [spec ...]
spec = varlist | (varname [, plot_options])
```

and variables in *varlist* or *varname* must be from the preceding mca and may refer to either a regular categorical variable or a crossed variable. The variables may also be supplementary.

options	Description
Options	
combine_options	affect the rendition of the combined graphs
<u>over</u> lay	overlay the plots of the variables; default is to produce separate plots
$\underline{\mathtt{dim}}\mathtt{ensions}(\#_1\ \#_2)$	display dimensions $\#_1$ and $\#_2$ ; default is dimensions (2 1)
$\underline{\mathtt{norm}}$ alize( $\underline{\mathtt{s}}$ tandard)	display standard coordinates
$\underline{\mathtt{norm}}\mathtt{alize}(\underline{\mathtt{p}}\mathtt{rincipal})$	display principal coordinates
<pre>maxlength(#)</pre>	<pre>use # as maximum number of characters for labels; default is maxlength(12)</pre>
<u>xneg</u> ate	negate the coordinates relative to the $x$ axis
ynegate	negate the coordinates relative to the $y$ axis
<u>or</u> igin	mark the origin and draw origin axes
<pre>originlopts(line_options)</pre>	affect the rendition of the origin axes
Y axis, X axis, Titles, Legend, Over	all
twoway_options	any options other than by() documented in [G-3] twoway_options
plot_options	Description
marker_options marker_label_options twoway_options	change look of markers (color, size, etc.) add marker labels; change look or position titles, legends, axes, added lines and text, regions, etc.

## Options for mcaplot

Dioto

plot\_options affect the rendition of markers, including their shape, size, color, and outline
 (see [G-3] marker\_options) and specify if and how the markers are to be labeled (see
 [G-3] marker\_label\_options). These options may be specified for each variable. If the overlay
 option is not specified, then for each variable you may also specify many of the twoway\_options
 excluding by(), name(), and aspectratio(); see [G-3] twoway\_options. See twoway\_options
 below for a warning against using options such as xlabel(), xscale(), ylabel(), and yscale().

Options

combine\_options affect the rendition of the combined plot; see [G-2] **graph combine**. combine\_options may not be specified with overlay.

overlay overlays the biplot graphs for the variables. The default is to produce a combined graph of the biplot graphs.

dimensions (#1 #2) identifies the dimensions to be displayed. For instance, dimensions (3 2) plots the third dimension (vertically) versus the second dimension (horizontally). The dimension number cannot exceed the number of extracted dimensions. The default is dimensions (2 1).

normalize(norm) specifies the normalization of the coordinates. normalize(standard) returns coordinates in standard normalization. normalize(principal) returns principal coordinates. The default is the normalization method specified with mca during estimation, or normalize(standard) if no method was specified.

maxlength(#) specifies the maximum number of characters for row and column labels; the default is maxlength(12).

xnegate specifies that the x-axis coordinates be negated (multiplied by -1).

ynegate specifies that the y-axis coordinates be negated (multiplied by -1).

origin marks the origin and draws the origin axes.

originlopts (line\_options) affect the rendition of the origin axes. See [G-3] line\_options.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options excluding by().

mcaplot automatically adjusts the aspect ratio on the basis of the range of the data and ensures that the axes are balanced. As an alternative, the  $twoway\_option$  aspectratio() can be used to override the default aspect ratio. mcaplot accepts the aspectratio() option as a suggestion only and will override it when necessary to produce plots with balanced axes; that is, distance on the x axis equals distance on the y axis.

twoway\_options such as xlabel(), xscale(), ylabel(), and yscale() should be used with caution. These options axis\_options are accepted but may have unintended side effects on the aspect ratio. See [G-3] twoway\_options.

## Description for mcaprojection

mcaprojection produces a projection plot of the coordinates of the categories of the MCA variables.

## Menu for mcaprojection

 ${\it Statistics} > {\it Multivariate analysis} > {\it Correspondence analysis} > {\it Postestimation after MCA or JCA} > {\it Dimension projection plot}$ 

## Syntax for mcaprojection

```
mcaprojection [speclist] [, options] where speclist = spec [spec ...] spec = varlist | (varname [, plot_options])
```

and variables in *varlist* or *varname* must be from the preceding mca and may refer to either a regular categorical variable or a crossed variable. The variables may also be supplementary.

options	Description
Options	
<pre>dimensions(numlist)</pre>	display numlist dimensions; default is all
<pre>normalize(principal)</pre>	scores (coordinates) should be in principal normalization
$\frac{-}{\texttt{norm}}$ alize( $\frac{-}{\texttt{s}}$ tandard)	scores (coordinates) should be in standard normalization
<u>alt</u> ernate	alternate labels
<pre>maxlength(#)</pre>	<pre>use # as maximum number of characters for labels; default is maxlength(12)</pre>
combine_options	affect the rendition of the combined graphs
Y axis, X axis, Titles, Legend, Ove	erall
twoway_options	any options other than by() documented in [G-3] twoway_options
plot_options	Description
marker_options	change look of markers (color, size, etc.)
marker_label_options	add marker labels; change look or position
twoway_options	titles, legends, axes, added lines and text, regions, etc.

## Options for mcaprojection

plot\_options affect the rendition of markers, including their shape, size, color, and outline (see [G-3] marker\_options) and specify if and how the markers are to be labeled (see [G-3] marker\_label\_options). These options may be specified for each variable. If the over-lay option is not specified then for each variable you may also specify twoway\_options excluding

Options

dimensions (numlist) identifies the dimensions to be displayed. By default, all dimensions are displayed.

normalize(norm) specifies the normalization of the coordinates. normalize(standard) returns coordinates in standard normalization. normalize(principal) returns principal coordinates. The default is the normalization method specified with mca during estimation, or normalize(standard) if no method was specified.

alternate causes adjacent labels to alternate sides.

by() and name(); see [G-3] twoway\_options.

maxlength(#) specifies the maximum number of characters for row and column labels; the default is maxlength(12).

*combine\_options* affect the rendition of the combined plot; see [G-2] **graph combine**. These options may not be used if only one variable is specified.

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by().

# Remarks and examples

Several examples of mcaplot were displayed in [MV] mca, so we will not give more examples here. The discussion in [MV] ca postestimation is also relevant.

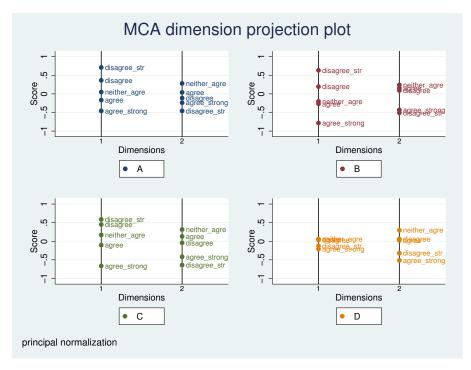
We will focus on mcaprojection, which is the mca analogue of caprojection, just as mcaplot is the analogue of cabiplot.

# Example 1: MCA dimension projection plot

mcaprojection produces a projection plot of the column coordinates after mca. We continue with example 1 of [MV] mca postestimation. Say that we want to examine the projections in the principal normalization.

- . use http://www.stata-press.com/data/r14/issp93
  (Selection from ISSP (1993))
- . mca A-D, method(joint)
   (output omitted)

. mcaprojection, norm(principal)



We would see the same alignment of points in the standard normalization, but the scale would be changed. We have noted previously that item D does not behave like the other variables in the MCA. Each of the first three variables, A, B, and C, has its responses arrayed in order from strong disagreement to strong agreement on the first dimension. Here again, variable D is the only one of the four that shows a different ordering in its projection. We do not see a nice projection from strong disagreement to strong agreement on the second dimension, but an inspection indicates that the first three variables are all in the same order, with the last, D, opposed to the remainder.

## Methods and formulas

See Methods and formulas in [MV] mca.

# References

See References in [MV] mca.

## Also see

[MV] mca — Multiple and joint correspondence analysis

[MV] mca postestimation — Postestimation tools for mca

[MV] ca — Simple correspondence analysis,

[MV] ca postestimation — Postestimation tools for ca and camat

4

## **Title**

mds — Multidimensional scaling for two-way data

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

mds performs multidimensional scaling (MDS) for dissimilarities between observations with respect to the specified variables. A wide selection of similarity and dissimilarity measures is available. mds performs classical metric MDS as well as modern metric and nonmetric MDS.

If your proximities are stored as variables in long format, see [MV] mdslong. For MDS with two-way proximity data in a matrix, see [MV] mdsmat.

## **Quick start**

Classical metric multidimensional scaling of variables v1, v2, v3, and v4 with observations identified by idvar

```
mds v1 v2 v3 v4, id(idvar)
```

As above, but use absolute-value distance and suppress the MDS configuration plot

mds v1 v2 v3 v4, id(idvar) measure(absolute) noplot

As above, but increase dimensions from 2 to 3 for approximating configuration

mds v1 v2 v3 v4, id(idvar) measure(absolute) noplot dimension(3)

Modern multidimensional scaling

```
mds v1 v2 v3 v4, id(idvar) method(modern)
```

As above, but Procrustes rotate toward classical solution instead of the default principal orientation mds v1 v2 v3 v4, id(idvar) method(modern) normalize(classical)

Modern multidimensional scaling with Sammon mapping for the loss criterion

```
mds v1 v2 v3 v4, id(idvar) loss(sammon)
```

Modern nonmetric multidimensional scaling

```
mds v1 v2 v3 v4, id(idvar) method(nonmetric)
```

## Menu

Statistics > Multivariate analysis > Multidimensional scaling (MDS) > MDS of data

mds varlist [if] [in], id(varname) [options]

# **Syntax**

```
options
                               Description
Model
*id(varname)
                               identify observations
 method (method)
                               method for performing MDS
 loss(loss)
                               loss function
 transform(tfunction)
                               permitted transformations of dissimilarities
 normalize(norm)
                               normalization method; default is normalize(principal)
 dimension(#)
                               configuration dimensions; default is dimension(2)
 addconstant
                               make distance matrix positive semidefinite
Model 2
 unit (varlist<sub>2</sub>)
                               scale variables to min = 0 and max = 1
 std[(varlist<sub>3</sub>)]
                               scale variables to mean = 0 and sd = 1
                               similarity or dissimilarity measure; default is L2 (Euclidean)
 measure(measure)
                               convert similarity to dissimilarity: \operatorname{dissim}_{ij} = \sqrt{\sin_{ij} + \sin_{jj} - 2\sin_{ij}};
 s2d(standard)
                                 the default
 s2d(oneminus)
                               convert similarity to dissimilarity: \operatorname{dissim}_{ij} = 1 - \operatorname{sim}_{ij}
Reporting
```

# <u>nopl</u>ot Minimization

config

neigen(#)

<pre>init ialize(initopt)</pre>	start with configuration given in initopt
<pre>tolerance(#)</pre>	tolerance for configuration matrix; default is tolerance(1e-4)
<pre>ltolerance(#)</pre>	tolerance for loss criterion; default is ltolerance(1e-8)
<u>iter</u> ate(#)	perform maximum # of iterations; default is iterate(1000)
<pre>protect(#)</pre>	perform # optimizations and report best solution; default is protect(1)
<u>nolo</u> g	suppress the iteration log
<u>tr</u> ace	display current configuration in iteration log
gradient	display current gradient matrix in iteration log
sdprotect(#)	advanced; see Options below

display table with configuration coordinates

suppress configuration plot

maximum number of eigenvalues to display; default is neigen(10)

bootstrap, by, jackknife, rolling, statsby, and xi are allowed; see [U] 11.1.10 Prefix commands. The maximum number of observations allowed in mds is the maximum matrix size; see [R] matsize. sdprotect(#) does not appear in the dialog box.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

<sup>\*</sup> id(varname) is required.

method	Description
<u>c</u> lassical	classical MDS; default if neither loss() nor transform() is specified
modern	<pre>modern MDS; default if loss() or transform() is specified; except when loss(stress) and transform(monotonic) are specified</pre>
nonmetric	nonmetric (modern) MDS; default when loss(stress) and transform(monotonic) are specified
loss	Description
stress	stress criterion, normalized by distances; the default
<u>nstr</u> ess	stress criterion, normalized by disparities
<u>sstr</u> ess	squared stress criterion, normalized by distances
<u>nsst</u> ress	squared stress criterion, normalized by disparities
<u>stra</u> in	strain criterion (with transform(identity) is equivalent to classical MDS)
sammon	Sammon mapping
tfunction	Description
<u>i</u> dentity	no transformation; disparity = dissimilarity; the default
<u>p</u> ower	power $\alpha$ : disparity = dissimilarity $^{\alpha}$
<u>m</u> onotonic	<pre>weakly monotonic increasing functions (nonmetric scaling); only   with loss(stress)</pre>
norm	Description
principal	principal orientation; location = 0; the default
classical	Procrustes rotation toward classical solution
<pre>target(matname)[, copy]</pre>	Procrustes rotation toward matname; ignore naming conflicts
	if copy is specified
initopt	Description
<u>c</u> lassical	start with classical solution; the default
$\underline{\underline{r}}$ andom $[(\#)]$	start at random configuration, setting seed to #
from(matname) [, copy]	start from <i>matname</i> ; ignore naming conflicts if copy is specified

# **Options**

Model

id(varname) is required and specifies a variable that identifies observations. A warning message is displayed if varname has duplicate values.

method(method) specifies the method for MDS.

method(classical) specifies classical metric scaling, also known as "principal coordinates analysis" when used with Euclidean proximities. Classical MDS obtains equivalent results to modern MDS with loss(strain) and transform(identity) without weights. The calculations for classical MDS are fast; consequently, classical MDS is generally used to obtain starting values for modern MDS. If the options loss() and transform() are not specified, mds computes the classical solution, likewise if method(classical) is specified loss() and transform() are not allowed.

method(modern) specifies modern scaling. If method(modern) is specified but not loss() or transform(), then loss(stress) and transform(identity) are assumed. All values of loss() and transform() are valid with method(modern).

method(nonmetric) specifies nonmetric scaling, which is a type of modern scaling. If method(nonmetric) is specified, loss(stress) and transform(monotonic) are assumed. Other values of loss() and transform() are not allowed.

loss (loss) specifies the loss criterion.

loss(stress) specifies that the stress loss function be used, normalized by the squared Euclidean distances. This criterion is often called Kruskal's stress-1. Optimal configurations for loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration paths may differ. loss(stress) is the default.

loss(nstress) specifies that the stress loss function be used, normalized by the squared disparities, that is, transformed dissimilarities. Optimal configurations for loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration paths may differ.

loss(sstress) specifies that the squared stress loss function be used, normalized by the fourth power of the Euclidean distances.

loss(nsstress) specifies that the squared stress criterion, normalized by the fourth power of the disparities (transformed dissimilarities) be used.

loss(strain) specifies the strain loss criterion. Classical scaling is equivalent to loss(strain) and transform(identity) but is computed by a faster noniterative algorithm. Specifying loss(strain) still allows transformations.

loss(sammon) specifies the Sammon (1969) loss criterion.

transform(tfunction) specifies the class of allowed transformations of the dissimilarities; transformed
dissimilarities are called disparities.

transform(identity) specifies that the only allowed transformation is the identity; that is, disparities are equal to dissimilarities. transform(identity) is the default.

transform(power) specifies that disparities are related to the dissimilarities by a power function,

$${\rm disparity}={\rm dissimilarity}^\alpha, \qquad \alpha>0$$

transform(monotonic) specifies that the disparities are a weakly monotonic function of the dissimilarities. This is also known as nonmetric MDS. Tied dissimilarities are handled by the primary method; that is, ties may be broken but are not necessarily broken. transform(monotonic) is valid only with loss(stress).

normalize(norm) specifies a normalization method for the configuration. Recall that the location and orientation of an MDS configuration is not defined ("identified"); an isometric transformation (that is, translation, reflection, or orthonormal rotation) of a configuration preserves interpoint Euclidean distances.

normalize(principal) performs a principal normalization, in which the configuration columns have zero mean and correspond to the principal components, with positive coefficient for the observation with lowest value of id(). normalize(principal) is the default.

- normalize(classical) normalizes by a distance-preserving Procrustean transformation of the configuration toward the classical configuration in principal normalization; see [MV] **procrustes**. normalize(classical) is not valid if method(classical) is specified.
- normalize(target(matname) [, copy]) normalizes by a distance-preserving Procrustean transformation toward matname; see [MV] **procrustes**. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is also specified.

Note on normalize(classical) and normalize(target()): the Procrustes transformation comprises any combination of translation, reflection, and orthonormal rotation—these transformations preserve distance. Dilation (uniform scaling) would stretch distances and is not applied. However, the output reports the dilation factor, and the reported Procrustes statistic is for the dilated configuration.

- dimension(#) specifies the dimension of the approximating configuration. The default # is 2 and should not exceed the number of observations; typically, # would be much smaller. With method(classical), it should not exceed the number of positive eigenvalues of the centered distance matrix.
- addconstant specifies that if the double-centered distance matrix is not positive semidefinite (psd), a constant should be added to the squared distances to make it psd and, hence, Euclidean. addconstant is allowed with classical MDS only.

Model 2

- unit[(varlist<sub>2</sub>)] specifies variables that are transformed to min = 0 and max = 1 before entering in the computation of similarities or dissimilarities. unit by itself, without an argument, is a shorthand for unit(\_all). Variables in unit() should not be included in std().
- std (varlist<sub>3</sub>) specifies variables that are transformed to mean = 0 and sd = 1 before entering in the computation of similarities or dissimilarities. std by itself, without an argument, is a shorthand for std(\_all). Variables in std() should not be included in unit().
- measure(*measure*) specifies the similarity or dissimilarity measure. The default is measure(L2), Euclidean distance. This option is not case sensitive. See [MV] *measure\_option* for detailed descriptions of the supported measures.

If a similarity measure is selected, the computed similarities will first be transformed into dissimilarities, before proceeding with the scaling; see the s2d() option below.

Classical metric MDS with Euclidean distance is equivalent to principal component analysis (see [MV] pca); the MDS configuration coordinates are the principal components.

s2d(standard | oneminus) specifies how similarities are converted into dissimilarities. By default, the command assumes dissimilarity data. Specifying s2d() indicates that your proximity data are similarities.

Dissimilarity data should have zeros on the diagonal (that is, an object is identical to itself) and nonnegative off-diagonal values. Dissimilarities need not satisfy the triangular inequality,  $D(i,j)^2 \leq D(i,h)^2 + D(h,j)^2$ . Similarity data should have ones on the diagonal (that is, an object is identical to itself) and have off-diagonal values between zero and one. In either case, proximities should be symmetric.

The available s2d() options, standard and oneminus, are defined as follows:

standard dissim
$$_{ij}=\sqrt{\sin_{ii}+\sin_{jj}-2\sin_{ij}}=\sqrt{2(1-\sin_{ij})}$$
 oneminus dissim $_{ij}=1-\sin_{ij}$ 

s2d(standard) is the default.

s2d() should be specified only with measures in similarity form.

Reporting

neigen(#) specifies the number of eigenvalues to be included in the table. The default is neigen(10). Specifying neigen(0) suppresses the table. This option is allowed with classical MDS only.

config displays the table with the coordinates of the approximating configuration. This table may also be displayed using the postestimation command estat config; see [MV] mds postestimation.

noplot suppresses the graph of the approximating configuration. The graph can still be produced later via mdsconfig, which also allows the standard graphics options for fine-tuning the plot; see [MV] mds postestimation plots.

Minimization

These options are available only with method(modern) or method(nonmetric):

initialize(initopt) specifies the initial values of the criterion minimization process.

initialize(classical), the default, uses the solution from classical metric scaling as initial
values. With protect(), all but the first run start from random perturbations from the classical
solution. These random perturbations are independent and normally distributed with standard
error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.
initialize(classical) is the default.

initialize(random) starts an optimization process from a random starting configuration. These random configurations are generated from independent normal distributions with standard error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities. The means of the configuration are irrelevant in MDS.

initialize(from(matname) [, copy]) sets the initial value to matname. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is specified. With protect(), the second-to-last runs start from random perturbations from matname. These random perturbations are independent normal distributed with standard error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.

tolerance(#) specifies the tolerance for the configuration matrix. When the relative change in the configuration from one iteration to the next is less than or equal to tolerance(), the tolerance() convergence criterion is satisfied. The default is tolerance(1e-4).

ltolerance(#) specifies the tolerance for the fit criterion. When the relative change in the fit
criterion from one iteration to the next is less than or equal to ltolerance(), the ltolerance()
convergence is satisfied. The default is ltolerance(1e-8).

Both the tolerance() and ltolerance() criteria must be satisfied for convergence.

iterate(#) specifies the maximum number of iterations. The default is iterate(1000).

protect(#) requests that # optimizations be performed and that the best of the solutions be reported. The default is protect(1). See option initialize() on starting values of the runs. The output contains a table of the run, return code, iteration, and criterion value reached. Specifying a large number, such as protect(50), provides reasonable insight whether the solution found is a global minimum and not just a local minimum.

If any of the options log, trace, or gradient is also specified, iteration reports will be printed for each optimization run. Beware: this option will produce a lot of output.

nolog suppresses the iteration log, showing the progress of the minimization process.

trace displays the configuration matrices in the iteration report. Beware: this option may produce a lot of output.

gradient displays the gradient matrices of the fit criterion in the iteration report. Beware: this option may produce a lot of output.

The following option is available with mds but is not shown in the dialog box:

sdprotect(#) sets a proportionality constant for the standard deviations of random configurations
 (init(random)) or random perturbations of given starting configurations (init(classical) or
 init(from())). The default is sdprotect(1).

# Remarks and examples

Remarks are presented under the following headings:

Introduction
Euclidean distances
Non-Euclidean dissimilarity measures
Introduction to modern MDS
Protecting from local minimums

#### Introduction

Multidimensional scaling (MDS) is a dimension-reduction and visualization technique. Dissimilarities (for instance, Euclidean distances) between observations in a high-dimensional space are represented in a lower-dimensional space (typically two dimensions) so that the Euclidean distance in the lower-dimensional space approximates the dissimilarities in the higher-dimensional space. See Kruskal and Wish (1978) for a brief nontechnical introduction to MDS. Young and Hamer (1987) and Borg and Groenen (2005) offer more advanced textbook-sized treatments.

If you already have the similarities or dissimilarities of the n objects, you should continue by reading [MV] **mdsmat**.

In many applications of MDS, however, the similarity or dissimilarity of objects is not measured but rather *defined* by the researcher in terms of variables ("attributes")  $x_1, \ldots, x_k$  that are measured on the objects. The pairwise dissimilarity of objects can be expressed using a variety of similarity or dissimilarity measures in the attributes (for example, Mardia, Kent, and Bibby [1979, sec. 13.4]; Cox and Cox [2001, sec. 1.3]). A common measure is the Euclidean distance L2 between the attributes of the objects i and j:

$$L2_{ij} = \left\{ (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ik} - x_{jk})^2 \right\}^{1/2}$$

A popular alternative is the L1 distance, also known as the cityblock or Manhattan distance. In comparison to L2, L1 gives less influence to larger differences in attributes:

$$L1_{ij} = |x_{i1} - x_{i1}| + |x_{i2} - x_{i2}| + \dots + |x_{ik} - x_{ik}|$$

In contrast, we may also define the extent of dissimilarity between 2 observations as the maximum absolute difference in the attributes and thus give a larger influence to larger differences:

Linfinity<sub>ij</sub> = 
$$\max(|x_{i1} - x_{j1}|, |x_{i2} - x_{j2}|, ..., |x_{ik} - x_{jk}|)$$

These three measures are special cases of the Minkowski distance L(q), for q=2 (L2), q=1 (L1), and  $q=\infty$  (Linfinity), respectively. Minkowski distances with other values of q may be used as well. Stata supports a wide variety of other similarity and dissimilarity measures, both for continuous variables and for binary variables. See [MV] *measure\_option* for details.

Multidimensional scaling constructs approximations for dissimilarities, not for similarities. Thus, if a similarity measure is specified, mds first transforms the similarities into dissimilarities. Two methods to do this are available. The default standard method,

$$\operatorname{dissim}_{ij} = \sqrt{\sin_{ii} - 2\sin_{ij} + \sin_{ij}}$$

has a useful property: if the similarity matrix is positive semidefinite, a property satisfied by most similarity measures, the standard dissimilarities are Euclidean.

Usually, the number of observations exceeds the number of variables on which the observations are compared, but this is not a requirement for MDS. MDS creates an  $n \times n$  dissimilarity matrix  $\mathbf{D}$  from the n observations on k variables. It then constructs an approximation of  $\mathbf{D}$  by the Euclidean distances in a matching configuration  $\mathbf{Y}$  of n points in p-dimensional space:

dissimilarity
$$(x_i, x_j) \approx L2(y_i, y_j)$$
 for all  $i, j$ 

Typically, of course,  $p \ll k$ , and most often p = 1, 2, or 3.

A wide variety of MDS methods have been proposed. mds performs classical and modern scaling. Classical scaling has its roots in Young and Householder (1938) and Torgerson (1952). MDS requires complete and symmetric dissimilarity interval-level data. To explore modern scaling, see Borg and Groenen (2005). Classical scaling results in an eigen decomposition, whereas modern scaling is accomplished by the minimization of a loss function. Consequently, eigenvalues are not available after modern MDS.

Computing the classical solution is straightforward, but with modern MDS the minimization of the loss criteria over configurations is a high-dimensional problem that is easily beset by convergence to local minimums. mds provides options to control the minimization process 1) by allowing the user to select the starting configuration and 2) by selecting the best solution among multiple minimization runs from random starting configurations.

#### **Euclidean distances**

## Example 1

The most popular dissimilarity measure is Euclidean distance. We illustrate with data from table 7.1 of Yang and Trewn (2004, 182). This dataset consists of eight variables with nutrition data on 25 breakfast cereals.

- . use http://www.stata-press.com/data/r14/cerealnut (Cereal Nutrition)
- . describe

Contains data from http://www.stata-press.com/data/r14/cerealnut.dta Cereal Nutrition obs: 24 Feb 2014 17:19 vars: a size: 1,050 (\_dta has notes)

variable name	storage type	display format	value label	variable label
brand	str25	%25s		Cereal Brand
calories	int	%9.0g		Calories (Cal/oz)
protein	byte	%9.0g		Protein (g)
fat	byte	%9.0g		Fat (g)
Na	int	%9.0g		Na (mg)
fiber	float	%9.0g		Fiber (g)
carbs	float	%9.0g		Carbs (g)
sugar	byte	%9.0g		Sugar (g)
К	int	%9.0g		K (mg)

#### Sorted by:

. summarize calories-K, sep(4)

Variable	Obs	Mean	Std. Dev.	Min	Max
calories	25	109.6	21.30728	50	160
protein	25	2.68	1.314027	1	6
fat	25	.92	.7593857	0	2
Na	25	195.8	71.32204	0	320
fiber	25	1.7	2.056494	0	9
carbs	25	15.3	4.028544	7	22
sugar	25	7.4	4.609772	0	14
K	25	90.6	77.5043	15	320

. replace brand = subinstr(brand, " ", "\_",.) (20 real changes made)

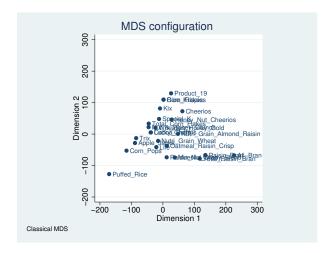
We replaced spaces in the cereal brand names with underscores to avoid confusing which words in the brand names are associated with which points in the graphs we are about to produce. Removing spaces is not required.

The default dissimilarity measure used by mds is the Euclidean distance L2 computed on the raw data (unstandardized). The summary of the eight nutrition variables shows that K, Na, and calories—having much larger standard deviations—will largely determine the Euclidean distances. . mds calories-K, id(brand)

Classical metric multidimensional scaling dissimilarity: L2, computed on 8 variables

		l	Number o	of c	bs		=	25
Eigenvalues > 0	=	8 N	Mardia 1	fit	measure	1	=	0.9603
Retained dimensions	=	2 N	Mardia 1	fit	measure	2	=	0.9970

		abs(eige	nvalue)	(eigenv	alue)^2
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.
1	158437.92	56.95	56.95	67.78	67.78
2	108728.77	39.08	96.03	31.92	99.70
3	10562.645	3.80	99.83	0.30	100.00
4	382.67849	0.14	99.97	0.00	100.00
5	69.761715	0.03	99.99	0.00	100.00
6	12.520822	0.00	100.00	0.00	100.00
7	5.7559984	0.00	100.00	0.00	100.00
8	2.2243244	0.00	100.00	0.00	100.00

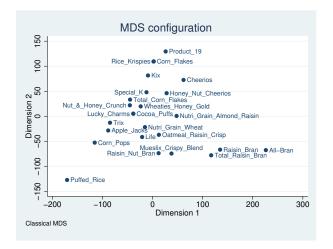


The default MDS configuration graph can be improved upon by using the mdsconfig postestimation command. We will demonstrate this in a moment. But first, we explain the output of mds.

mds has performed classical metric scaling and extracted two dimensions, which is the default action. To assess goodness of fit, the two statistics proposed by Mardia are reported (see Mardia, Kent, and Bibby [1979, sec. 14.4]). The statistics are defined in terms of the eigenvalues of the double-centered distance matrix. If the dissimilarities are truly Euclidean, all eigenvalues are nonnegative. Look at the eigenvalues. We may interpret these as the extent to which the dimensions account for dissimilarity between the cereals. Depending on whether you look at the eigenvalues or squared eigenvalues, it takes two or three dimensions to account for more than 99% of the dissimilarity.

We can produce a prettier configuration plot with the mdsconfig command; see [MV] mds postestimation plots for details.

```
. generate place = 3
. replace place = 9 if inlist(brand, "Rice_Krispies", "Nut_&_Honey_Crunch",
> "Special_K", "Raisin_Nut_Bran", "Lucky_Charms")
(5 real changes made)
. replace place = 12 if inlist(brand, "Mueslix_Crispy_Blend")
(1 real change made)
. mdsconfig, autoaspect mlabypos(place)
```



The  $marker\_label\_option$  mlabvposition() allowed fine control over the placement of the cereal brand names. We created a variable called place giving clock positions where the cereal names were to appear in relation to the plotted point. We set these to minimize overlap of the names. We also requested the autoaspect option to obtain better use of the graphing region while preserving the scale of the x and y axes.

MDS has placed the cereals so that all the brands fall within a triangle defined by Product 19, All-Bran, and Puffed Rice. You can examine the graph to see how close your favorite cereal is to the other cereals.

But, as we saw from the variable summary, three of the eight variables are controlling the distances. If we want to provide for a more equal footing for the eight variables, we can request that mds compute the Euclidean distances on standardized variables. Euclidean distance based on standardized variables is also known as the *Karl Pearson distance* (Pearson 1900). We obtain standardized measures with the option std.

```
. mds calories-K, id(brand) std noplot
Classical metric multidimensional scaling
    dissimilarity: L2, computed on 8 variables
```

			Number	of	obs		=	25
Eigenvalues > 0	=	8	Mardia	fit	${\tt measure}$	1	=	0.5987
Retained dimensions	=	2	Mardia	fit	${\tt measure}$	2	=	0.7697

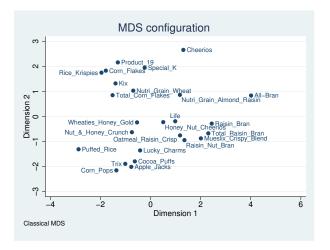
		abs(eige	nvalue)	(eigenv	ralue)^2
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.
1	65.645395	34.19	34.19	49.21	49.21
2	49.311416	25.68	59.87	27.77	76.97
3	38.826608	20.22	80.10	17.21	94.19
4	17.727805	9.23	89.33	3.59	97.78
5	11.230087	5.85	95.18	1.44	99.22
6	8.2386231	4.29	99.47	0.78	99.99
7	.77953426	0.41	99.87	0.01	100.00
8	. 24053137	0.13	0.13 100.00 0.0		100.00

In this and the previous example, we did not specify a method() for mds and got classical metric scaling. Classical scaling is the default when method() is omitted and neither the loss() nor transform() option is specified.

Accounting for more than 99% of the underlying distances now takes more MDS-retained dimensions. For this example, we have still retained only two dimensions. We specified the noplot option because we wanted to exercise control over the configuration plot by using the mdsconfig command. We generate a variable named pos that will help minimize cereal brand name overlap.

```
. generate pos = 3
. replace pos = 5 if inlist(brand, "Honey_Nut_Cheerios", "Raisin_Nut_Bran",
> "Nutri_Grain_Almond_Raisin")
(3 real changes made)
. replace pos = 8 if inlist(brand, "Oatmeal_Raisin_Crisp")
(1 real change made)
. replace pos = 9 if inlist(brand, "Corn_Pops", "Trix", "Nut_&_Honey_Crunch",
> "Rice_Krispies", "Wheaties_Honey_Gold")
(5 real changes made)
. replace pos = 12 if inlist(brand, "Life")
(1 real change made)
```

. mdsconfig, autoaspect mlabvpos(pos)



This configuration plot, based on the standardized variables, better incorporates all the nutrition data. If you are familiar with these cereal brands, spotting groups of similar cereals appearing near each other is easy. The bottom-left corner has several of the most sweetened cereals. The brands containing the word "Bran" all appear to the right of center. Rice Krispies and Puffed Rice are the farthest to the left.

Classical multidimensional scaling based on standardized Euclidean distances is actually equivalent to a principal component analysis of the correlation matrix of the variables. See Mardia, Kent, and Bibby (1979, sec. 14.3) for details.

We now demonstrate this property by doing a principal component analysis extracting the leading two principal components. See [MV] pca for details.

. pca calories-K, comp(2)

Principal components/correlation

Number of obs = 25

Number of comp. = 2

Trace = 8

Rotation: (unrotated = principal)

Rho = 0.5987

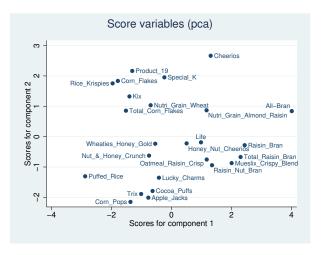
Component	Eigenvalue	Difference	Proportion	Cumulative
Comp1	2.73522	.680583	0.3419	0.3419
Comp2	2.05464	.436867	0.2568	0.5987
Comp3	1.61778	.879117	0.2022	0.8010
Comp4	.738659	.270738	0.0923	0.8933
Comp5	.46792	.124644	0.0585	0.9518
Comp6	.343276	.310795	0.0429	0.9947
Comp7	.0324806	.0224585	0.0041	0.9987
Comp8	.0100221		0.0013	1.0000

Variable	Comp1	Comp2	Unexplained
calories	0.1992	-0.0632	.8832
protein	0.3376	0.4203	.3253
fat	0.3811	-0.0667	. 5936
Na	0.0962	0.5554	.3408
fiber	0.5146	0.0913	.2586
carbs	-0.2574	0.4492	.4043
sugar	0.2081	-0.5426	.2765
K	0.5635	0.0430	.1278

Principal components (eigenvectors)

The proportion and cumulative proportion of the eigenvalues in the PCA match the percentages from MDS. We will ignore the interpretation of the principal components but move directly to the principal coordinates, also known as the scores of the PCA. We make a plot of the first and second scores, using the scoreplot command; see [MV] scoreplot. We specify the mlabel() option to label the cereals and the mlabvpos() option for fine control over placement of the brand names.

- . replace pos = 11 if inlist(brand, "All-Bran")
  (1 real change made)
- . scoreplot, mlabel(brand) mlabvpos(pos)



Compare this PCA score plot with the MDS configuration plot. Apart from some differences in how the graphs were rendered, they are the same.

# Non-Euclidean dissimilarity measures

With non-Euclidean dissimilarity measures, the parallel between PCA and MDS no longer holds.

# ▶ Example 2

To illustrate MDS with non-Euclidean distance measures, we will analyze books on multivariate statistics. Gifi (1990) reports on the number of pages devoted to six topics in 20 textbooks on multivariate statistics. We added similar data on five more recent books.

4

- . use http://www.stata-press.com/data/r14/mvstatsbooks, clear
- . describe

Contains data from http://www.stata-press.com/data/r14/mvstatsbooks.dta obs:

8 15 Mar 2014 16:27 vars: 725 size: (\_dta has notes)

variable name	storage type	display format	value label	variable label
author	str17	%17s		
math	int	%9.0g		<pre>math other than statistics (e.g., linear algebra)</pre>
corr	int	%9.0g		correlation and regression, including linear structural and functional equations
fact	byte	%9.0g		factor analysis and principal component analysis
cano	byte	%9.0g		canonical correlation analysis
disc	int	%9.0g		discriminant analysis, classification, and cluster analysis
stat	int	%9.0g		<pre>statistics, incl. dist. theory,   hypothesis testing &amp; est.;   categorical data</pre>
mano	int	%9.0g		manova and the general linear model

Sorted by:

A brief description of the topics is given in the variable labels. For more details, we refer to Gifi (1990, 15). Here are the data:

#### . list, noobs

author	math	corr	fact	cano	disc	stat	mano
Roy57	31	0	0	0	0	164	11
Kendal157	0	16	54	18	27	13	14
Kendal175	0	40	32	10	42	60	0
Anderson58	19	0	35	19	28	163	52
CooleyLohnes62	14	7	35	22	17	0	56
•		(0)	utput omi	tted)			
GreenCarol176	290	10	6	0	8	0	2
CailliezPages76	184	48	82	42	134	0	0
Giri77	29	0	0	0	41	211	32
Gnanadesikan77	0	19	56	0	39	75	0
Kshirsagar78	0	22	45	42	60	230	59
Thorndike78	30	128	90	28	48	0	0
MardiaKentBibby79	34	28	68	19	67	131	55
Seber84	16	0	59	13	116	129	101
Stevens96	23	87	67	21	30	43	249
EverittDunn01	0	54	65	0	56	20	30
Rencher02	38	0	71	19	105	135	131

For instance, the 1979 book by Mardia, Kent, and Bibby has 34 pages on mathematics (mostly linear algebra); 28 pages on correlation, regression, and related topics (in this particular case, simultaneous equations); etc. In most of these books, some pages are not classified. Anyway, the number of pages and the amount of information per page vary widely among the books. A Euclidean distance measure is not appropriate here. Standardization does not help us here—the problem is not differences in the scales of the variables but those in the observations. One possibility is to transform the data into compositional data by dividing the variables by the total number of classified pages. See Mardia, Kent, and Bibby (1979, 377–380) for a discussion of specialized dissimilarity measures for compositional data. However, we can also use the correlation between observations (not between variables) as the similarity measure. The higher the correlation between the attention given to the various topics, the more similar two textbooks are. We do a classical MDS, suppressing the plot to first assess the quality of a two-dimensional representation.

```
. mds math-mano, id(author) measure(corr) noplot

Classical metric multidimensional scaling
    similarity: correlation, computed on 7 variables
    dissimilarity: sqrt(2(1-similarity))
```

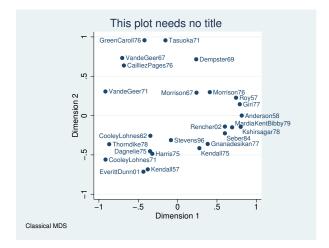
			Number	OI ODS		_	25
Eigenvalues > 0	=	6	${\tt Mardia}$	fit measure	1	=	0.6680
Retained dimensions	=	2	Mardia	fit measure	2	=	0.8496

		abs(eigenvalue)		(eigenvalue)^2	
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.
1	8.469821	38.92	38.92	56.15	56.15
2	6.0665813	27.88	66.80	28.81	84.96
3	3.8157101	17.53	84.33	11.40	96.35
4	1.6926956	7.78	92.11	2.24	98.60
5	1.2576053	5.78	97.89	1.24	99.83
6	. 45929376	2.11	100.00	0.17	100.00

Again the quality of a two-dimensional approximation is somewhat unsatisfactory, with 67% and 85% of the variation accounted for according to the two Mardia criteria. Still, let's look at the plot, using a title that refers to the self-referential aspect of the analysis (Smullyan 1986). We reposition some of the author labels to enhance readability by using the mlabvpos() option.

```
. generate spot = 3
. replace spot = 5 if inlist(author, "Seber84", "Kshirsagar78", "Kendal175")
(3 real changes made)
. replace spot = 2 if author=="MardiaKentBibby79"
(1 real change made)
. replace spot = 9 if inlist(author, "Dagnelie75", "Rencher02",
> "GreenCarol176", "EverittDunn01", "CooleyLohnes62", "Morrison67")
(6 real changes made)
```

. mdsconfig, mlabvpos(spot) title(This plot needs no title)



A striking characteristic of the plot is that the textbooks seem to be located on a circle. This is a phenomenon that is regularly encountered in multidimensional scaling and was labeled the "horseshoe effect" by Kendall (1971, 215–251). This phenomenon seems to occur especially in situations in which a one-dimensional representation of objects needs to be constructed, for example, in *seriation* applications, from data in which small dissimilarities were measured accurately but moderate and larger dissimilarities are "lumped together".

#### □ Technical note

These data could also be analyzed differently. A particularly interesting method is correspondence analysis (CA), which seeks a simultaneous geometric representation of the rows (textbooks) and columns (topics). We used camat to analyze these data. The results for the textbooks were not much different. Textbooks that were mapped as similar using MDS were also mapped this way by CA. The Green and Carroll book that appeared much different from the rest was also displayed away from the rest by CA. In the CA biplot, it was immediately clear that this book was so different because its pages were classified by Gifi (1990) as predominantly mathematical. But CA also located the topics in this space. The pattern was easy to interpret and was expected. The seven topics were mapped in three groups. math and stat appear as two groups by themselves, and the five applied topics were mapped close together. See [MV] ca for information on the ca command.

#### Introduction to modern MDS

We return to the data on breakfast cereals explored above to introduce modern MDS. We repeat some steps taken previously and then perform estimation using options loss(strain) and transform(identity), which we demonstrate are equivalent to classical MDS.

mds is an estimation or eclass command; see program define in [P] program. You can display its stored results using ereturn list. The configuration is stored as e(Y) and we will compare the configuration obtained from classical MDS with the equivalent one from modern MDS.

4

#### Example 3

```
. use http://www.stata-press.com/data/r14/cerealnut, clear
(Cereal Nutrition)
. replace brand = subinstr(brand, " ", "_",.)
(20 real changes made)
. quietly mds calories-K, id(brand) noplot
. mat Yclass = e(Y)
. mds calories-K, id(brand) meth(modern) loss(strain) trans(ident) noplot
Iteration 1:
               strain = 594.12657
               strain = 594.12657
Modern multidimensional scaling
    dissimilarity: L2, computed on 8 variables
    Loss criterion: strain = loss for classical MDS
    Transformation: identity (no transformation)
                                                                              25
                                                  Number of obs
                                                  Dimensions
                                                                              2
    Normalization: principal
                                                  Loss criterion
                                                                       594.1266
. mat Ymod = e(Y)
. assert mreldif(Yclass, Ymod) < 1e-6
```

Note the output differences between modern and classical MDS. In modern MDS we have an iteration log from the minimization of the loss function. The method, measure, observations, dimensions, and number of variables are reported as before, but we do not have or display eigenvalues. The normalization is always reported in modern MDS and with normalize(target()) for classical MDS. The loss criterion is simply the value of the loss function at the minimum.

4

# Protecting from local minimums

Modern MDS can sometimes converge to a local rather than a global minimum. To protect against this, multiple runs can be made, giving the best of the runs as the final answer. The option for performing this is protect(#), where # is the number of runs to be performed. The nolog option is of particular use with protect(), because the iteration logs from the runs will create a lot of output. Repeating the minimization can take some time, depending on the number of runs selected and the number of iterations it takes to converge.

# ▶ Example 4

We choose loss(stress), and transform(identity) is assumed with modern MDS. We omit the iteration logs to avoid a large amount of output. The number of iterations is available after estimation in e(ic). We first do a run without the protect() option, and then we use protect(50) and compare our results.

```
. mds calories-K, id(brand) method(modern) loss(stress) nolog noplot
(transform(identity) assumed)
Modern multidimensional scaling
    dissimilarity: L2, computed on 8 variables
    Loss criterion: stress = raw_stress/norm(distances)
    Transformation: identity (no transformation)
                                                 Number of obs
                                                                             25
                                                                              2
                                                 Dimensions
                                                 Loss criterion =
                                                                         0.0263
    Normalization: principal
. di e(ic)
45
. mat Ystress = e(Y)
. set seed 123456789
. mds calories-K, id(brand) method(modern) loss(stress) nolog protect(50)
(transform(identity) assumed)
```

run	mrc	#iter	lossval
1	0	68	.02626681
2	0	73	.02626681
3	0	65	.02626681
4	0	156	.02626681
5	0	45	.02626681
6	0	72	.02626681
7	0	77	.02626682
8	0	66	.02626682
9	0	60	.02626682
10	0	55	.02626682
11	0	57	.02626682
12	0	74	.02626682
13	0	65	.02626682
14	0	72	.02626682
15	0	59	.02626682
16	0	59	.02626682
17	0	68	.02626682
18	0	52	.02626682
19	0	53	.02626683
20	0	51	.02626683
21	0	57	.02626683
22	0	71	.026303
23	0	89	.026303
24	0	143	.026303
25	0	60	.026303
26	0	55	.026303
27	0	81	.026303
28	0	163	.026303
29	0	68	.026303
30	0	72	.026303
31	0	63	.026303
32	0	97	.026303
33	0	51	.026303
34	0	61	.026303
35	0	55	.026303
36	0	139	.026303
37	0	53	.026303
38	0	76	.026303
39	0	47	.02630301
40	0	59	.02630301
41	0	59	.02630301
42	0	70	.02630302
43	0	106	.18601022

44	0	137	.19899066
45	0	131	.19899067
46	0	115	.19899067
47	0	143	.19899067
48	0	113	.22087176
49	0	151	.22453361
50	0	203	.23810368

Modern multidimensional scaling

Normalization: principal

dissimilarity: L2, computed on 8 variables

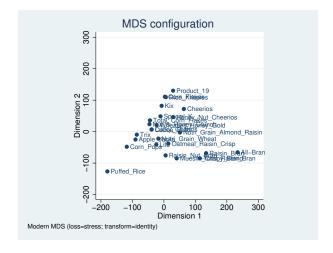
Loss criterion: stress = raw\_stress/norm(distances)

Transformation: identity (no transformation)

Number of obs = 25 Dimensions = 2 Loss criterion = 0.0263

. mat YstressP = e(Y)

. assert mreldif(Ystress, YstressP) < 2e-3</pre>



The output provided when protect() is specified includes a table with information on each run, sorted by the loss criterion value. The first column simply counts the runs. The second column gives the internal return code from modern MDS. This example only has values of 0, which indicate converged results. The column header mrc is clickable and opens a help file explaining the various MDS return codes. The number of iterations is in the third column. These runs converged in as few as 45 iterations to as many as 203. The loss criterion values are in the fourth column.

In this example, the results from our original run versus the protected run did not differ by much. However, looking at runs 43–50, we see loss criterion values that are much higher than the rest.

The graph from this protected modern MDS run may be compared with the first one produced. There are obvious similarities, though inspection indicates that the two are not the same.

### Stored results

mds stores the following in e():

```
Scalars
                          number of observations
    e(N)
                          number of dimensions in the approximating configuration
    e(p)
                          number of strictly positive eigenvalues
    e(np)
    e(addcons)
                          constant added to squared dissimilarities to force positive semidefiniteness
    e(mardia1)
                          Mardia measure 1
    e(mardia2)
                          Mardia measure 2
    e(critval)
                          loss criterion value
    e(alpha)
                          parameter of transform(power)
    e(ic)
                          iteration count
    e(rc)
                          return code
    e(converged)
                          1 if converged, 0 otherwise
Macros
    e(cmd)
                          mds
    e(cmdline)
                          command as typed
                          classical or modern MDS method
    e(method)
    e(method2)
                          nonmetric, if method(nonmetric)
    e(loss)
                          loss criterion
    e(losstitle)
                          description loss criterion
                          identity, power, or monotonic, transformation function
    e(tfunction)
                          description of transformation
    e(transftitle)
    e(id)
                          ID variable name (mds)
    e(idtype)
                          int or str; type of id() variable
    e(duplicates)
                          1 if duplicates in id(), 0 otherwise
    e(labels)
                          labels for ID categories
    e(strfmt)
                          format for category labels
    e(mxlen)
                          maximum length of category labels
    e(varlist)
                          variables used in computing similarities or dissimilarities
    e(dname)
                          similarity or dissimilarity measure name
                          similarity or dissimilarity
    e(dtype)
    e(s2d)
                          standard or oneminus (when e(dtype) is similarity)
    e(unique)
                          1 if eigenvalues are distinct, 0 otherwise
                          initialization method
    e(init)
                          initial random-number state used for init(random)
    e(irngstate)
    e(rngstate)
                          random-number state for solution
    e(norm)
                          normalization method
    e(targetmatrix)
                          name of target matrix for normalize(target)
    e(properties)
                          nob noV for modern or nonmetric MDS; nob noV eigen for classical MDS
    e(estat_cmd)
                          program used to implement estat
    e(predict)
                          program used to implement predict
    e(marginsnotok)
                          predictions disallowed by margins
```

## Methods and formulas

mds creates a dissimilarity matrix **D** according to the *measure* specified in option measure(). See [MV] *measure\_option* for descriptions of these measures. Subsequently, mds uses the same subroutines as mdsmat to compute the MDS solution for **D**. See *Methods and formulas* in [MV] **mdsmat** for information.

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Also see References in [MV] mdsmat.

Joseph Bernard Kruskal (1928–2010) was born in New York. His brothers were statistician William Henry Kruskal (1919–2005) and mathematician and physicist Martin David Kruskal (1925–2006). He earned degrees in mathematics from Chicago and Princeton and worked at Bell Labs until his retirement in 1993. In statistics, Kruskal made major contributions to multidimensional scaling. In computer science, he devised an algorithm for computing the minimal spanning tree of a weighted graph. His other interests include clustering and statistical linguistics.

# Also see

- [MV] mds postestimation Postestimation tools for mds, mdsmat, and mdslong
- [MV] mds postestimation plots Postestimation plots for mds, mdsmat, and mdslong
- [MV] **biplot** Biplots
- [MV] ca Simple correspondence analysis
- [MV] **factor** Factor analysis
- [MV] mdslong Multidimensional scaling of proximity data in long format
- [MV] mdsmat Multidimensional scaling of proximity data in a matrix
- [MV] **pca** Principal component analysis
- [U] 20 Estimation and postestimation commands

# **Title**

mds postestimation — Postestimation tools for mds, mdsmat, and mdslong

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

# **Postestimation commands**

The following postestimation commands are of special interest after mds, mdslong, and mdsmat:

Command	Description
estat config	coordinates of the approximating configuration
estat correlations	correlations between dissimilarities and approximating distances
estat pairwise	pairwise dissimilarities, approximating distances, and raw residuals
estat quantiles	quantiles of the residuals per object
estat stress	Kruskal stress (loss) measure (only after classical MDS)
*estat summarize	estimation sample summary
mdsconfig	plot of approximating configuration
mdsshepard	Shepard diagram
screeplot	plot eigenvalues (only after classical MDS)

<sup>\*</sup> estat summarize is not available after mdsmat.

The following standard postestimation commands are also available:

Command	Description
*estimates predict	cataloging estimation results approximating configuration, disparities, dissimilarities, distances, and residuals

<sup>\*</sup> All estimates subcommands except table and stats are available.

# predict

# **Description for predict**

predict creates new variables containing predictions such as approximating configurations in Euclidean space and selected pairwise statistics.

## Menu for predict

Statistics > Postestimation

# Syntax for predict

statistic	Description		
Sittlistic	Description		
Main			
<u>con</u> fig	approximating configuration; specify dimension() or fewer variables		
pairwise(pstats)	selected pairwise statistics; specify same number of variables		
pstats	Description		
disparities	disparities = transformed(dissimilarities)		
dissimilarities	dissimilarities		
<u>dist</u> ances	Euclidean distances between configuration points		
<u>rr</u> esiduals	raw residual = dissimilarity - distance		
<u>tr</u> esiduals	transformed residual = disparity - distance		
weights	weights		
options	Description		
Main			
* <u>sav</u> ing( <i>filename</i> , replace)	save results to filename; use replace to overwrite existing filename		
full	create predictions for all pairs of objects; pairwise() only		

<sup>\*</sup> saving() is required after mdsmat, after mds if pairwise() is selected, and after mdslong if config is selected.

# **Options for predict**

Main

config generates variables containing the approximating configuration in Euclidean space. Specify as many new variables as approximating dimensions (as determined by the dimension() option of mds, mdsmat, or mdslong), though you may specify fewer. estat config displays the same information but does not store the information in variables. After mdsmat and mdslong, you must also specify the saving() option.

pairwise (pstats) generates new variables containing pairwise statistics. The number of new variables should be the same as the number of specified statistics. The following statistics are allowed:

disparities generates the disparities, that is, the transformed dissimilarities. If no transformation is applied (modern MDS with transform(identity)), disparities are the same as dissimilarities.

dissimilarities generates the dissimilarities used in MDS. If mds, mdslong, or mdsmat was invoked on similarity data, the associated dissimilarities are returned.

distances generates the (unsquared) Euclidean distances between the fitted configuration points.

rresiduals generates the raw residuals: dissimilarities — distances.

tresiduals generates the transformed residuals: disparities — distances.

weights generates the weights. Missing proximities are represented by zero weights.

estat pairwise displays some of the same information but does not store the information in variables.

After mds and mdsmat, you must also specify the saving() option. With n objects, the pairwise dataset has n(n-1)/2 observations. In addition to the three requested variables, predict produces variables id1 and id2, which identify pairs of objects. With mds, id is the name of the identification variable (id() option), and with mdsmat, it is "Category".

saving (filename, replace) is required after mdsmat, after mds if pairwise() is selected, and after mdslong if config is selected. saving() indicates that the generated variables are to be created in a new Stata dataset and saved in the file named filename. Unless saving() is specified, the variables are generated in the current dataset.

replace indicates that filename specified in saving() may be overwritten.

full creates predictions for all pairs of objects  $(j_1, j_2)$ . The default is to generate predictions only for pairs  $(j_1, j_2)$  where  $j_1 > j_2$ . full may be specified only with pairwise().

#### estat

# Description for estat

estat config lists the coordinates of the approximating configuration.

estat correlations lists the Pearson and Spearman correlations between the disparities or dissimilarities and the Euclidean distances for each object.

estat pairwise lists the pairwise statistics: the disparities, the distances, and the residuals.

estat quantiles lists the quantiles of the residuals per object.

estat stress displays the Kruskal stress (loss) measure between the (transformed) dissimilarities and fitted distances per object (only after classical MDS).

estat summarize summarizes the variables in the MDS over the estimation sample. After mds, estat summarize also reports whether and how variables were transformed before computing similarities or dissimilarities.

#### Menu for estat

Statistics > Postestimation

## Syntax for estat

```
List the coordinates of the approximating configuration
```

```
estat config [, maxlength(#) format(%fmt)]
```

List the Pearson and Spearman correlations

```
estat <u>cor</u>relations [, <u>max</u>length(#) <u>for</u>mat(%fmt) <u>notrans</u>form <u>nototal</u>]
```

List the pairwise statistics: disparities, distances, and residuals

```
estat pairwise | , maxlength(#) notransform full separator |
```

List the quantiles of the residuals

```
estat quantiles [, maxlength(#) format(%fmt) nototal notransform]
```

Display the Kruskal stress (loss) measure per point (only after classical MDS)

```
estat stress [, maxlength(#) format(%fmt) nototal notransform]
```

Summarize the variables in MDS

```
estat <u>summarize</u> [, <u>lab</u>els]
```

options	Description
<pre>maxlength(#)</pre>	maximum number of characters for displaying object names; default is 12
<pre>format(%fmt)</pre>	display format
<u>notot</u> al	suppress display of overall summary statistics
$\underline{\mathtt{notrans}}\mathtt{form}$	use dissimilarities instead of disparities
<u>f</u> ull	display all pairs $(j_1, j_2)$ ; default is $(j_1 > j_2)$ only
$\underline{\mathtt{s}}\mathtt{e}\mathtt{parator}$	draw separating lines
<u>lab</u> els	display variable labels

# Options for estat

maxlength(#), an option used with all but estat summarize, specifies the maximum number of characters of the object names to be displayed; the default is maxlength(12).

format(% fmt), an option used with estat config, estat correlations, estat quantiles, and estat stress, specifies the display format; the default differs between the subcommands.

nototal, an option used with estat correlations, estat quantiles, and estat stress, suppresses the overall summary statistics.

notransform, an option used with estat correlations, estat pairwise, estat quantiles, and estat stress, specifies that the untransformed dissimilarities be used instead of the transformed dissimilarities (disparities).

full, an option used with estat pairwise, displays a row for all pairs  $(j_1, j_2)$ . The default is to display rows only for pairs where  $j_1 > j_2$ .

separator, an option used with estat pairwise, draws separating lines between blocks of rows corresponding to changes in the first of the pair of objects.

labels, an option used with estat summarize, displays variable labels.

# Remarks and examples

Remarks are presented under the following headings:

Postestimation statistics Predictions

#### Postestimation statistics

After an MDS analysis, several facilities can help you better understand the analysis and, in particular, to assess the quality of the lower-dimensional Euclidean representation. We display results after classical MDS. All are available after modern MDS except for estat stress.

## Example 1: estat

We illustrate the MDS postestimation facilities with the Morse code digit-similarity dataset; see example 1 in [MV] mdslong.

- . use http://www.stata-press.com/data/r14/morse\_long (Morse data (Rothkopf 1957))
- . generate sim = freqsame/100
- . mdslong sim, id(digit1 digit2) s2d(standard) noplot (output omitted)

MDS has produced a two-dimensional configuration with Euclidean distances approximating the dissimilarities between the Morse codes for digits. This configuration may be examined using the estat config command; see mdsconfig if you want to plot the configuration.

. estat config Configuration in 2-dimensional Euclidean space (principal normalization)

digit1	dim1	dim2
0	0.5690	0.0162
1	0.4561	-0.3384
2	0.0372	-0.5854
3	-0.3878	-0.4516
4	-0.5800	-0.0770
5	-0.5458	-0.0196
6	-0.3960	0.4187
7	-0.0963	0.5901
8	0.3124	0.3862
9	0.6312	0.0608

This configuration is not unique. A translation, a reflection, and an orthonormal rotation of the configuration do not affect the interpoint Euclidean distances. All such transformations are equally reasonable MDS solutions. Thus you should not interpret aspects of these numbers (or of the configuration plot) that are not invariant to these transformations.

We now turn to the three estat subcommands that analyze the MDS residuals, that is, the differences between the disparities or dissimilarities and the matching Euclidean distances. There is a catch here. The raw residuals of MDS are not well behaved. For instance, the sum of the raw residuals is not zero—often it is not even close. The MDS solution does *not* minimize the sum of squares of the raw residuals Mardia, Kent, and Bibby (1979, 406–408). To create reasonable residuals with MDS, the dissimilarities can be transformed to disparities approximating the Euclidean distances. In classical MDS we use a linear transform f, fit by least squares. This is equivalent to Kruskal's Stress1 loss function. The modified residuals are defined as the differences between the linearly transformed dissimilarities and the matching Euclidean distances.

In modern MDS we have three types of transformations from dissimilarities to disparities to choose from: the identity (which does not transform the dissimilarities), a power transformation, and a monotonic transformation.

The three estat subcommands summarize the residuals in different ways. After classical MDS, estat stress displays the Kruskal loss or stress measures for each object and the overall total.

# . estat stress Stress between disparities and Euclidean distances

digit1	Kruskal
0	0.1339
1	0.1255
2	0.1972
3	0.2028
4	0.2040
5	0.2733
6	0.1926
7	0.1921
8	0.1715
9	0.1049
Total	0.1848

Second, after classical or modern MDS, the quantiles of the residuals are available, both overall and for the subgroup of object pairs in which an object is involved.

# . estat quantiles Quantiles of transformed residuals

digit1	N	min	p25	q50	q75	max
0	9	111732	088079	028917	.11202	.220399
1	9	170063	137246	041244	.000571	.11202
2	9	332717	159472	072359	.074999	.234867
3	9	136251	120398	072359	.105572	.365833
4	9	160797	014099	.03845	.208215	.355053
5	9	09971	035357	.176337	.325043	.365833
6	9	137246	113564	075008	.177448	.325043
7	9	332717	170063	124129	.03845	.176337
8	9	186452	134831	041244	.075766	.220399
9	9	160797	104403	088079	064316	030032
Total	90	332717	113564	041244	.105572	.365833

The dissimilarities for the Morse code of digit 5 are fit considerably worse than for all other Morse codes. Digit 5 has the largest Kruskal stress (0.273) and median residual (0.176).

Finally, after classical or modern MDS, estat correlations displays the Pearson and Spearman correlations between the (transformed or untransformed) dissimilarities and the Euclidean distances.

. estat correlations

Correlations of disparities and Euclidean distances

digit1	N	Pearson	Spearman
0	9	0.9510	0.9540
1	9	0.9397	0.7782
2	9	0.7674	0.4017
3	9	0.7922	0.7815
4	9	0.9899	0.9289
5	9	0.9412	0.9121
6	9	0.8226	0.8667
7	9	0.8444	0.4268
8	9	0.8505	0.7000
9	9	0.9954	0.9333
Total	90	0.8602	0.8301

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#### **Predictions**

It is possible to generate variables containing the results from the MDS analysis. MDS operates at two levels: first at the level of the objects and second at the level of relations between the objects or pairs of objects. You can generate variables at both of these levels.

The config option of predict after an MDS requests that the coordinates of the objects in the matching configuration be stored in variables. You may specify as many variables as there are retained dimensions. You may also specify fewer variables. The first variable will store the coordinates from the first dimension. The second variable, if any, will store the coordinates from the second dimension, and so on.

The pairwise() option specifies that a given selection of the pairwise statistics are stored in variables. The statistics available are the disparities, dissimilarities, fitted distances, raw residuals, transformed residuals, and weights. The raw residuals are the difference between dissimilarities and the fitted distances, and the transformed residuals are the difference between the disparities and the fitted distances.

There is a complicating issue. With n objects, there are n(n-1)/2 pairs of objects. So, to store properties of objects, you need n observations, but to store properties of pairs of objects, you need n(n-1)/2 observations. So, where do you store the variables? predict after MDS commands can save the predicted variables in a new dataset. Specify the option saving (filename). Such a dataset will automatically have the appropriate object identification variable or variables.

Sometimes it is also possible to store the variables in the dataset you have in memory: object-level variables in an object-level dataset and pairwise-level variables in a pairwise-level dataset.

After mds you have a dataset in memory in which the observations are associated with the MDS objects. Here you can store object-level variables directly in the dataset in memory. To do so, you just omit the saving() option. Here it is not possible to store the pairwise statistics in the dataset in memory. The pairwise statistics have to be stored in a new dataset.

After mdslong, the dataset in memory is in a pairwise form, so the variables predicted with the option pairwise() can be stored in the dataset in memory. It is, of course, also possible to store the pairwise variables in a new dataset; the choice is yours. With pairwise data in memory, you cannot store the object-level predicted variables into the data in memory; you need to specify the name of a new dataset.

After mdsmat, you always need to save the predicted variables in a new dataset.

# ▶ Example 2: Predictions

Continuing with example 1; the dataset in memory is in long form. Thus we can store the pairwise statistics with the dataset in memory.

- . predict tdissim eudist resid, pairwise
- . list in 1/10

	digit1	digit2	freqsame	sim	tdissim	eudist	resid
1.	2	1	62	.62	.3227682	.4862905	1635224
2.	3	1	16	.16	.957076	.851504	.105572
3.	3	2	59	.59	.3732277	.4455871	0723594
4.	4	1	6	.06	1.069154	1.068583	.0005709
5.	4	2	23	.23	.8745967	.7995979	.0749988
6.	4	3	38	.38	.6841489	.4209922	.2631567
7.	5	1	12	.12	1.002667	1.051398	048731
8.	5	2	8	.08	1.047234	.8123672	.2348665
9.	5	3	27	.27	.8257753	.4599419	.3658335
10.	5	4	56	.56	.4218725	.0668193	.3550532

Because we used mdslong, the object-level statistics must be saved in a file.

- . predict d1 d2, config saving(digitdata)
- . describe digit\* d1 d2 using digitdata

variable name	_	display format	value label	variable label	
digit1	byte float	%9.0g %9.0g		MDS dimension 1	
d2	float	%9.0g		MDS dimension 2	

The information in these variables was already shown with estat config. The dataset created has variables d1 and d2 with the coordinates of the Morse digits on the two retained dimensions and an identification variable digit1. Use merge to add these variables to the data in memory; see [D] merge.

# Stored results

estat correlations stores the following in r():

Matrices

r(R) statistics per object; columns with # of obs., Pearson corr., and Spearman corr.

r(T) overall statistics; # of obs., Pearson corr., and Spearman corr.

estat quantiles stores the following in r():

Macros

r(dtype) adjusted or raw; dissimilarity transformation

Matrices

r(Q) statistics per object; columns with # of obs., min., p25, p50, p75, and max.

r(T) overall statistics; # of obs., min., p25, p50, p75, and max.

estat stress stores the following in r():

Macros

r(dtype) adjusted or raw; dissimilarity transformation

Matrices

r(S) Kruskal's stress/loss measure per object

r(T) 1×1 matrix with the overall Kruskal stress/loss measure

## Methods and formulas

See [MV] mdsmat for information on the methods and formulas for multidimensional scaling.

For classical MDS, let  $D_{ij}$  be the dissimilarity between objects i and j,  $1 \le i, j \le n$ . We assume  $D_{ii} = 0$  and  $D_{ij} = D_{ji}$ . Let  $E_{ij}$  be the Euclidean distance between rows i and j of the matching configuration  $\mathbf{Y}$ . In classical MDS,  $\mathbf{D} - \mathbf{E}$  is not a well-behaved residual matrix. We follow the approach used in metric and nonmetric MDS to transform  $D_{ij}$  to "optimally match"  $E_{ij}$ , with  $\widehat{D}_{ij} = a + bD_{ij}$ , where a and b are chosen to minimize the residual sum of squares. This is a simple regression problem and is equivalent to minimizing Kruskal's stress measure (Kruskal 1964; Cox and Cox 2001, 63)

$$\mathrm{Kruskal}(\widehat{\mathbf{D}},\mathbf{E}) = \left\{ \frac{\sum (E_{ij} - \widehat{D}_{ij})^2}{\sum E_{ij}^2} \right\}^{1/2}$$

with summation over all pairs (i, j). We call the  $\widehat{D}_{ij}$  the adjusted or transformed dissimilarities. If the transformation step is skipped by specifying the option notransform, we set  $\widehat{D}_{ij} = D_{ij}$ .

In estat stress, the decomposition of Kruskal's stress measure over the objects is displayed. Kruskal $(\widehat{\mathbf{D}}, \mathbf{E})_i$  is defined analogously with summation over all  $j \neq i$ .

For modern MDS, the optimal transformation to disparities,  $f(\mathbf{D}) \to \widehat{\mathbf{D}}$ , is calculated during the estimation. See [MV] **mdsmat** for details. For transform(power), the power is stored in e(alpha). For transform(monotonic), the disparities themselves are stored as e(Disparities).

# References

Borg, I., and P. J. F. Groenen. 2005. Modern Multidimensional Scaling: Theory and Applications. 2nd ed. New York: Springer.

Cox, T. F., and M. A. A. Cox. 2001. Multidimensional Scaling. 2nd ed. Boca Raton, FL: Chapman & Hall/CRC.

Kruskal, J. B. 1964. Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis. *Psychometrika* 29: 1–27.

Mardia, K. V., J. T. Kent, and J. M. Bibby. 1979. Multivariate Analysis. London: Academic Press.

Also see References in [MV] mdsmat.

# Also see

- [MV] mds Multidimensional scaling for two-way data
- [MV] mdslong Multidimensional scaling of proximity data in long format
- [MV] mdsmat Multidimensional scaling of proximity data in a matrix
- [MV] mds postestimation plots Postestimation plots for mds, mdsmat, and mdslong
- [MV] screeplot Scree plot
- [U] 20 Estimation and postestimation commands

## Title

mds postestimation plots — Postestimation plots for mds, mdsmat, and mdslong

Postestimation commands mdsconfig mdsshepard Remarks and examples References Also see

## Postestimation commands

The following postestimation commands are of special interest after mds, mdslong, and mdsmat:

Command	Description
mdsconfig	plot of approximating configuration
mdsshepard	Shepard diagram

For more information on these commands, see below. Also see [MV] mds postestimation.

# mdsconfig

## **Description for mdsconfig**

mdsconfig produces a plot of the approximating Euclidean configuration. By default, dimensions 1 and 2 are plotted.

# Menu for mdsconfig

 ${\it Statistics} > {\it Multivariate analysis} > {\it Multidimensional scaling (MDS)} > {\it Postestimation} > {\it Approximating configuration plot}$ 

# Syntax for mdsconfig

mdsconfig [, options]

options	Description
Main	
<pre>dimensions(# #)</pre>	two dimensions to be displayed; default is dimensions(2 1)
xnegate	negate data relative to the $x$ axis
ynegate	negate data relative to the $y$ axis
<u>auto</u> aspect	adjust aspect ratio on the basis of the data; default aspect ratio is 1
<pre>maxlength(#)</pre>	maximum number of characters used in marker labels
cline_options	affect rendition of the lines connecting points
marker_options	change look of markers (color, size, etc.)
marker_label_options	change look or position of marker labels
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by () documented in [G-3] twoway_options

### Options for mdsconfig

Main

dimensions (##) identifies the dimensions to be displayed. For instance, dimensions (3 2) plots the third dimension (vertically) versus the second dimension (horizontally). The dimension number cannot exceed the number of extracted dimensions. The default is dimensions (2 1).

xnegate specifies that the data be negated relative to the x axis.

ynegate specifies that the data be negated relative to the y axis.

autoaspect specifies that the aspect ratio be automatically adjusted based on the range of the data to be plotted. This option can make some plots more readable. By default, mdsconfig uses an aspect ratio of one, producing a square plot. Some plots will have little variation in the y-axis direction, and use of the utoaspect option will better fill the available graph space while preserving the equivalence of distance in the x and y axes.

As an alternative to autoaspect, the  $twoway\_option$  aspectratio() can be used to override the default aspect ratio. mdsconfig accepts the aspectratio() option as a suggestion only and will override it when necessary to produce plots with balanced axes; that is, distance on the x axis equals distance on the y axis.

*twoway\_options*, such as xlabel(), xscale(), ylabel(), and yscale(), should be used with caution. These *axis\_options* are accepted but may have unintended side effects on the aspect ratio. See [G-3] *twoway\_options*.

maxlength(#) specifies the maximum number of characters for object names used to mark the
points; the default is maxlength(12).

cline\_options affect the rendition of the lines connecting the plotted points; see [G-3] cline\_options.
If you are drawing connected lines, the appearance of the plot depends on the sort order of the data.

marker\_options affect the rendition of the markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] marker\_options.

marker\_label\_options specify if and how the markers are to be labeled; see [G-3] marker\_label\_options.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These
include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk
(see [G-3] saving\_option). See autoaspect above for a warning against using options such as
xlabel(), xscale(), ylabel(), and yscale().

# mdsshepard

### **Description for mdsshepard**

mdsshepard produces a Shepard diagram of the disparities against the Euclidean distances. Ideally, the points in the plot should be close to the y=x line. Optionally, separate plots are generated for each "row" (value of id()).

### Menu for mdsshepard

Statistics > Multivariate analysis > Multidimensional scaling (MDS) > Postestimation > Shepard diagram

# Syntax for mdsshepard

mdsshepard [, options]

options	Description
Main	
<u>notrans</u> form	use dissimilarities instead of disparities
<u>auto</u> aspect	adjust aspect ratio on the basis of the data; default aspect ratio is 1
separate	draw separate Shepard diagrams for each object
marker_options	change look of markers (color, size, etc.)
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by () documented in [G-3] twoway_options
<pre>byopts(by_option)</pre>	affect the rendition of combined graphs; separate only

# **Options for mdsshepard**

Main

notransform uses dissimilarities instead of disparities, that is, suppresses the transformation of the dissimilarities.

autoaspect specifies that the aspect ratio be automatically adjusted based on the range of the data to be plotted. By default, mdsshepard uses an aspect ratio of one, producing a square plot.

See the description of the autoaspect option of mdsconfig for more details.

separate displays separate plots of each value of the ID variable. This may be time consuming if the number of distinct ID values is not small.

marker\_options affect the rendition of the markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] marker\_options.

```
Y axis, X axis, Titles, Legend, Overall
```

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option). See the autoaspect option of mdsconfig for a warning against using options such as xlabel(), xscale(), ylabel(), and yscale().

byopts(by\_option) is documented in [G-3] by\_option. This option affects the appearance of the combined graph and is allowed only with the separate option.

# Remarks and examples

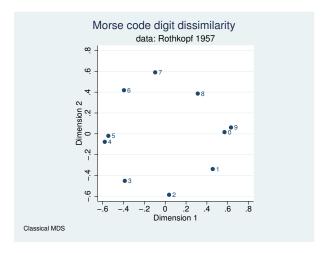
The matching configuration plot and Shepard diagram are easily obtained after an MDS analysis.

### Example 1: configuration plot

By default, mds, mdsmat, and mdslong display the MDS matching configuration plot. If you want to exercise control over the graph, you can specify the noplot option of mds, mdsmat, or mdslong and then use the mdsconfig postestimation graph command.

Continuing with example 1 of [MV] **mds postestimation**, we produce a configuration plot with an added title and subtitle.

- . use http://www.stata-press.com/data/r14/morse\_long
  (Morse data (Rothkopf 1957))
- . generate sim = freqsame/100
- . mdslong sim, id(digit1 digit2) s2d(standard) noplot (output omitted)
- . mdsconfig, title(Morse code digit dissimilarity) subtitle(data: Rothkopf 1957)



The plot has an aspect ratio of one so that 1 unit on the horizontal dimension equals 1 unit on the vertical dimension. Thus the "straight-line" distance in the plot is really (proportional to) the Euclidean distance between the points in the configuration and hence approximates the dissimilarities between the objects—here the Morse codes for digits.

# Example 2: Shepard diagram

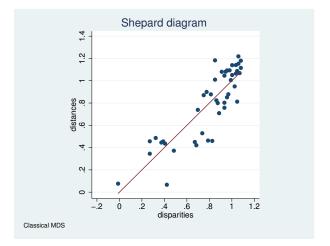
A second popular plot for MDS is the Shepard diagram. This is a plot of the Euclidean distances in the matching configuration against the "observed" dissimilarities. As we explained before, in classical MDS a linear transformation is applied to the dissimilarities to fit the Euclidean distances as close

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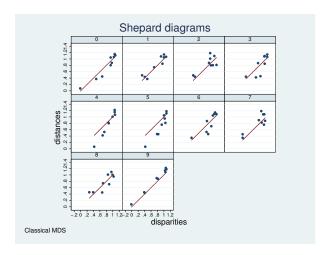
as possible (in the least-squares sense). In modern MDS the transformation may be the identity (no transformation), a power function, or a monotonic function. A Shepard diagram is a plot of the n(n-1)/2 transformed dissimilarities, called disparities, against the Euclidean distances.

. mdsshepard



If the Euclidean configuration is close to the disparities between the objects, all points would be close to the y=x line. Deviations indicate lack of fit. To simplify the diagnosis of whether there are specific objects that are poorly represented, Shepard diagrams can be produced for each object separately. Such plots consist of n small plots with n-1 points each, namely, the disparities and Euclidean distances to all other objects.

. mdsshepard, separate (mdsshepard is producing a separate plot for each obs; this may take a while)



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Other examples of mdsconfig are found in [MV] mds, [MV] mdslong, and [MV] mdsmat.

Roger Newland Shepard (1929–) was born in Palo Alto, California, earned degrees at Stanford and Yale, and worked at Bell Labs and Harvard before returning to Stanford in 1968. One of the world's leading psychologists and cognitive scientists, he has worked on perception, mental imagery, representation, learning, and generalization. Shepard is noted within statistical science primarily for his work on nonmetric multidimensional scaling. He is a member of the U.S. National Academy of Sciences and a recipient of the National Medal of Science.

### References

See References in [MV] mds.

### Also see

```
[MV] mds — Multidimensional scaling for two-way data
```

[MV] mdslong — Multidimensional scaling of proximity data in long format

[MV] mdsmat — Multidimensional scaling of proximity data in a matrix

[MV] mds postestimation — Postestimation tools for mds, mdsmat, and mdslong

[MV] **screeplot** — Scree plot

### **Title**

mdslong — Multidimensional scaling of proximity data in long format

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

mdslong performs multidimensional scaling (MDS) for two-way proximity data in long format with an explicit measure of similarity or dissimilarity between objects. mdslong performs classical metric MDS as well as modern metric and nonmetric MDS.

For MDS with two-way proximity data in a matrix, see [MV] **mdsmat**. If you are looking for MDS on a dataset, based on dissimilarities between observations over variables, see [MV] **mds**.

#### **Quick start**

Classical multidimensional scaling based on dissimilarities in variable d between subjects identified by variables i and j

```
mdslong d, id(i j)
```

As above, but suppress the MDS configuration plot and use 3 dimensions for the approximating configuration

```
mdslong d, id(i j) noplot dimension(3)
```

Modern multidimensional scaling

```
mdslong d, id(i j) method(modern)
```

As above, but with Sammon mapping loss criterion and Procrustes rotation toward the classical solution

```
mdslong d, id(i j) loss(sammon) normalize(classical)
```

Nonmetric modern multidimensional scaling

```
mdslong d, id(i j) method(nonmetric)
```

#### Menu

Statistics > Multivariate analysis > Multidimensional scaling (MDS) > MDS of proximity-pair data

# **Syntax**

```
mdslong depvar [if] [in] [weight], id(var<sub>1</sub> var<sub>2</sub>) [options]
 options
                           Description
Model
*id(var_1 var_2)
                           identify comparison pairs (object<sub>1</sub>, object<sub>2</sub>)
 method(method)
                           method for performing MDS
 loss(loss)
                           loss function
 transform(tfunction)
                           permitted transformations of dissimilarities
 normalize(norm)
                           normalization method; default is normalize(principal)
                           convert similarity to dissimilarity: \operatorname{dissim}_{ij} = \sqrt{\sin_{ij} + \sin_{jj} - 2\sin_{ij}};
 s2d(standard)
                              the default
 s2d(oneminus)
                           convert similarity to dissimilarity: dissim_{ij} = 1 - sim_{ij}
                           correct problems in proximity information
 force
 dimension(#)
                           configuration dimensions; default is dimension(2)
 addconstant
                           make distance matrix positive semidefinite (classical MDS only)
Reporting
                           maximum number of eigenvalues to display; default is neigen(10)
 neigen(#)
                              (classical MDS only)
                           display table with configuration coordinates
 config
 noplot
                           suppress configuration plot
Minimization
 initialize(initopt)
                           start with configuration given in initopt
 tolerance(#)
                           tolerance for configuration matrix; default is tolerance(1e-4)
 ltolerance(#)
                           tolerance for loss criterion; default is ltolerance(1e-8)
 iterate(#)
                           perform maximum # of iterations; default is iterate(1000)
 protect(#)
                           perform # optimizations and report best solution; default is protect(1)
                           suppress the iteration log
 nolog
                           display current configuration in iteration log
 trace
                           display current gradient matrix in iteration log
 gradient
 sdprotect(#)
                           advanced; see description below
```

by and statsby are allowed; see [U] 11.1.10 Prefix commands.

aweights and fweights are allowed for methods modern and nonmetric; see [U] 11.1.6 weight.

The maximum number of compared objects allowed is the maximum matrix size; see [R] matsize. sdprotect(#) does not appear in the dialog box.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

<sup>\*</sup> id(var<sub>1</sub> var<sub>2</sub>) is required.

#### 506 mdslong — Multidimensional scaling of proximity data in long format

method	Description
<u>c</u> lassical	classical MDS; default if neither loss() nor transform() is specified
modern	<pre>modern MDS; default if loss() or transform() is specified; except when loss(stress) and transform(monotonic) are specified</pre>
<u>n</u> onmetric	nonmetric (modern) MDS; default when loss(stress) and transform(monotonic) are specified
loss	Description
stress	stress criterion, normalized by distances; the default
<u>nstr</u> ess	stress criterion, normalized by disparities
<u>sstr</u> ess	squared stress criterion, normalized by distances
<u>nsst</u> ress	squared stress criterion, normalized by disparities
<u>stra</u> in	strain criterion (with transform(identity) is equivalent to classical MDS)
<u>sam</u> mon	Sammon mapping
tfunction	Description
<u>i</u> dentity	no transformation; disparity = dissimilarity; the default
$\underline{\mathbf{p}}$ ower	power $\alpha$ : disparity = dissimilarity $^{\alpha}$
<u>m</u> onotonic	<pre>weakly monotonic increasing functions (nonmetric scaling); only   with loss(stress)</pre>
norm	Description
principal	principal orientation; location = 0; the default
<u>c</u> lassical	Procrustes rotation toward classical solution
$\underline{\underline{t}}$ arget(matname)[, copy]	Procrustes rotation toward <i>matname</i> ; ignore naming conflicts
	if copy is specified
initopt	Description
<u>c</u> lassical	start with classical solution; the default
$\underline{\mathbf{r}}$ andom $[$ (#) $]$	start at random configuration, setting seed to #
<u>from(matname)</u> , copy	start from matname; ignore naming conflicts if copy is specified

# **Options**

Model

 $id(var_1 \ var_2)$  is required. The pair of variables  $var_1$  and  $var_2$  should uniquely identify comparisons.  $var_1$  and  $var_2$  are string or numeric variables that identify the objects to be compared.  $var_1$  and  $var_2$  should be of the same data type; if they are value labeled, they should be labeled with the same value label. Using value-labeled variables or string variables is generally helpful in identifying the points in plots and tables.

Example data layout for mdslong proxim, id(i1 i2).

proxim	i1	i2
7	1	2
10	1	3
12	1	4
4	2	3
6	2	4
3	3	4

If you have multiple measurements per pair, we suggest that you specify the mean of the measures as the proximity and the inverse of the variance as the weight.

method(method) specifies the method for MDS.

method(classical) specifies classical metric scaling, also known as "principal coordinates analysis" when used with Euclidean proximities. Classical MDS obtains equivalent results to modern MDS with loss(strain) and transform(identity) without weights. The calculations for classical MDS are fast; consequently, classical MDS is generally used to obtain starting values for modern MDS. If the options loss() and transform() are not specified, mds computes the classical solution, likewise if method(classical) is specified loss() and transform() are not allowed.

method(modern) specifies modern scaling. If method(modern) is specified but not loss() or transform(), then loss(stress) and transform(identity) are assumed. All values of loss() and transform() are valid with method(modern).

method(nonmetric) specifies nonmetric scaling, which is a type of modern scaling. If
method(nonmetric) is specified, loss(stress) and transform(monotonic) are assumed.
Other values of loss() and transform() are not allowed.

loss (loss) specifies the loss criterion.

loss(stress) specifies that the stress loss function be used, normalized by the squared Euclidean distances. This criterion is often called Kruskal's stress-1. Optimal configurations for
loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration
paths may differ. loss(stress) is the default.

loss(nstress) specifies that the stress loss function be used, normalized by the squared disparities, that is, transformed dissimilarities. Optimal configurations for loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration paths may differ.

loss(sstress) specifies that the squared stress loss function be used, normalized by the fourth power of the Euclidean distances.

loss(nsstress) specifies that the squared stress criterion, normalized by the fourth power of the disparities (transformed dissimilarities) be used.

loss(strain) specifies the strain loss criterion. Classical scaling is equivalent to loss(strain) and transform(identity) but is computed by a faster noniterative algorithm. Specifying loss(strain) still allows transformations.

loss(sammon) specifies the Sammon (1969) loss criterion.

transform(tfunction) specifies the class of allowed transformations of the dissimilarities; transformed dissimilarities are called disparities.

transform(identity) specifies that the only allowed transformation is the identity; that is, disparities are equal to dissimilarities. transform(identity) is the default.

transform(power) specifies that disparities are related to the dissimilarities by a power function,

disparity = dissimilarity
$$^{\alpha}$$
,  $\alpha > 0$ 

transform(monotonic) specifies that the disparities are a weakly monotonic function of the dissimilarities. This is also known as nonmetric MDS. Tied dissimilarities are handled by the primary method; that is, ties may be broken but are not necessarily broken. transform(monotonic) is valid only with loss(stress).

normalize(norm) specifies a normalization method for the configuration. Recall that the location and orientation of an MDS configuration is not defined ("identified"); an isometric transformation (that is, translation, reflection, or orthonormal rotation) of a configuration preserves interpoint Euclidean distances.

normalize(principal) performs a principal normalization, in which the configuration columns have zero mean and correspond to the principal components, with positive coefficient for the observation with lowest value of id(). normalize(principal) is the default.

normalize(classical) normalizes by a distance-preserving Procrustean transformation of the configuration toward the classical configuration in principal normalization; see [MV] **procrustes**. normalize(classical) is not valid if method(classical) is specified.

normalize(target(matname) [, copy]) normalizes by a distance-preserving Procrustean transformation toward matname; see [MV] **procrustes**. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is also specified.

Note on normalize(classical) and normalize(target()): the Procrustes transformation comprises any combination of translation, reflection, and orthonormal rotation—these transformations preserve distance. Dilation (uniform scaling) would stretch distances and is not applied. However, the output reports the dilation factor, and the reported Procrustes statistic is for the dilated configuration.

s2d(standard | oneminus) specifies how similarities are converted into dissimilarities. By default, the command assumes dissimilarity data. Specifying s2d() indicates that your proximity data are similarities.

Dissimilarity data should have zeros on the diagonal (that is, an object is identical to itself) and nonnegative off-diagonal values. Dissimilarities need not satisfy the triangular inequality,  $D(i,j)^2 \leq D(i,h)^2 + D(h,j)^2$ . Similarity data should have ones on the diagonal (that is, an object is identical to itself) and have off-diagonal values between zero and one. In either case, proximities should be symmetric. See option force if your data violate these assumptions.

The available s2d() options, standard and oneminus, are defined as follows:

standard dissim
$$_{ij} = \sqrt{\sin_{ii} + \sin_{jj} - 2\sin_{ij}} = \sqrt{2(1 - \sin_{ij})}$$
 oneminus dissim $_{ij} = 1 - \sin_{ij}$ 

s2d(standard) is the default.

s2d() should be specified only with measures in similarity form.

force corrects problems with the supplied proximity information. In the long format used by mdslong, multiple measurements on (i, j) may be available. Including both (i, j) and (j, i) would be treated as multiple measurements. This is an error, even if the measures are identical. Option force uses

the mean of the measurements. force also resolves problems on the diagonal, that is, comparisons of objects with themselves; these should have zero dissimilarity or unit similarity. force does not resolve incomplete data, that is, pairs (i,j) for which no measurement is available. Out-of-range values are also not fixed.

- dimension(#) specifies the dimension of the approximating configuration. The default is dimension(2), and # should not exceed the number of positive eigenvalues of the centered distance matrix.
- addconstant specifies that if the double-centered distance matrix is not positive semidefinite (psd), a constant should be added to the squared distances to make it psd and, hence, Euclidean. This option is allowed with classical MDS only.

Reporting

- neigen(#) specifies the number of eigenvalues to be included in the table. The default is neigen(10). Specifying neigen(0) suppresses the table. This option is allowed with classical MDS only.
- config displays the table with the coordinates of the approximating configuration. This table may also be displayed using the postestimation command estat config; see [MV] mds postestimation.
- noplot suppresses the graph of the approximating configuration. The graph can still be produced later via mdsconfig, which also allows the standard graphics options for fine-tuning the plot; see [MV] mds postestimation plots.

Minimization

These options are available only with method(modern) or method(nonmetric):

initialize (initopt) specifies the initial values of the criterion minimization process.

- initialize(classical), the default, uses the solution from classical metric scaling as initial
   values. With protect(), all but the first run start from random perturbations from the classical
   solution. These random perturbations are independent and normally distributed with standard
   error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.
   initialize(classical) is the default.
- initialize(random) starts an optimization process from a random starting configuration. These random configurations are generated from independent normal distributions with standard error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities. The means of the configuration are irrelevant in MDS.
- initialize(from(matname) [, copy]) sets the initial value to matname. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is specified. With protect(), the second-to-last runs start from random perturbations from matname. These random perturbations are independent normal distributed with standard error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.
- tolerance(#) specifies the tolerance for the configuration matrix. When the relative change in the configuration from one iteration to the next is less than or equal to tolerance(), the tolerance() convergence criterion is satisfied. The default is tolerance(1e-4).
- ltolerance(#) specifies the tolerance for the fit criterion. When the relative change in the fit
   criterion from one iteration to the next is less than or equal to ltolerance(), the ltolerance()
   convergence is satisfied. The default is ltolerance(1e-8).

Both the tolerance() and ltolerance() criteria must be satisfied for convergence.

iterate(#) specifies the maximum number of iterations. The default is iterate(1000).

protect(#) requests that # optimizations be performed and that the best of the solutions be reported.
The default is protect(1). See option initialize() on starting values of the runs. The output
contains a table of the return code, the criterion value reached, and the seed of the random number
used to generate the starting value. Specifying a large number, such as protect(50), provides
reasonable insight whether the solution found is a global minimum and not just a local minimum.

If any of the options log, trace, or gradient is also specified, iteration reports will be printed for each optimization run. Beware: this option will produce a lot of output.

nolog suppresses the iteration log, showing the progress of the minimization process.

trace displays the configuration matrices in the iteration report. Beware: this option may produce a lot of output.

gradient displays the gradient matrices of the fit criterion in the iteration report. Beware: this option may produce a lot of output.

The following option is available with mdslong but is not shown in the dialog box:

sdprotect(#) sets a proportionality constant for the standard deviations of random configurations
 (init(random)) or random perturbations of given starting configurations (init(classical) or
 init(from())). The default is sdprotect(1).

# Remarks and examples

Remarks are presented under the following headings:

Introduction
Proximity data in long format
Modern nonmetric MDS

#### Introduction

Multidimensional scaling (MDS) is a dimension-reduction and visualization technique. Dissimilarities (for instance, Euclidean distances) between observations in a high-dimensional space are represented in a lower-dimensional space (typically two dimensions) so that the Euclidean distance in the lower-dimensional space approximates the dissimilarities in the higher-dimensional space. See Kruskal and Wish (1978) for a brief nontechnical introduction to MDS. Young and Hamer (1987) and Borg and Groenen (2005) are more advanced textbook-sized treatments.

mdslong performs MDS on data in long format. depvar specifies proximity data in either dissimilarity or similarity form. The comparison pairs are identified by two variables specified in the required option id(). Exactly 1 observation with a nonmissing depvar should be included for each pair (i,j). Pairs are unordered; you do not include observations for both (i,j) and (j,i). Observations for comparisons of objects with themselves (i,i) are optional. See option force if your data violate these assumptions.

When you have multiple independent measurements of the dissimilarities, you may specify the mean of these dissimilarity measurements as the combined measurement and specify 1/(#of measurements) or 1/variance(measurements) as weights. For more discussion of weights in MDS, we refer to Borg and Groenen (2005, sec. 11.3). Weights should be irreducible; that is, it is not possible to split the objects into disjointed groups with all intergroup weights 0.

In some applications, the similarity or dissimilarity of objects is defined by the researcher in terms of variables (attributes) measured on the objects. If you need MDS of this form, you should continue by reading [MV] mds.

Often, however, proximities—that is, similarities or dissimilarities—are measured directly. For instance, psychologists studying the similarities or dissimilarities in a set of stimuli—smells, sounds, faces, concepts, etc.—may have subjects rate the dissimilarity of pairs of stimuli. Linguists have subjects rate the similarity or dissimilarity of pairs of dialects. Political scientists have subjects rate the similarity or dissimilarity of political parties or candidates for political office. In other fields, relational data are studied that may be interpreted as proximities in a more abstract sense. For instance, sociologists study interpersonal contact frequencies in groups ("social networks"); these measures are sometimes interpreted in terms of similarities.

A wide variety of MDS methods have been proposed. mdslong performs classical and modern scaling. Classical scaling has its roots in Young and Householder (1938) and Torgerson (1952). MDS requires complete and symmetric dissimilarity interval-level data. To explore modern scaling, see Borg and Groenen (2005). Classical scaling results in an eigen decomposition, whereas modern scaling is accomplished by the minimization of a loss function. Consequently, eigenvalues are not available after modern MDS.

Computing the classical solution is straightforward, but with modern MDS the minimization of the loss criteria over configurations is a high-dimensional problem that is easily beset by convergence to local minimums. mdslong provides options to control the minimization process 1) by allowing the user to select the starting configuration and 2) by selecting the best solution among multiple minimization runs from random starting configurations.

# Proximity data in long format

One format for proximity data is called the "long format", with an observation recording the dissimilarity  $d_{ij}$  of the "objects" i and j. This requires three variables: one variable to record the dissimilarities and two variables to identify the comparison pair. The MDS command mdslong requires

- Complete data without duplicates: there is exactly 1 observation for each combination (i, j) or (j, i).
- Optional diagonal: you may, but need not, specify dissimilarities for the reflexive pairs (i, i). If you do, you need not supply values for all (i, i).

# Example 1

We illustrate the use of mdslong with a popular dataset from the MDS literature. Rothkopf (1957) had 598 subjects listen to pairs of Morse codes for the 10 digits and for the 26 letters, recording for each pair of codes the percentage of subjects who declared the codes to be the same. The data on the 10 digits are reproduced in Mardia, Kent, and Bibby (1979, 395).

. use http://www.stata-press.com/data/r14/morse\_long
(Morse data (Rothkopf 1957))

. list in 1/10

	digit1	digit2	freqsame
1. 2. 3. 4.	2 3 3 4	1 1 2 1	62 16 59 6
5.	4	2	23
6. 7. 8. 9.	4 5 5 5 5	3 1 2 3 4	38 12 8 27 56

Sixty-two percent of the subjects declare that the Morse codes for 1 and 2 are the same, 16% declare that 1 and 3 are the same, 59% declare 2 and 3 to be the same, etc. We may think that these percentages are similarity measures between the Morse codes: the more similar two Morse codes, the higher the percentage is of subjects who do not distinguish them. The reported percentages suggest, for example, that 1 and 2 are similar to approximately the same extent as 2 and 3, whereas 1 and 3 are much less similar. This is the kind of relationship you would expect with data that can be adequately represented with MDS.

We transform our data to a zero-to-one scale.

. generate sim = freqsame/100

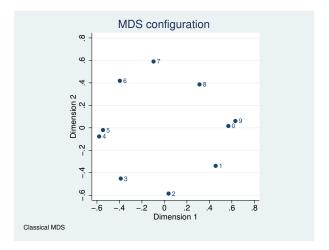
and invoke mdslong on sim, specifying that the proximity variable sim be interpreted as similarities, and we use option s2d(standard) to convert to dissimilarities by using the standard conversion.

. mdslong sim, id(digit1 digit2) s2d(standard)

Classical metric multidimensional scaling similarity variable: sim in long format dissimilarity: sqrt(2(1-similarity))

			Number	of	obs		=	10
Eigenvalues > 0	=	9	Mardia	fit	measure	1	=	0.5086
Retained dimensions	=	2	Mardia	fit	measure	2	=	0.7227

		abs(eige	nvalue)	(eigenv	ralue)^2
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.
1	1.9800226	30.29	30.29	49.47	49.47
2	1.344165	20.57	50.86	22.80	72.27
3	1.063133	16.27	67.13	14.26	86.54
4	.66893922	10.23	77.36	5.65	92.18
5	.60159396	9.20	86.56	4.57	96.75
6	.42722301	6.54	93.10	2.30	99.06
7	.21220785	3.25	96.35	0.57	99.62
8	.1452025	2.22	98.57	0.27	99.89
9	.09351288	1.43	100.00	0.11	100.00



The two-dimensional representation provides a reasonable, but certainly not impressive, fit to the data. The plot itself is interesting, though, with the digits being roughly 45 degrees apart, except for the pairs (0,9) and (4,5), which are mapped almost at the same locations. Interpretation is certainly helped if you see the circular structure in the Morse codes.

digit	morse code
1	
2	
3	
4	
5	
6	
7	
8	
9	
0	

4

#### Example 2

You might have your data in wide instead of long format. The Morse code dataset in wide format has 10 observations, 10 data variables d1, ..., d9, d0, and one case identifier.

. use http://www.stata-press.com/data/r14/morse\_wide, clear (Morse data (Rothkopf 1957))

. describe

Contains data from http://www.stata-press.com/data/r14/morse\_wide.dta obs: 10 Morse data (Rothkopf 1957)

vars: 11 size: 110

14 Feb 2014 20:28 (\_dta has notes)

variable name	storage type	display format	value label	variable label
digit	byte	%9.0g		
d1	byte	%9.0g		
d2	byte	%9.0g		
d3	byte	%9.0g		
d4	byte	%9.0g		
d5	byte	%9.0g		
d6	byte	%9.0g		
d7	byte	%9.0g		
d8	byte	%9.0g		
d9	byte	%9.0g		
d0	byte	%9.0g		

Sorted by:

. list

	digit	d1	d2	d3	d4	d5	d6	d7	d8	d9	d0
1.	1	84	62	16	6	12	12	20	37	57	52
2.	2	62	89	59	23	8	14	25	25	28	18
3.	3	16	59	86	38	27	33	17	16	9	9
4.	4	6	23	38	89	56	34	24	13	7	7
5.	5	12	8	27	56	90	30	18	10	5	5
6.	6	12	14	33	34	30	86	65	22	8	18
7.	7	20	25	17	24	18	65	85	65	31	15
8.	8	37	25	16	13	10	22	65	88	58	39
9.	9	57	28	9	7	5	8	31	58	91	79
10.	0	52	18	9	7	5	18	15	39	79	94

Stata does not provide an MDS command to deal directly with the wide format because it is easy to convert the wide format into the long format with the reshape command; see [D] reshape.

. reshape long d, i(digit) j(other)
(note: j = 0 1 2 3 4 5 6 7 8 9)

Data	wide	->	long	
Number of obs.	10	->	100	
Number of variables	11	->	3	
<pre>j variable (10 values) xij variables:</pre>		->	other	
	d0 d1 d9	->	d	

Now our data are in long format, and we can use mdslong to obtain a MDS analysis.

```
. generate sim = d/100
. mdslong sim, id(digit other) s2d(standard) noplot
objects should have unit similarity to themselves
r(198);
```

mdslong complains. The wide data—and hence also the long data that we now have—also contain the frequencies in which two identical Morse codes were recognized as the same. This is not 100%. Auditive memory is not perfect, posing a problem for the standard MDS model. We can solve this by ignoring the diagonal observations:

```
. mdslong ... if digit != other ...
```

We may also specify the force option. The force option will take care of a problem that has not yet surfaced, namely, that mdslong requires 1 observation for each pair (i, j). In the long data as now created, we have duplicates observations (i, j) and (j, i). force will symmetrize the proximity information, but it will not deal with multiple measurements in general; having 2 or more observations for (i, j) is an error. If you have multiple measurements, you may average the measurements and use weights.

```
. mdslong sim, id(digit other) s2d(standard) force noplot
Classical metric multidimensional scaling
    similarity variable: sim in long format
          dissimilarity: sqrt(2(1-similarity))
```

			Number	of obs	=	= 10
Eigenvalues > 0	=	9	Mardia	fit measure	1 =	0.5086
Retained dimensions	=	2	Mardia	fit measure	2 =	0.7227

		abs(eigenvalue)				
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.	
1	1.9800226	30.29	30.29	49.47	49.47	
2	1.344165	20.57	50.86	22.80	72.27	
3	1.063133	16.27	67.13	14.26	86.54	
4	.66893922	10.23	77.36	5.65	92.18	
5	.60159396	9.20	86.56	4.57	96.75	
6	.42722301	6.54	93.10	2.30	99.06	
7	.21220785	3.25	96.35	0.57	99.62	
8	.1452025	2.22	98.57	0.27	99.89	
9	.09351288	1.43	100.00	0.11	100.00	

The output produced by mdslong here is identical to what we saw earlier.

1

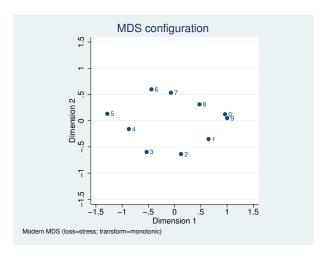
#### Modern nonmetric MDS

Unlike classical MDS, modern MDS is calculated via the minimization of the loss function. Eigenvalues are no longer calculated. We look at nonmetric MDS, which is a type of modern MDS in which the transformation from distances to disparities is not an identifiable function as in modern metric MDS but is instead a general monotonic function.

#### Example 3

We return to the Rothkopf (1957) Morse codes in long format. When we specify method(nonmetric), we assume loss(stress) and transform(monotonic).

```
. use http://www.stata-press.com/data/r14/morse_long, clear
(Morse data (Rothkopf 1957))
. generate sim = freqsame/100
. mdslong sim, id(digit1 digit2) s2d(standard) meth(nonmetric)
(loss(stress) assumed)
(transform(monotonic) assumed)
Iteration 1t:
                stress =
                           .14719847
Iteration 1c:
                stress =
                          .11378737
 (output omitted)
Iteration 89t:
                 stress = .07228281
Iteration 89c:
                 stress =
                           .07228281
Modern multidimensional scaling
    similarity variable: sim in long format
          dissimilarity: sqrt(2(1-similarity))
    Loss criterion: stress = raw_stress/norm(distances)
    Transformation: monotonic (nonmetric)
                                                  Number of obs
                                                                              10
                                                  Dimensions
                                                                               2
                                                                          0.0723
    Normalization: principal
                                                  Loss criterion
```



Each iteration has two steps associated with it. The two parts to each iteration consist of modifying the transformation (the T-step) and modifying the configuration (the C-step). If the transform(identity) option had been used, there would not be a T-step. In the iteration log, you see these as *Iteration 1t* and *Iteration 1c*. The rest of the output from modern MDS is explained in [MV] mds.

Although there is a resemblance between this graph and the first graph, the points are not as circular or as evenly spaced as they are in the first example, and a great deal more distance is seen between points 4 and 5. Nonmetric MDS depends only on the ordinal properties of the data and admits transformations that may radically change the appearance of the configuration.

After mdslong, all MDS postestimation tools are available. For instance, you may analyze residuals with estat quantile, you may produce a Shepard diagram, etc.; see [MV] mds postestimation and [MV] mds postestimation plots.

### Stored results

mdslong stores the following in e():

```
e(N)
                          number of underlying observations
                          number of dimensions in the approximating configuration
    e(p)
    e(np)
                          number of strictly positive eigenvalues
                          constant added to squared dissimilarities to force positive semidefiniteness
    e(addcons)
                          Mardia measure 1
    e(mardia1)
    e(mardia2)
                          Mardia measure 2
    e(critval)
                          loss criterion value
                          number of pairs with positive weights
    e(npos)
    e(wsum)
                          sum of weights
    e(alpha)
                          parameter of transform(power)
    e(ic)
                          iteration count
    e(rc)
                          return code
                          1 if converged, 0 otherwise
    e(converged)
Macros
    e(cmd)
                          mdslong
    e(cmdline)
                          command as typed
                          classical or modern MDS method
    e(method)
    e(method2)
                          nonmetric, if method(nonmetric)
    e(loss)
                          loss criterion
                          description loss criterion
    e(losstitle)
    e(tfunction)
                          identity, power, or monotonic, transformation function
    e(transftitle)
                          description of transformation
    e(id)
                          two ID variable names identifying compared object pairs
    e(idtype)
                          int or str; type of id() variable
    e(duplicates)
                          1 if duplicates in id(), 0 otherwise
    e(labels)
                          labels for ID categories
    e(mxlen)
                          maximum length of category labels
    e(depvar)
                          dependent variable containing dissimilarities
                          similarity or dissimilarity; type of proximity data
    e(dtype)
    e(s2d)
                          standard or oneminus (when e(dtype) is similarity)
                          weight type
    e(wtype)
    e(wexp)
                          weight expression
                          1 if eigenvalues are distinct, 0 otherwise
    e(unique)
                          initialization method
    e(init)
                          initial random-number state used for init(random)
    e(irngstate)
    e(rngstate)
                          random-number state for solution
    e(norm)
                          normalization method
    e(targetmatrix)
                          name of target matrix for normalize(target)
                          nob noV for modern or nonmetric MDS; nob noV eigen for classical MDS
    e(properties)
    e(estat_cmd)
                          program used to implement estat
                          program used to implement predict
    e(predict)
    e(marginsnotok)
                          predictions disallowed by margins
```

Matrices	
e(D) e(Disparities) e(Y)	dissimilarity matrix disparity matrix for nonmetric MDS approximating configuration coordinates
e(Ev) e(W) e(idcoding) e(norm_stats)	eigenvalues weight matrix coding for integer identifier variable normalization statistics
e(linearf)	two-element vector defining the linear transformation; distance equals first element plus second element times dissimilarity
Functions e(sample)	marks estimation sample

#### Methods and formulas

See Methods and formulas in [MV] mdsmat for information.

#### References

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Young, G., and A. S. Householder. 1938. Discussion of a set of points in terms of their mutual distances. *Psychometrika* 3: 19–22.

See [MV] mdsmat for more references.

### Also see

```
[MV] mds postestimation — Postestimation tools for mds, mdsmat, and mdslong
```

[MV] mds postestimation plots — Postestimation plots for mds, mdsmat, and mdslong

[MV] **biplot** — Biplots

[MV] ca — Simple correspondence analysis

[MV] **factor** — Factor analysis

[MV] mds — Multidimensional scaling for two-way data

[MV] mdsmat — Multidimensional scaling of proximity data in a matrix

[MV] **pca** — Principal component analysis

[U] 20 Estimation and postestimation commands

#### Title

mdsmat — Multidimensional scaling of proximity data in a matrix

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# **Description**

mdsmat performs multidimensional scaling (MDS) for two-way proximity data with an explicit measure of similarity or dissimilarity between objects, where the proximities are found in a user-specified matrix. mdsmat performs classical metric MDS as well as modern metric and nonmetric MDS.

If your proximities are stored as variables in long format, see [MV] mdslong. If you are looking for MDS on a dataset on the basis of dissimilarities between observations over variables, see [MV] mds.

#### **Quick start**

Classical multidimensional scaling based on dissimilarities in matrix M mdsmat M

As above, but suppress the MDS configuration plot and use 3 dimensions for the approximating configuration

mdsmat M, noplot dimension(3)

Modern multidimensional scaling based on dissimilarities in matrix M mdsmat M, method(modern)

As above, but with Sammon mapping loss criterion and Procrustes rotation toward the classical solution

```
mdsmat M, loss(sammon) normalize(classical)
```

Nonmetric modern multidimensional scaling based on dissimilarities in matrix M mdsmat M, method(nonmetric)

#### Menu

Statistics > Multivariate analysis > Multidimensional scaling (MDS) > MDS of proximity matrix

# **Syntax**

mdsmat matname [	, options]
options	Description
Model	
<pre>method(method)</pre>	method for performing MDS
loss(loss)	loss function
$\underline{\mathtt{trans}}$ form( $\mathit{tfunction}$ )	permitted transformations of dissimilarities
$\underline{\mathtt{norm}}$ alize( $norm$ )	normalization method; default is normalize(principal)
<u>nam</u> es( <i>namelist</i> )	variable names corresponding to row and column names of the matrix; required with all but shape(full)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{f}}\mathtt{ull})$	matname is a square symmetric matrix; the default
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{l}}\mathtt{ower})$	matname is a vector with the rowwise lower triangle (with diagonal)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{ll}}\mathtt{ower})$	matname is a vector with the rowwise strictly lower triangle (no diagonal)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{u}}\mathtt{pper})$	matname is a vector with the rowwise upper triangle (with diagonal)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{uu}}\mathtt{pper})$	matname is a vector with the rowwise strictly upper triangle (no diagonal)
s2d( <u>st</u> andard)	convert similarity to dissimilarity: $d_{ij} = \sqrt{s_{ii} + s_{jj} - 2s_{ij}}$
s2d( <u>one</u> minus)	convert similarity to dissimilarity: $d_{ij} = 1 - s_{ij}$
Model 2	
<pre>dimension(#)</pre>	configuration dimensions; default is dimension(2)
force	fix problems in proximity information
$\underline{\mathtt{add}}\mathtt{constant}$	make distance matrix positive semidefinite (classical MDS only)
weight( <i>matname</i> )	specifies a weight matrix with the same shape as the proximity matrix
Reporting	
neigen(#)	maximum number of eigenvalues to display; default is neigen(10) (classical MDS only)
<u>con</u> fig	display table with configuration coordinates
<u>nopl</u> ot	suppress configuration plot
Minimization	
<pre>initialize(initopt)</pre>	start with configuration given in initopt
<pre>tolerance(#)</pre>	tolerance for configuration matrix; default is tolerance(1e-4)
<pre>ltolerance(#)</pre>	tolerance for loss criterion; default is ltolerance(1e-8)
<pre>iterate(#)</pre>	perform maximum # of iterations; default is iterate(1000)
<pre>protect(#)</pre>	perform # optimizations and report best solution; default is protect(1)
<u>nolo</u> g	suppress the iteration log
<u>tr</u> ace	display current configuration in iteration log
$\underline{\mathtt{grad}}\mathtt{ient}$	display current gradient matrix in iteration log
<pre>sdprotect(#)</pre>	advanced; see Options below

sdprotect(#) does not appear in the dialog box.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

method	Description		
<u>c</u> lassical	classical MDS; default if neither loss() nor transform() is specified		
<u>m</u> odern	modern MDS; default if loss() or transform() is specified; except when loss(stress) and transform(monotonic) specified		
<u>n</u> onmetric	nonmetric (modern) MDS; default when loss(stress) and transform(monotonic) are specified		
loss	Description		
stress	stress criterion, normalized by distances; the default		
nstress	stress criterion, normalized by disparities		
<u>sstr</u> ess	squared stress criterion, normalized by distances		
<u>nsst</u> ress	squared stress criterion, normalized by disparities		
<u>stra</u> in	strain criterion (with transform(identity) is equivalent to classical MDS)		
<u>sam</u> mon	Sammon mapping		
tfunction	Description		
<u>i</u> dentity	no transformation; disparity = dissimilarity; the default		
<u>p</u> ower	power $\alpha$ : disparity = dissimilarity $^{\alpha}$		
<u>m</u> onotonic	<pre>weakly monotonic increasing functions (nonmetric scaling); only   with loss(stress)</pre>		
norm	Description		
principal	principal orientation; location = 0; the default		
_ classical	Procrustes rotation toward classical solution		
target(matname)[, copy]	Procrustes rotation toward <i>matname</i> ; ignore naming conflicts if copy is specified		
initopt	Description		
<u>c</u> lassical	start with classical solution; the default		
$\underline{\mathbf{r}}$ andom $[$ (#) $]$	start at random configuration, setting seed to #		
$\underline{\mathbf{f}}$ rom(matname)[, copy]	start from matname; ignore naming conflicts if copy is specified		

# **Options**

Model

method(method) specifies the method for MDS.

method(classical) specifies classical metric scaling, also known as "principal coordinates analysis" when used with Euclidean proximities. Classical MDS obtains equivalent results to modern MDS with loss(strain) and transform(identity) without weights. The calculations for classical MDS are fast; consequently, classical MDS is generally used to obtain starting values

for modern MDS. If the options loss() and transform() are not specified, mds computes the classical solution, likewise if method(classical) is specified loss() and transform() are not allowed.

method(modern) specifies modern scaling. If method(modern) is specified but not loss() or transform(), then loss(stress) and transform(identity) are assumed. All values of loss() and transform() are valid with method(modern).

method(nonmetric) specifies nonmetric scaling, which is a type of modern scaling. If
method(nonmetric) is specified, loss(stress) and transform(monotonic) are assumed.
Other values of loss() and transform() are not allowed.

loss (loss) specifies the loss criterion.

loss(stress) specifies that the stress loss function be used, normalized by the squared Euclidean distances. This criterion is often called Kruskal's stress-1. Optimal configurations for loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration paths may differ. loss(stress) is the default.

loss(nstress) specifies that the stress loss function be used, normalized by the squared disparities, that is, transformed dissimilarities. Optimal configurations for loss(stress) and for loss(nstress) are equivalent up to a scale factor, but the iteration paths may differ.

loss(sstress) specifies that the squared stress loss function be used, normalized by the fourth power of the Euclidean distances.

loss(nsstress) specifies that the squared stress criterion, normalized by the fourth power of the disparities (transformed dissimilarities) be used.

loss(strain) specifies the strain loss criterion. Classical scaling is equivalent to loss(strain) and transform(identity) but is computed by a faster noniterative algorithm. Specifying loss(strain) still allows transformations.

loss(sammon) specifies the Sammon (1969) loss criterion.

transform(*tfunction*) specifies the class of allowed transformations of the dissimilarities; transformed dissimilarities are called disparities.

transform(identity) specifies that the only allowed transformation is the identity; that is,
disparities are equal to dissimilarities. transform(identity) is the default.

transform(power) specifies that disparities are related to the dissimilarities by a power function,

disparity = dissimilarity
$$^{\alpha}$$
,  $\alpha > 0$ 

transform(monotonic) specifies that the disparities are a weakly monotonic function of the dissimilarities. This is also known as nonmetric MDS. Tied dissimilarities are handled by the primary method; that is, ties may be broken but are not necessarily broken. transform(monotonic) is valid only with loss(stress).

normalize(norm) specifies a normalization method for the configuration. Recall that the location and orientation of an MDS configuration is not defined ("identified"); an isometric transformation (that is, translation, reflection, or orthonormal rotation) of a configuration preserves interpoint Euclidean distances.

normalize(principal) performs a principal normalization, in which the configuration columns have zero mean and correspond to the principal components, with positive coefficient for the observation with lowest value of id(). normalize(principal) is the default.

normalize(classical) normalizes by a distance-preserving Procrustean transformation of the configuration toward the classical configuration in principal normalization; see [MV] **procrustes**. normalize(classical) is not valid if method(classical) is specified.

normalize(target(matname) [, copy]) normalizes by a distance-preserving Procrustean transformation toward matname; see [MV] **procrustes**. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is also specified.

Note on normalize(classical) and normalize(target()): the Procrustes transformation comprises any combination of translation, reflection, and orthonormal rotation—these transformations preserve distance. Dilation (uniform scaling) would stretch distances and is not applied. However, the output reports the dilation factor, and the reported Procrustes statistic is for the dilated configuration.

names(namelist) is required with all but shape(full). The number of names should equal the number of rows (and columns) of the full similarity or dissimilarity matrix and should not contain duplicates.

shape(*shape*) specifies the storage mode of the existing similarity or dissimilarity matrix *matname*. The following storage modes are allowed:

full specifies that *matname* is a symmetric  $n \times n$  matrix.

lower specifies that *matname* is a row or column vector of length n(n+1)/2, with the rowwise lower triangle of the similarity or dissimilarity matrix including the diagonal.

$$D_{11} D_{21} D_{22} D_{31} D_{32} D_{33} \dots D_{n1} D_{n2} \dots D_{nn}$$

llower specifies that *matname* is a row or column vector of length n(n-1)/2, with the rowwise lower triangle of the similarity or dissimilarity matrix excluding the diagonal.

$$D_{21} \ D_{31} \ D_{32} \ D_{41} \ D_{42} \ D_{43} \ \dots \ D_{n1} \ D_{n2} \ \dots \ D_{n,n-1}$$

upper specifies that *matname* is a row or column vector of length n(n+1)/2, with the rowwise upper triangle of the similarity or dissimilarity matrix including the diagonal.

$$D_{11} D_{12} \dots D_{1n} D_{22} D_{23} \dots D_{2n} D_{33} D_{34} \dots D_{3n} \dots D_{nn}$$

uupper specifies that *matname* is a row or column vector of length n(n-1)/2, with the rowwise upper triangle of the similarity or dissimilarity matrix excluding the diagonal.

$$D_{12} \ D_{13} \ \dots \ D_{1n} \ D_{23} \ D_{24} \ \dots \ D_{2n} \ D_{34} \ D_{35} \ \dots \ D_{3n} \ \dots \ D_{n-1,n}$$

s2d(standard oneminus) specifies how similarities are converted into dissimilarities. By default, the command assumes dissimilarity data. Specifying s2d() indicates that your proximity data are similarities.

Dissimilarity data should have zeros on the diagonal (that is, an object is identical to itself) and nonnegative off-diagonal values. Dissimilarities need not satisfy the triangular inequality,  $D(i,j)^2 \leq D(i,h)^2 + D(h,j)^2$ . Similarity data should have ones on the diagonal (that is, an object is identical to itself) and have off-diagonal values between zero and one. In either case, proximities should be symmetric. See option force if your data violate these assumptions.

The available s2d() options, standard and oneminus, are defined as follows:

standard dissim
$$_{ij}=\sqrt{\mathrm{sim}_{ii}+\mathrm{sim}_{jj}-2\mathrm{sim}_{ij}}=\sqrt{2(1-\mathrm{sim}_{ij})}$$
 oneminus dissim $_{ij}=1-\mathrm{sim}_{ij}$ 

s2d(standard) is the default.

s2d() should be specified only with measures in similarity form.

Model 2

- dimension(#) specifies the dimension of the approximating configuration. The default is dimension(2), and # should not exceed the number of positive eigenvalues of the centered distance matrix.
- force corrects problems with the supplied proximity information. force specifies that the dissimilarity matrix be symmetrized; the mean of  $D_{ij}$  and  $D_{ji}$  is used. Also, problems on the diagonal (similarities:  $D_{ii} \neq 1$ ; dissimilarities:  $D_{ii} \neq 0$ ) are fixed. force does not fix missing values or out-of-range values (that is,  $D_{ij} < 0$  or similarities with  $D_{ij} > 1$ ). Analogously, force symmetrizes the weight matrix.
- addconstant specifies that if the double-centered distance matrix is not positive semidefinite (psd), a constant should be added to the squared distances to make it psd and, hence, Euclidean.
- weight (matname) specifies a symmetric weight matrix with the same shape as the proximity matrix; that is, if shape(lower) is specified, the weight matrix must have this shape. Weights should be nonnegative. Missing weights are assumed to be 0. Weights must also be irreducible; that is, it is not possible to split the objects into disjointed groups with all intergroup weights 0. weight() is not allowed with method(classical), but see loss(strain).

Reporting

- neigen(#) specifies the number of eigenvalues to be included in the table. The default is neigen(10).
  Specifying neigen(0) suppresses the table. This option is allowed with classical MDS only.
- config displays the table with the coordinates of the approximating configuration. This table may also be displayed using the postestimation command estat config; see [MV] mds postestimation.
- noplot suppresses the graph of the approximating configuration. The graph can still be produced later via mdsconfig, which also allows the standard graphics options for fine-tuning the plot; see [MV] mds postestimation plots.

Minimization

These options are available only with method(modern) or method(nonmetric):

initialize(initopt) specifies the initial values of the criterion minimization process.

- initialize(classical), the default, uses the solution from classical metric scaling as initial
   values. With protect(), all but the first run start from random perturbations from the classical
   solution. These random perturbations are independent and normally distributed with standard
   error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.
   initialize(classical) is the default.
- initialize(random) starts an optimization process from a random starting configuration. These
  random configurations are generated from independent normal distributions with standard error
  equal to the product of sdprotect(#) and the standard deviation of the dissimilarities. The
  means of the configuration are irrelevant in MDS.

- initialize(from(matname) [, copy]) sets the initial value to matname. matname should be an  $n \times p$  matrix, where n is the number of observations and p is the number of dimensions, and the rows of matname should be ordered with respect to id(). The rownames of matname should be set correctly but will be ignored if copy is specified. With protect(), the second-to-last runs start from random perturbations from matname. These random perturbations are independent normal distributed with standard error equal to the product of sdprotect(#) and the standard deviation of the dissimilarities.
- tolerance(#) specifies the tolerance for the configuration matrix. When the relative change in the
  configuration from one iteration to the next is less than or equal to tolerance(), the tolerance()
  convergence criterion is satisfied. The default is tolerance(1e-4).
- ltolerance(#) specifies the tolerance for the fit criterion. When the relative change in the fit
  criterion from one iteration to the next is less than or equal to ltolerance(), the ltolerance()
  convergence is satisfied. The default is ltolerance(1e-8).

Both the tolerance() and ltolerance() criteria must be satisfied for convergence.

iterate(#) specifies the maximum number of iterations. The default is iterate(1000).

protect(#) requests that # optimizations be performed and that the best of the solutions be reported.
The default is protect(1). See option initialize() on starting values of the runs. The output
contains a table of the return code, the criterion value reached, and the seed of the random number
used to generate the starting value. Specifying a large number, such as protect(50), provides
reasonable insight whether the solution found is a global minimum and not just a local minimum.

If any of the options log, trace, or gradient is also specified, iteration reports will be printed for each optimization run. Beware: this option will produce a lot of output.

nolog suppresses the iteration log, showing the progress of the minimization process.

trace displays the configuration matrices in the iteration report. Beware: this option may produce a lot of output.

gradient displays the gradient matrices of the fit criterion in the iteration report. Beware: this option may produce a lot of output.

The following option is available with mdsmat but is not shown in the dialog box:

sdprotect(#) sets a proportionality constant for the standard deviations of random configurations
 (init(random)) or random perturbations of given starting configurations (init(classical) or
 init(from())). The default is sdprotect(1).

# Remarks and examples

Remarks are presented under the following headings:

Introduction
Proximity data in a Stata matrix
Modern MDS and local minimums

#### Introduction

Multidimensional scaling (MDS) is a dimension-reduction and visualization technique. Dissimilarities (for instance, Euclidean distances) between observations in a high-dimensional space are represented in a lower-dimensional space (typically two dimensions) so that the Euclidean distance in the lower-dimensional space approximates the dissimilarities in the higher-dimensional space. See Kruskal and Wish (1978) for a brief nontechnical introduction to MDS. Young and Hamer (1987) and Borg and Groenen (2005) are more advanced textbook-sized treatments.

mdsmat performs MDS on a similarity or dissimilarity matrix matname. You may enter the matrix as a symmetric square matrix or as a vector (matrix with one row or column) with only the upper or lower triangle; see option shape() for details. matname should not contain missing values. The diagonal elements should be 0 (dissimilarities) or 1 (similarities). If you provide a square matrix (that is, shape(full)), names of the objects are obtained from the matrix row and column names. The row names should all be distinct, and the column names should equal the row names. Equation names, if any, are ignored. In any of the vectorized shapes, names are specified with option names(), and the matrix row and column names are ignored.

See option force if your matrix violates these assumptions.

In some applications, the similarity or dissimilarity of objects is defined by the researcher in terms of variables (attributes) measured on the objects. If you need to do MDS of this form, you should continue by reading [MV] mds.

Often, however, proximities—that is, similarities or dissimilarities—are measured directly. For instance, psychologists studying the similarities or dissimilarities in a set of stimuli—smells, sounds, faces, concepts, etc.—may have subjects rate the dissimilarity of pairs of stimuli. Linguists have subjects rate the similarity or dissimilarity of pairs of dialects. Political scientists have subjects rate the similarity or dissimilarity of political parties or candidates for political office. In other fields, relational data are studied that may be interpreted as proximities in a more abstract sense. For instance, sociologists study interpersonal contact frequencies in groups ("social networks"); these measures are sometimes interpreted in terms of similarities.

A wide variety of MDS methods have been proposed mdsmat performs classical and modern scaling. Classical scaling has its roots in Young and Householder (1938) and Torgerson (1952). MDS requires complete and symmetric dissimilarity interval-level data. To explore modern scaling, see Borg and Groenen (2005). Classical scaling results in an eigen decomposition, whereas modern scaling is accomplished by the minimization of a loss function. Consequently, eigenvalues are not available after modern MDS.

Computing the classical solution is straightforward, but with modern MDS the minimization of the loss criteria over configurations is a high-dimensional problem that is easily beset by convergence to local minimums. mdsmat provides options to control the minimization process 1) by allowing the user to select the starting configuration and 2) by selecting the best solution among multiple minimization runs from random starting configurations.

# Proximity data in a Stata matrix

To perform MDS of relational data, you must enter the data in a suitable format. One convenient format is a Stata matrix. You may want to use this format for analyzing data that you obtain from a printed source.

# Example 1

Many texts on multidimensional scaling illustrate how locations can be inferred from a table of geographic distances. We will do this too, using an example of distances in miles between 14 locations in Texas, representing both manufactured and natural treasures:

```
Big Bend
                        0
                            523
                                 551
                                       243
                                             322
                                                   412
                                                         263
                                                              596
                                                                    181
                                                                          313
                                                                                553
                      523
                                                   232
                                                              226
  Corpus Christi
                              0
                                 396
                                       280
                                             705
                                                         619
                                                                    342
                                                                          234
                                                                                 30
           Dallas
                      551
                            396
                                    0
                                       432
                                             643
                                                   230
                                                         532
                                                               243
                                                                    494
                                                                          317
                                                                                426
          Del Rio
                      243
                            280
                                 432
                                          0
                                             427
                                                   209
                                                         339
                                                              353
                                                                     62
                                                                           70
                                                                                310
          El Paso
                      322
                           705
                                 643
                                       427
                                               Λ
                                                   528
                                                         110
                                                              763
                                                                    365
                                                                          525
                                                                                735
                            232
                                 230
                                       209
                                                         398
                                                                    271
  Enchanted Rock
                      412
                                             528
                                                     0
                                                              260
                                                                           69
                                                                                262
   Guadalupe Mnt
                      263
                            619
                                 532
                                       339
                                             110
                                                   398
                                                           0
                                                              674
                                                                    277
                                                                          280
                                                                                646
          Houston
                      596
                            226
                                 243
                                       353
                                             763
                                                   260
                                                         674
                                                                 0
                                                                    415
                                                                          292
                                                                                256
                      181
                            342
                                  494
                                        62
                                             365
                                                   271
                                                         277
                                                               415
                                                                       0
                                                                          132
                                                                                372
          Langtry
     Lost Maples
                      313
                            234
                                  317
                                        70
                                             525
                                                    69
                                                         280
                                                               292
                                                                    132
                                                                            0
                                                                                264
    Padre Island
                      553
                             30
                                  426
                                       310
                                             735
                                                   262
                                                         646
                                                               256
                                                                    372
                                                                          264
                                                                                  0
                      434
                                 235
                                                    40
                                                         420
                                                               202
                                                                    293
                                                                          115
                                                                                246
Pedernales Falls
                            216
                                       231
                                             550
                      397
                            141
                                             564
                                                         475
                                                               199
                                                                           93
     San Antonio
                                 274
                                       154
                                                    91
                                                                    216
                                                                                171
        StataCorp
                      426
                            205
                                 151
                                       287
                                             606
                                                   148
                                                         512
                                                                83
                                                                    318
                                                                          202
                                                                                316
```

Big Bend	434	397	426
Corpus Christi	216	141	205
Dallas	235	274	151
Del Rio	231	154	287
El Paso	550	564	606
Enchanted Rock	40	91	148
Guadalupe Mnt	420	475	512
Houston	202	199	83
Langtry	293	216	318
Lost Maples	115	93	202
Padre Island	246	171	316
Pedernales Falls	0	75	116
San Antonio	75	0	154
StataCorp	116	154	0

Note the inclusion of StataCorp, which is located in the twin cities of Bryan/College Station (BCS). To get the data into Stata, we will enter only the strictly upper triangle as a Stata one-dimensional matrix and collect the names in a global macro for later use. We are using the strictly upper triangle (that is, omitting the diagonal) because the diagonal of a dissimilarity matrix contains all zeros—there is no need to enter them.

```
matrix input D = (
>
           551
                 243
                       322
                            412
                                  263
                                        596
                                              181
                                                    313
                                                         553
                                                               434
                                                                     397
                                                                           426
>
           396
                 280
                       705
                             232
                                  619
                                        226
                                              342
                                                    234
                                                          30
                                                               216
                                                                     141
                                                                           205
>
                 432
                       643
                             230
                                  532
                                        243
                                              494
                                                    317
                                                         426
                                                               235
                                                                     274
                                                                           151
                       427
                            209
                                               62
                                                     70
                                                         310
                                                               231
                                                                           287
>
                                  339
                                        353
                                                                     154
                             528
                                  110
                                        763
                                              365
                                                   525
                                                         735
                                                               550
                                                                     564
                                                                           606
                                  398
                                        260
                                              271
                                                     69
                                                         262
                                                                40
                                                                      91
                                                                           148
                                        674
                                              277
                                                   280
                                                         646
                                                               420
                                                                     475
                                                                          512
>
                                              415
                                                   292
                                                         256
                                                               202
                                                                     199
                                                                            83
                                                    132
                                                         372
                                                               293
                                                                     216
                                                                           318
>
                                                         264
                                                               115
                                                                      93
                                                                          202
                                                               246
                                                                     171
                                                                          316
>
>
                                                                      75
                                                                          116
                                                                           154 )
  global names
                                                        Del Rio
     Big Bend
                    Corpus_Christi
                                       Dallas
>
     El Paso
                    Enchanted_Rock
                                       Guadalupe_Mnt
                                                        Houston
>
     Langtry
                    Lost_Maples
                                       Padre_Island
                                                        Pedernales_Falls
     San_Antonio
                    StataCorp
```

The triangular data entry is just typographical and is useful for catching data entry errors. As far as Stata is concerned, we could have typed all the numbers in one long row. We use matrix input

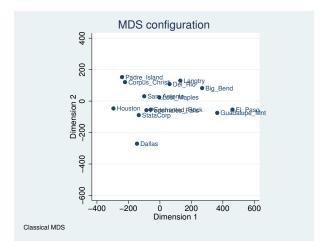
D = rather than matrix define D = or just matrix D = so that we do not have to separate entries with commas.

With the data now in Stata, we may use mdsmat to infer the locations in Texas and produce a map:

. mdsmat D, names(\$names) shape(uupper)
Classical metric multidimensional scaling
dissimilarity matrix: D

		Nur	nber of	obs		=	14
Eigenvalues > 0	=	8 Mai	rdia fi	it measure	1	=	0.7828
Retained dimensions	=	2 Max	rdia fi	it measure	2	=	0.9823

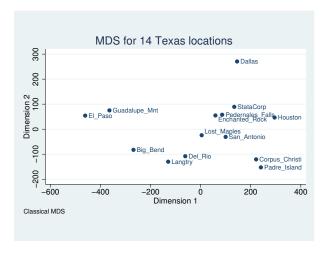
		abs(eige	nvalue)	(eigenv	alue)^2
Dimension	Eigenvalue	Percent	Cumul.	Percent	Cumul.
1	691969.62	62.63	62.63	92.45	92.45
2	172983.05	15.66	78.28	5.78	98.23
3	57771.995	5.23	83.51	0.64	98.87
4	38678.916	3.50	87.01	0.29	99.16
5	19262.579	1.74	88.76	0.07	99.23
6	9230.7695	0.84	89.59	0.02	99.25
7	839.70996	0.08	89.67	0.00	99.25
8	44.989372	0.00	89.67	0.00	99.25



The representation of the distances in two dimensions provides a reasonable, but not great, fit; the percentage of eigenvalues accounted for is 78%.

By default, mdsmat produces a configuration plot. Enhancements to the configuration plot are possible using the mdsconfig postestimation graphics command; see [MV] mds postestimation plots. We present the configuration plot with the autoaspect option to obtain better use of the available space while preserving the equivalence of distance in the x and y axes. We negate the direction of the x axis with the xnegate option to flip the configuration horizontally and flip the direction of the y axis with the ynegate option. We also change the default title and control the placement of labels.

```
. set obs 14
number of observations (_N) was 0, now 14
. generate pos = 3
. replace pos = 4 in 6
(1 real change made)
. replace pos = 2 in 10
(1 real change made)
. mdsconfig, autoaspect xnegate ynegate mlabvpos(pos)
> title(MDS for 14 Texas locations)
```



Look at the graph produced by mdsconfig after mdsmat. You will probably recognize a twisted (and slightly distorted) map of Texas. The vertical orientation of the map is not correctly north—south; you would probably want to turn the map some 20 degrees clockwise. Why didn't mdsmat get it right? It could not have concluded the correct rotation from the available distance information. Any orthogonal rotation of the map would produce the same distances. The orientation of the map is not identified. Finally, the "location" of the map cannot be inferred from the distances. Translating the coordinates does not change the distances. As far as mdsmat is concerned, Texas could be part of China.

#### Modern MDS and local minimums

Modern MDS can converge to a local rather than a global minimum. We give an example where this happens and show how the protect() option can guard against this. protect(#) performs multiple minimizations and reports the best one. The output is explained in [MV] mds.

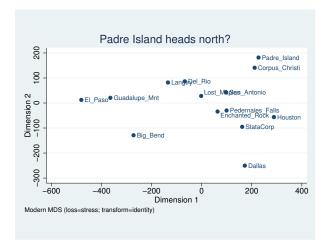
# Example 2

Continuing from where we left off, we perform modern MDS, using an initial random configuration with the init(random(512308)) option. The number 512,308 sets the seed so that this run may be replicated.

4

```
. mdsmat D, names($names) shape(uupper) meth(modern) init(random(512308)) nolog
> noplot
(loss(stress) assumed)
(transform(identity) assumed)
Modern multidimensional scaling
    dissimilarity matrix: D
    Loss criterion: stress = raw_stress/norm(distances)
    Transformation: identity (no transformation)
                                                  Number of obs
                                                                              14
                                                  Dimensions
                                                                              2
    Normalization: principal
                                                  Loss criterion
                                                                         0.0858
. mdsconfig, autoaspect xnegate ynegate mlabvpos(pos)
```

- title(Padre Island heads north?)



This graph has some resemblance to the one we saw before, but any Texan can assure you that Padre Island should not end up north of Dallas.

We check this result by rerunning with protect (10). This will repeat the minimization and report the best result. Larger values of protect() give us more assurance that we have found the global minimum, but here protect(10) is sufficient to tell us that our original mdsmat found a local, not a global, minimum.

```
. mdsmat D, names($names) shape(uupper) meth(modern) init(random(512308)) nolog
> protect(10) noplot
```

(loss(stress) assumed) 

(transform(identity) assumed)

run	mrc	#iter	lossval
1	0	61	.06180059
2	0	48	.0618006
3	0	49	.0618006
4	0	42	.0618006
5	0	52	.0618006
6	0	84	.08581202
7	0	83	.08581202
8	0	70	.08581202
9	0	89	.12189371
10	0	66	.12189371

Modern multidimensional scaling dissimilarity matrix: D

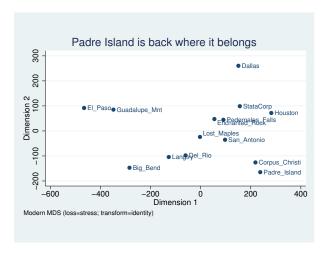
Normalization: principal

Loss criterion: stress = raw\_stress/norm(distances)

Transformation: identity (no transformation)

Number of obs 14 Dimensions 2 0.0618 Loss criterion

- . mdsconfig, autoaspect xnegate ynegate mlabvpos(pos)
- > title(Padre Island is back where it belongs)



The original run had a loss criterion of 0.0858, but after using the protect() option the loss criterion was much lower—0.0618. We also see that Padre Island is back down south where it belongs. It is clear that the original run converged to a local minimum. You can see the original results appear as the final output line of the first table in the output after using protect(10). The seed in the table is a hexadecimal representation of how the seed is stored internally. The number 512,308 in init(random(512308)) is convenient shorthand for specifying the seed; the two are equivalent. If we wish, we could repeat the command with a larger value of protect() to assure ourselves that 0.0618 is indeed the global minimum.

After mdsmat, all MDS postestimation tools are available. For instance, you may analyze residuals with estat quantile, you may produce a Shepard diagram, etc.; see [MV] mds postestimation and [MV] mds postestimation plots.

#### Stored results

mdsmat stores the following in e():

```
e(N)
                          number of rows or columns (i.e., number of observations)
                          number of dimensions in the approximating configuration
    e(p)
    e(np)
                          number of strictly positive eigenvalues
                          constant added to squared dissimilarities to force positive semidefiniteness
    e(addcons)
    e(mardia1)
    e(mardia2)
                          Mardia measure 2
    e(critval)
                          loss criterion value
    e(wsum)
                          sum of weights
    e(alpha)
                          parameter of transform(power)
                          iteration count
    e(ic)
    e(rc)
                          return code
    e(converged)
                          1 if converged, 0 otherwise
Macros
    e(cmd)
                          mdsmat
    e(cmdline)
                          command as typed
    e(method)
                          classical or modern MDS method
    e(method2)
                          nonmetric, if method(nonmetric)
                          loss criterion
    e(loss)
                          description loss criterion
    e(losstitle)
    e(dmatrix)
                          name of analyzed matrix
    e(tfunction)
                          identity, power, or monotonic, transformation function
                          description of transformation
    e(transftitle)
    e(mxlen)
                          maximum length of category labels
                          similarity or dissimilarity; type of proximity data
    e(dtype)
    e(s2d)
                          standard or oneminus (when e(dtype) is similarity)
    e(unique)
                          1 if eigenvalues are distinct, 0 otherwise
    e(init)
                          initialization method
    e(irngstate)
                          initial random-number state used for init(random)
    e(rngstate)
                          random-number state for solution
    e(norm)
                          normalization method
    e(targetmatrix)
                          name of target matrix for normalize(target)
                          nob noV for modern or nonmetric MDS; nob noV eigen for classical MDS
    e(properties)
    e(estat_cmd)
                          program used to implement estat
                          program used to implement predict
    e(predict)
    e(marginsnotok)
                          predictions disallowed by margins
Matrices
    e(D)
                          dissimilarity matrix
                          disparity matrix for nonmetric MDS
    e(Disparities)
    e(Y)
                          approximating configuration coordinates
    e(Ev)
                          eigenvalues
                          weight matrix
    e(W)
    e(norm_stats)
                          normalization statistics
                          two element vector defining the linear transformation; distance
    e(linearf)
                            equals first element plus second element times dissimilarity
```

# Methods and formulas

Methods and formulas are presented under the following headings:

Classical multidimensional scaling Modern multidimensional scaling Conversion of similarities to dissimilarities

### Classical multidimensional scaling

Let **D** be an  $n \times n$  dissimilarity matrix. The matrix **D** is said to be *Euclidean* if there are coordinates **Y** so that

$$D_{ij}^2 = (\mathbf{Y}_i - \mathbf{Y}_j)(\mathbf{Y}_i - \mathbf{Y}_j)'$$

Here  $\mathbf{Y}_i$  and  $\mathbf{Y}_j$  are the *i*th and *j*th column vectors extracted from  $\mathbf{Y}$ . Let  $\mathbf{A} = -(1/2)\mathbf{D} \odot \mathbf{D}$ , with  $\odot$  being the Hadamard or elementwise matrix product, and define  $\mathbf{B}$  as the double-centered distance matrix

$$\mathbf{B} = \mathbf{H}\mathbf{A}\mathbf{H}$$
 with  $\mathbf{H} = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}'$ 

 ${\bf D}$  is Euclidean if and only if  ${\bf B}$  is positive semidefinite. Assume for now that  ${\bf D}$  is indeed Euclidean. The spectral or eigen decomposition of  ${\bf B}$  is written as  ${\bf B}={\bf U}\Lambda{\bf U}'$ , with  ${\bf U}$  the orthonormal matrix of eigenvectors normed to 1, and  $\Lambda$  a diagonal matrix with nonnegative values (the eigenvalues of  ${\bf B}$ ) in decreasing order. The coordinates  ${\bf Y}$  are defined in terms of the spectral decomposition  ${\bf Y}={\bf U}\Lambda^{1/2}$ . These coordinates are centered  ${\bf Y}'{\bf 1}={\bf 0}$ .

The spectral decomposition can also be used to obtain a low-dimensional configuration  $\widetilde{\mathbf{Y}}$ ,  $n \times p$ , so that the interrow distances of  $\widetilde{\mathbf{Y}}$  approximate  $\mathbf{D}$ . Mardia, Kent, and Bibby (1979, sec. 14.4) discuss some characterizations under which the leading p columns of  $\mathbf{Y}$  are an optimal choice of  $\widetilde{\mathbf{Y}}$ . These characterizations also apply to the case when  $\mathbf{B}$  is not positive semidefinite, so some of the  $\lambda$ 's are negative; we require that  $\lambda_p > 0$ .

Various other approaches have been proposed to deal with the case when the matrix  $\bf B$  is not positive semidefinite, that is, when  $\bf B$  has negative eigenvalues (see Cox and Cox 2001, 45–48). An easy solution is to add a constant to the off-diagonal elements of  $\bf D\odot \bf D$  to make  $\bf B$  positive semidefinite. The smallest such constant is  $-2\lambda_n$ , where  $\lambda_n$  is the smallest eigenvalue of  $\bf B$  (Lingoes 1971). See Cailliez (1983) for a solution to the additive constant problem in terms of the dissimilarities instead of the squared dissimilarities.

Goodness-of-fit statistics for a configuration in p dimensions have been proposed by Mardia (1978) in characterizations of optimality properties of the classical solution

$$Mardia_1 = \frac{\sum_{i=1}^{p} |\lambda_i|}{\sum_{i=1}^{n} |\lambda_i|}$$

and

$$Mardia_2 = \frac{\sum_{i=1}^{p} \lambda_i^2}{\sum_{i=1}^{n} \lambda_i^2}$$

# Modern multidimensional scaling

Let  $\mathbf{D}$  be a symmetric  $n \times n$  matrix of observed dissimilarities. We assume that proximity data in the form of similarities have already been transformed into dissimilarities. Let  $\mathbf{W}$  be an  $n \times n$  matrix of nonnegative weights. With unweighted MDS, we define  $W_{ij} = 1$ . For a configuration of n points in k-dimensional space represented by the  $n \times k$  matrix  $\mathbf{Y}$ , let  $\mathbf{B}(\mathbf{Y})$  be the  $n \times n$  matrix of Euclidean distances between the rows of  $\mathbf{Y}$ . We consider  $\mathcal{F}$  to be some class of permitted transformations from  $n \times n$  real matrices to  $n \times n$  real matrices.

Modern metric and nonmetric multidimensional scaling involves the minimization of a loss criterion

$$L\{f(\mathbf{D}), \mathbf{B}(\mathbf{Y}), \mathbf{W}\}\$$

over the configurations Y and transformations  $f \in \mathcal{F}$ . Whether a scaling method is labeled metric or nonmetric depends on the class  $\mathcal{F}$ . In nonmetric scaling,  $\mathcal{F}$  is taken to be the class of monotonic functions. If  $\mathcal{F}$  is a regular parametrized set of functions, one commonly labels the scaling as metric.

 ${\bf D}$  is the matrix of proximities or dissimilarities,  ${\bf B}({\bf Y})$  is the matrix of distances, and the result of  $f({\bf D})=\widehat{{\bf D}}$  is the matrix of disparities.

The mdsmat command supports the following loss criteria:

1. **stress** specifies Kruskal's stress-1 criterion: the Euclidean norm of the difference between the distances and the disparities, normalized by the Euclidean norm of the distances.

$$\mathbf{stress}(\widehat{\mathbf{D}}, \mathbf{B}, \mathbf{W}) = \left\{ \frac{\sum_{ij} W_{ij} (B_{ij} - \widehat{D}_{ij})^2}{\sum_{ij} W_{ij} B_{ij}^2} \right\}^{1/2}$$

nstress specifies the square root of the normalized stress criterion: the Euclidean norm of the difference between the distances and the disparities, normalized by the Euclidean norm of the disparities.

$$\mathbf{nstress}(\widehat{\mathbf{D}}, \mathbf{B}, \mathbf{W}) = \left\{ \frac{\sum_{ij} W_{ij} (B_{ij} - \widehat{D}_{ij})^2}{\sum_{ij} W_{ij} \widehat{D}_{ij}^2} \right\}^{1/2}$$

nstress normalizes with the disparities, stress with the distances.

3. **sammon** specifies the Sammon mapping criterion (Sammon 1969; Neimann and Weiss 1979): the sum of the scaled, squared differences between the distances and the disparities, normalized by the sum of the disparities.

$$\mathbf{sammon}(\widehat{\mathbf{D}}, \mathbf{B}, \mathbf{W}) = \frac{\sum_{ij} W_{ij} (B_{ij} - \widehat{D}_{ij})^2 / \widehat{D}_{ij}}{\sum_{ij} W_{ij} \widehat{D}_{ij}}$$

4. **sstress** specifies the squared stress criterion: the Euclidean norm of the difference between the squared distances and the squared disparities, normalized by the Euclidean norm of the squared distances.

$$\mathbf{sstress}(\widehat{\mathbf{D}}, \mathbf{B}, \mathbf{W}) = \left\{ \frac{\sum_{ij} W_{ij} (B_{ij}^2 - \widehat{D}_{ij}^2)^2}{\sum_{ij} W_{ij} B_{ij}^4} \right\}^{1/2}$$

5. **nsstress** specifies the normalized squared stress criterion: the Euclidean norm of the difference between the squared distances and the squared disparities, normalized by the Euclidean norm of the squared disparities.

$$\mathbf{nsstress}(\widehat{\mathbf{D}},\mathbf{B},\mathbf{W}) = \left\{\frac{\sum_{ij} W_{ij} (B_{ij}^2 - \widehat{D}_{ij}^2)^2}{\sum_{ij} W_{ij} \widehat{D}_{ij}^4}\right\}^{1/2}$$

**nsstress** normalizes with the disparities, **sstress** with the distances.

6. **strain** specifies the strain criterion,

$$\mathrm{strain}(\widehat{\mathbf{D}},\mathbf{B},\mathbf{W}) = \frac{\sqrt{\mathrm{trace}(\mathbf{X}'\mathbf{X})}}{\sum_{ij} W_{ij}}$$

where

$$\mathbf{X} = \mathbf{W} \odot \left\{ \widehat{\mathbf{D}} - \mathbf{B}(\widetilde{\mathbf{Y}}) \right\}$$

where  $\widetilde{\mathbf{Y}}$  is the centered configuration of  $\mathbf{Y}$ . Without weights,  $W_{ij}=1$ , and without transformation, that is,  $\widehat{\mathbf{D}}=\mathbf{D}$ , minimization of the strain criterion is equivalent to classical metric scaling.

The mdsmat command supports three classes of permitted transformations,  $f \in \mathcal{F}$ : 1) the class of all weakly monotonic transformations, 2) the power class of functions where f is defined elementwise on  $\mathbf{D}$  as  $f(D_{ij}, \alpha) = D_{ij}^{\alpha}$  (Critchley 1978; Cox and Cox 2001), and 3) the trivial identity case of  $f(\mathbf{D}) = \mathbf{D}$ .

Minimization of a loss criterion with respect to the configuration  $\mathbf{Y}$  and the permitted transformation  $f \in \mathcal{F}$  is performed with an alternating algorithm in which the configuration  $\mathbf{Y}$  is modified (the C-step) and the transformation f is adjusted (the T-step) to reduce loss. Obviously, no T-step is made with the identity transformation. The classical solution is the default starting configuration. Iteration continues until the C-step and T-step reduce loss by less than the tolerance for convergence or the maximum number of iterations is performed. The C-step is taken by steepest descent using analytical gradients and an optimal stepsize computed using Brent's bounded minimization (Brent 1973). The implementation of the T-step varies with the specified class of transformations. In the nonmetric case of monotonic transformations, we use isotonic regression (Kruskal 1964a, 1964b; Cox and Cox 2001), using the primary approach to ties (Borg and Groenen 2005, 40). For power transformations, we again apply Brent's minimization method.

Given enough iterations, convergence is usually not a problem. However, the alternating algorithm may not converge to a global minimum.  $\mathtt{mdsmat}$  provides some protection by repeated runs from different initial configurations. However, as Euclidean distances B(Y) are invariant with respect to isometric transformations (rotations, translations) of Y, some caution is required to compare different runs and, similarly, to compare the configurations obtained from different scaling methods.  $\mathtt{mdsmat}$  normalizes the optimal configuration by centering and via the orthogonal Procrustean rotation without dilation toward the classical or a user-specified solution; see  $[\mathtt{MV}]$  procrustes.

#### Conversion of similarities to dissimilarities

If a similarity measure was selected, it is turned into a dissimilarity measure by using one of two methods. The *standard* conversion method is

$$\operatorname{dissim}_{ij} = \sqrt{\operatorname{sim}_{ii} + \operatorname{sim}_{jj} - 2\operatorname{sim}_{ij}}$$

With the similarity of an object to itself being 1, this is equivalent to

$$\operatorname{dissim}_{ij} = \sqrt{2(1-\operatorname{sim}_{ij})}$$

This conversion method has the attractive property that it transforms a positive-semidefinite similarity matrix into a Euclidean distance matrix (see Mardia, Kent, and Bibby 1979, 402).

We also offer the one-minus method

$$\operatorname{dissim}_{ij} = 1 - \operatorname{sim}_{ij}$$

### References

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### Also see

[MV] mds postestimation — Postestimation tools for mds, mdsmat, and mdslong

[MV] mds postestimation plots — Postestimation plots for mds, mdsmat, and mdslong

[MV] **biplot** — Biplots

[MV] ca — Simple correspondence analysis

[MV] **factor** — Factor analysis

[MV] mds — Multidimensional scaling for two-way data

[MV] mdslong — Multidimensional scaling of proximity data in long format

[MV] **pca** — Principal component analysis

[U] 20 Estimation and postestimation commands

## **Title**

measure\_option — Option for similarity and dissimilarity measures

command ..., ... measure(measure) ...

Description Syntax Options References Also see

# **Description**

Several commands have options that allow you to specify a similarity or dissimilarity measure designated as *measure* in the syntax; see [MV] **cluster**, [MV] **mds**, [MV] **discrim knn**, and [MV] **matrix dissimilarity**. These options are documented here. Most analysis commands (for example, cluster and mds) transform similarity measures to dissimilarity measures as needed.

# **Syntax**

or			
command,	command, measure		
measure	Description		
cont_measure	similarity or dissimilarity measure for continuous data		
binary_measure	similarity measure for binary data		
mixed_measure	dissimilarity measure for a mix of binary and continuous data		
cont_measure	Description		
 L2	Euclidean distance (Minkowski with argument 2)		
<u>Euc</u> lidean	alias for L2		
L(2)	alias for L2		
L2squared	squared Euclidean distance		
Lpower(2)	alias for L2squared		
L1	absolute-value distance (Minkowski with argument 1)		
<u>abs</u> olute	alias for L1		
cityblock	alias for L1		
<u>manhat</u> tan	alias for L1		
L(1)	alias for L1		
Lpower(1)	alias for L1		
<u>Linf</u> inity	maximum-value distance (Minkowski with infinite argument)		
$\underline{\mathtt{max}}\mathtt{imum}$	alias for Linfinity		
L(#)	Minkowski distance with # arguments		
<u>Lpow</u> er(#)	Minkowski distance with # arguments raised to # power		
<u>Canb</u> erra	Canberra distance		
<u>corr</u> elation	correlation coefficient similarity measure		
angular	angular separation similarity measure		
angle	alias for angular		

# **Options**

Measures are divided into those for continuous data and binary data. *measure* is not case sensitive. Full definitions are presented in *Similarity and dissimilarity measures for continuous data*, *Similarity measures for binary data*, and *Dissimilarity measures for mixed data*.

The similarity or dissimilarity measure is most often used to determine the similarity or dissimilarity between observations. However, sometimes the similarity or dissimilarity between variables is of interest.

## Similarity and dissimilarity measures for continuous data

Here are the similarity and dissimilarity measures for continuous data available in Stata. In the following formulas, p represents the number of variables, N is the number of observations, and  $x_{iv}$  denotes the value of observation i for variable v.

The formulas are presented in two forms. The first is the formula used when computing the similarity or dissimilarity between observations. The second is the formula used when computing the similarity or dissimilarity between variables.

#### L2 (aliases Euclidean and L(2))

requests the Minkowski distance metric with argument 2. For comparing observations i and j, the formula is

$$\left\{ \sum_{i=1}^{p} (x_{ia} - x_{ja})^2 \right\}^{1/2}$$

and for comparing variables u and v the formula is

$$\left\{ \sum_{k=1}^{N} (x_{ku} - x_{kv})^2 \right\}^{1/2}$$

L2 is best known as Euclidean distance and is the default dissimilarity measure for discrim knn, mds, matrix dissimilarity, and all the cluster subcommands except for centroidlinkage, medianlinkage, and wardslinkage, which default to using L2squared; see [MV] discrim knn, [MV] mds, [MV] matrix dissimilarity, and [MV] cluster.

#### L2squared (alias Lpower(2))

requests the square of the Minkowski distance metric with argument 2. For comparing observations i and j, the formula is

$$\sum_{a=1}^{p} (x_{ia} - x_{ja})^2$$

and for comparing variables u and v, the formula is

$$\sum_{k=1}^{N} (x_{ku} - x_{kv})^2$$

L2squared is best known as squared Euclidean distance and is the default dissimilarity measure for the centroidlinkage, medianlinkage, and wardslinkage subcommands of cluster; see [MV] cluster.

L1 (aliases absolute, cityblock, manhattan, L(1), and Lpower(1)) requests the Minkowski distance metric with argument 1. For comparing observations i and j, the formula is

$$\sum_{a=1}^{p} |x_{ia} - x_{ja}|$$

and for comparing variables u and v, the formula is

$$\sum_{k=1}^{N} |x_{ku} - x_{kv}|$$

L1 is best known as absolute-value distance.

#### Linfinity (alias maximum)

requests the Minkowski distance metric with infinite argument. For comparing observations i and j, the formula is

$$\max_{a=1,\ldots,p} |x_{ia} - x_{ja}|$$

and for comparing variables u and v, the formula is

$$\max_{k=1,\ldots,N} |x_{ku} - x_{kv}|$$

Linfinity is best known as maximum-value distance.

#### L(#)

requests the Minkowski distance metric with argument #. For comparing observations i and j, the formula is

$$\left(\sum_{i=1}^{p} |x_{ia} - x_{ja}|^{\#}\right)^{1/\#} \qquad \# \ge 1$$

and for comparing variables u and v, the formula is

$$\left(\sum_{k=1}^{N} |x_{ku} - x_{kv}|^{\#}\right)^{1/\#} \qquad \# \ge 1$$

We discourage using extremely large values for #. Because the absolute value of the difference is being raised to the value of #, depending on the nature of your data, you could experience numeric overflow or underflow. With a large value of #, the L() option will produce results similar to those of the Linfinity option. Use the numerically more stable Linfinity option instead of a large value for # in the L() option.

See Anderberg (1973) for a discussion of the Minkowski metric and its special cases.

#### Lpower(#)

requests the Minkowski distance metric with argument #, raised to the # power. For comparing observations i and j, the formula is

$$\sum_{a=1}^{p} |x_{ia} - x_{ja}|^{\#} \qquad \# \ge 1$$

and for comparing variables u and v, the formula is

$$\sum_{k=1}^{N} |x_{ku} - x_{kv}|^{\#} \qquad \# \ge 1$$

As with L(#), we discourage using extremely large values for #; see the discussion above.

#### Canberra

requests the following distance metric when comparing observations i and j

$$\sum_{a=1}^{p} \frac{|x_{ia} - x_{ja}|}{|x_{ia}| + |x_{ja}|}$$

and the following distance metric when comparing variables u and v

$$\sum_{k=1}^{N} \frac{|x_{ku} - x_{kv}|}{|x_{ku}| + |x_{kv}|}$$

When comparing observations, the Canberra metric takes values between 0 and p, the number of variables. When comparing variables, the Canberra metric takes values between 0 and N, the number of observations; see Gordon (1999) and Gower (1985). Gordon (1999) explains that the Canberra distance is sensitive to small changes near zero.

#### correlation

requests the correlation coefficient similarity measure. For comparing observations i and j, the formula is

$$\frac{\sum_{a=1}^{p} (x_{ia} - \overline{x}_{i.})(x_{ja} - \overline{x}_{j.})}{\left\{\sum_{a=1}^{p} (x_{ia} - \overline{x}_{i.})^{2} \sum_{b=1}^{p} (x_{jb} - \overline{x}_{j.})^{2}\right\}^{1/2}}$$

and for comparing variables u and v, the formula is

$$\frac{\sum_{k=1}^{N} (x_{ku} - \overline{x}_{.u})(x_{kv} - \overline{x}_{.v})}{\left\{\sum_{k=1}^{N} (x_{ku} - \overline{x}_{.u})^2 \sum_{l=1}^{N} (x_{lv} - \overline{x}_{.v})^2\right\}^{1/2}}$$

where 
$$\overline{x}_{i.} = (\sum_{a=1}^{p} x_{ia})/p$$
 and  $\overline{x}_{.u} = (\sum_{k=1}^{N} x_{ku})/N$ .

The correlation similarity measure takes values between -1 and 1. With this measure, the relative direction of the two vectors is important. The correlation similarity measure is related to the angular separation similarity measure (described next). The correlation similarity measure gives the cosine of the angle between the two vectors measured from the mean; see Gordon (1999).

#### angular (alias angle)

requests the angular separation similarity measure. For comparing observations i and j, the formula is

$$\frac{\sum_{a=1}^{p} x_{ia} x_{ja}}{\left(\sum_{a=1}^{p} x_{ia}^{2} \sum_{b=1}^{p} x_{jb}^{2}\right)^{1/2}}$$

and for comparing variables u and v, the formula is

$$\frac{\sum_{k=1}^{N} x_{ku} x_{kv}}{\left(\sum_{k=1}^{N} x_{ku}^{2} \sum_{l=1}^{N} x_{lv}^{2}\right)^{1/2}}$$

The angular separation similarity measure is the cosine of the angle between the two vectors measured from zero and takes values from -1 to 1; see Gordon (1999).

### Similarity measures for binary data

Similarity measures for binary data are based on the four values from the cross-tabulation of observation i and j (when comparing observations) or variables u and v (when comparing variables).

For comparing observation i and j, the cross-tabulation is

		obs 1	. j 0
obs.	1	$\begin{bmatrix} a \\ c \end{bmatrix}$	d

a is the number of variables where observations i and j both had ones, and d is the number of variables where observations i and j both had zeros. The number of variables where observation i is one and observation j is zero is b, and the number of variables where observation i is zero and observation j is one is c.

For comparing variables u and v, the cross-tabulation is

		var. 1	$\begin{array}{c} v \\ 0 \end{array}$
var.	1	$\begin{pmatrix} a \\ c \end{pmatrix}$	$\frac{b}{d}$

a is the number of observations where variables u and v both had ones, and d is the number of observations where variables u and v both had zeros. The number of observations where variable u is one and variable v is zero is b, and the number of observations where variable u is zero and variable v is one is c.

Stata treats nonzero values as one when a binary value is expected. Specifying one of the binary similarity measures imposes this behavior unless some other option overrides it (for instance, the allbinary option of matrix dissimilarity; see [MV] matrix dissimilarity).

Hubálek (1982) gives an extensive list of binary similarity measures. Gower (1985) lists 15 binary similarity measures, 14 of which are implemented in Stata. (The excluded measure has many cases where the quantity is undefined, so it was not implemented.) Anderberg (1973) gives an interesting table where many of these measures are compared based on whether the zero-zero matches are included in the numerator, whether these matches are included in the denominator, and how the weighting of matches and mismatches is handled. Hilbe (1992b, 1992a) implemented an early Stata command for computing some of these (as well as other) binary similarity measures.

The formulas for some of these binary similarity measures are undefined when either one or both of the vectors (observations or variables depending on which are being compared) are all zeros (or, sometimes, all ones). Gower (1985) says concerning these cases, "These coefficients are then conventionally assigned some appropriate value, usually zero."

The following binary similarity coefficients are available. Unless stated otherwise, the similarity measures range from 0 to 1.

#### matching

requests the simple matching (Zubin 1938, Sokal and Michener 1958) binary similarity coefficient

$$\frac{a+d}{a+b+c+d}$$

which is the proportion of matches between the 2 observations or variables.

#### Jaccard

requests the Jaccard (1901, 1908) binary similarity coefficient

$$\frac{a}{a+b+c}$$

which is the proportion of matches when at least one of the vectors had a one. If both vectors are all zeros, this measure is undefined. Stata then declares the answer to be one, meaning perfect agreement. This is a reasonable choice for most applications and will cause an all-zero vector to have similarity of one only with another all-zero vector. In all other cases, an all-zero vector will have Jaccard similarity of zero to the other vector.

The Jaccard coefficient was discovered earlier by Gilbert (1884).

#### Russell

requests the Russell and Rao (1940) binary similarity coefficient

$$\frac{a}{a+b+c+d}$$

#### Hamann

requests the Hamann (1961) binary similarity coefficient

$$\frac{(a+d) - (b+c)}{a+b+c+d}$$

which is the number of agreements minus disagreements divided by the total. The Hamann coefficient ranges from -1, perfect disagreement, to 1, perfect agreement. The Hamann coefficient is equal to twice the simple matching coefficient minus 1.

#### Dice

requests the Dice binary similarity coefficient

$$\frac{2a}{2a+b+c}$$

suggested by Czekanowski (1932), Dice (1945), and Sørensen (1948). The Dice coefficient is similar to the Jaccard similarity coefficient but gives twice the weight to agreements. Like the Jaccard coefficient, the Dice coefficient is declared by Stata to be one if both vectors are all zero, thus avoiding the case where the formula is undefined.

#### antiDice

requests the binary similarity coefficient

$$\frac{a}{a+2(b+c)}$$

which is credited to Anderberg (1973) but was shown earlier by Sokal and Sneath (1963, 129). We did not call this the Anderberg coefficient because there is another coefficient better known by that name; see the Anderberg option. The name antiDice is our creation. This coefficient takes the opposite view from the Dice coefficient and gives double weight to disagreements. As with the Jaccard and Dice coefficients, the anti-Dice coefficient is declared to be one if both vectors are all zeros.

#### Sneath

requests the Sneath and Sokal (1962) binary similarity coefficient

$$\frac{2(a+d)}{2(a+d)+(b+c)}$$

which is similar to the simple matching coefficient but gives double weight to matches. Also compare the Sneath and Sokal coefficient with the Dice coefficient, which differs only in whether it includes d.

#### Rogers

requests the Rogers and Tanimoto (1960) binary similarity coefficient

$$\frac{a+d}{(a+d)+2(b+c)}$$

which takes the opposite approach from the Sneath and Sokal coefficient and gives double weight to disagreements. Also compare the Rogers and Tanimoto coefficient with the anti-Dice coefficient, which differs only in whether it includes d.

#### Ochiai

requests the Ochiai (1957) binary similarity coefficient

$$\frac{a}{\left\{(a+b)(a+c)\right\}^{1/2}}$$

The formula for the Ochiai coefficient is undefined when one or both of the vectors being compared are all zeros. If both are all zeros, Stata declares the measure to be one, and if only one of the two vectors is all zeros, the measure is declared to be zero.

The Ochiai coefficient was presented earlier by Driver and Kroeber (1932).

#### Yule

requests the Yule (see Yule [1900] and Yule and Kendall [1950]) binary similarity coefficient

$$\frac{ad - bc}{ad + bc}$$

which ranges from -1 to 1. The formula for the Yule coefficient is undefined when one or both of the vectors are either all zeros or all ones. Stata declares the measure to be 1 when b+c=0, meaning that there is complete agreement. Stata declares the measure to be -1 when a+d=0, meaning that there is complete disagreement. Otherwise, if ad-bc=0, Stata declares the measure to be 0. These rules, applied before using the Yule formula, avoid the cases where the formula would produce an undefined result.

#### Anderberg

requests the Anderberg binary similarity coefficient

$$\left(\frac{a}{a+b} + \frac{a}{a+c} + \frac{d}{c+d} + \frac{d}{b+d}\right) / 4$$

The Anderberg coefficient is undefined when one or both vectors are either all zeros or all ones. This difficulty is overcome by first applying the rule that if both vectors are all ones (or both vectors are all zeros), the similarity measure is declared to be one. Otherwise, if any of the marginal totals (a + b, a + c, c + d, b + d) are zero, then the similarity measure is declared to be zero.

Though this similarity coefficient is best known as the Anderberg coefficient, it appeared earlier in Sokal and Sneath (1963, 130).

#### Kulczynski

requests the Kulczyński (1927) binary similarity coefficient

$$\left(\frac{a}{a+b} + \frac{a}{a+c}\right)/2$$

The formula for this measure is undefined when one or both of the vectors are all zeros. If both vectors are all zeros, Stata declares the similarity measure to be one. If only one of the vectors is all zeros, the similarity measure is declared to be zero.

#### Pearson

requests Pearson's (1900)  $\phi$  binary similarity coefficient

$$\frac{ad - bc}{\{(a+b)(a+c)(d+b)(d+c)\}^{1/2}}$$

which ranges from -1 to 1. The formula for this coefficient is undefined when one or both of the vectors are either all zeros or all ones. Stata declares the measure to be 1 when b+c=0, meaning that there is complete agreement. Stata declares the measure to be -1 when a+d=0, meaning that there is complete disagreement. Otherwise, if ad-bc=0, Stata declares the measure to be 0. These rules, applied before using Pearson's  $\phi$  coefficient formula, avoid the cases where the formula would produce an undefined result.

#### Gower2

requests the binary similarity coefficient

$$\frac{ad}{\{(a+b)(a+c)(d+b)(d+c)\}^{1/2}}$$

which is presented by Gower (1985) but appeared earlier in Sokal and Sneath (1963, 130). Stata uses the name Gower2 to avoid confusion with the better-known Gower coefficient, which is used with a mix of binary and continuous data.

The formula for this similarity measure is undefined when one or both of the vectors are all zeros or all ones. This is overcome by first applying the rule that if both vectors are all ones (or both vectors are all zeros) then the similarity measure is declared to be one. Otherwise, if ad = 0, the similarity measure is declared to be zero.

### Dissimilarity measures for mixed data

Here is one measure that works with a mix of binary and continuous data. Binary variables are those containing only zeros, ones, and missing values; all other variables are treated as continuous.

#### Gower

requests the Gower (1971) dissimilarity coefficient for a mix of binary and continuous variables. For comparing observations i and j, the formula is

$$\frac{\sum_{v} \delta_{ijv} d_{ijv}}{\sum_{v} \delta_{ijv}}$$

where  $\delta_{ijv}$  is a binary indicator equal to 1 whenever both observations i and j are nonmissing for variable v, and zero otherwise. Observations with missing values are not included when using cluster or mds, and so if an observation is included,  $\delta_{ijv}=1$  and  $\sum_v \delta_{ijv}$  is the number of variables. However, using matrix dissimilarity with the Gower option does not exclude observations with missing values. See [MV] cluster, [MV] mds, and [MV] matrix dissimilarity.

For binary variables v,

$$d_{ijv} = \begin{cases} 0 & \text{if } x_{iv} = x_{jv} \\ 1 & \text{otherwise} \end{cases}$$

This is the same as the matching measure.

For continuous variables v,

$$d_{ijv} = \frac{|x_{iv} - x_{jv}|}{\left\{\max_k(x_{kv}) - \min_k(x_{kv})\right\}}$$

 $d_{ijv}$  is set to 0 if  $\max_k(x_{kv}) - \min_k(x_{kv}) = 0$ , that is, if the range of the variable is zero. This is the L1 measure divided by the range of the variable.

For comparing variables u and v, the formula is

$$\frac{\sum_{i} \delta_{iuv} d_{iuv}}{\sum_{i} \delta_{iuv}}$$

where  $\delta_{iuv}$  is a binary indicator equal to 1 whenever both variables u and v are nonmissing for observation i, and zero otherwise. If there are no missing values,  $\sum_i \delta_{iuv}$  is the number of observations; otherwise, it is the number of observations for which neither variable u nor v has a missing value.

If all the variables are binary,

$$d_{iuv} = \begin{cases} 0 & \text{if } x_{iu} = x_{iv} \\ 1 & \text{otherwise} \end{cases}$$

If at least one variable is continuous,

$$d_{iuv} = \frac{|x_{iu} - x_{iv}|}{\left\{\max_v(x_{iv}) - \min_v(x_{iv})\right\}}$$

 $d_{iuv}$  is set to 0 if  $\max_{v}(x_{iv}) - \min_{v}(x_{iv}) = 0$ , that is, if the range of the observation is zero.

The Gower measure interprets binary variables as those with only 0, 1, or missing values. All other variables are treated as continuous.

In [MV] matrix dissimilarity, missing observations are included only in the calculation of the Gower dissimilarity, but the formula for this dissimilarity measure is undefined when all the values of  $\delta_{ijv}$  or  $\delta_{iuv}$  are zero. The dissimilarity is then set to missing.

☐ Technical note: Matrix dissimilarity and the Gower measure

Normally the commands

- . matrix dissimilarity gm = x1 x2 y1, Gower
- . clustermat waverage gm, add

and

. cluster waverage x1 x2 y1, measure(Gower)

will yield the same results, and likewise with mdsmat and mds. However, if any of the variables contain missing observations, this will not be the case. cluster and mds exclude all observations that have missing values for any of the variables of interest, whereas matrix dissimilarity with the Gower option does not. See [MV] cluster, [MV] mds, and [MV] matrix dissimilarity for more information.

Note: matrix dissimilarity without the Gower option does exclude all observations that have missing values for any of the variables of interest.

□ Technical note: Binary similarity measures applied to averages

Some cluster-analysis methods (such as Stata's kmeans and kmedians clustering) need to compute the similarity or dissimilarity between observations and group averages or group medians; see [MV] cluster. With binary data, a group average is interpreted as a proportion.

A group median for binary data will be zero or one, except when there are an equal number of zeros and ones. Here Stata calls the median 0.5, which can also be interpreted as a proportion.

In Stata's cluster kmeans and cluster kmedians commands for comparing a binary observation to a group proportion (see *Partition cluster-analysis methods* in [MV] **cluster**), the values of a, b, c, and d are obtained by assigning the appropriate fraction of the count to these values. In our earlier table showing the relationship of a, b, c, and d in the cross-tabulation of observation i and observation j, we replace observation j by the group-proportions vector. Then when observation i is 1, we add the corresponding proportion to a and add one minus that proportion to a. When observation a is 0, we add the corresponding proportion to a and add one minus that proportion to a. After the values of a, a, a, a, and a are computed in this way, the binary similarity measures are computed using the formulas as already described.

Paul Jaccard (1868–1944) was a Swiss botanist who was born in Sainte-Croix (Vaud) and died in Zürich. He studied at Lausanne, Zürich, and Paris before being appointed to posts at Lausanne in 1894, where he specialized in plant geography, undertaking fieldwork in Egypt, Sweden, and Turkestan. In 1903, Jaccard returned to Zürich to a chair in general botany and plant physiology at ETH. His interests there centered on the microscopic analysis of wood, and anatomical and physiological studies of the growth of trees.

Robert Reuven Sokal (1926–2012) was born in Vienna to a Jewish family. He gained degrees from St. John's University in Shanghai and the University of Chicago. Sokal worked at the University of Kansas–Lawrence and (from 1969) the State University of New York–Stony Brook. He was one of the leaders in the development of numerical taxonomy (Sokal and Sneath 1963; Sneath and Sokal 1973) and was prominent in the application of statistical methods within biological systematics. With F. J. Rohlf, he authored one of the leading biometrics texts (Sokal and Rohlf 2011). In the latter stages of his career, his interests centered on genetic variation in human populations, European ethnohistory, and spatial statistics. Sokal was a member of the U.S. National Academy of Sciences.

Peter Henry Andrews Sneath (1923–2011) was born in Ceylon (now Sri Lanka) and studied medicine in Cambridge and London. After military service, he specialized in microbial systematics and the application of computers to biomedical science, working for the Medical Research Council in the UK and the University of Leicester. With Robert Sokal, Sneath wrote the two initial texts on numerical taxonomy. He is a Fellow of the Royal Society. A bacterial taxon, the genus *Sneathia*, was named after him in 2002.

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### Also see

- [MV] matrix dissimilarity Compute similarity or dissimilarity measures
- [MV] cluster Introduction to cluster-analysis commands
- [MV] **clustermat** Introduction to clustermat commands

### **Title**

### **mvreg** — Multivariate regression

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

Reference Also see

# **Description**

mvreg fits a multivariate regression model for several dependent variables with the same independent variables.

## **Quick start**

Multivariate regression of three y variables on two x variables

$$mvreg y1 y2 y3 = x1 x2$$

Add indicator variables for each level of categorical variable catvar

$$mvreg y1 y2 y3 = x1 x2 i.catvar$$

Model of three y variables on five x variables reporting the correlations between the residuals and the Breusch-Pagan test of independence

$$mvreg y1 y2 y3 = x1 x2 x3 x4 x5, corr$$

### Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Multivariate regression

# **Syntax**

```
mvreg depvars = indepvars [if] [in] [weight] [, options]
```

options	Description
Model	
$\underline{\mathtt{nocon}}\mathtt{stant}$	suppress constant term
Reporting	
<u>l</u> evel(#)	set confidence level; default is level(95)
<u>cor</u> r	report correlation matrix
display_options	control columns and column formats, row spacing, line width, display of omitted variables and base and empty cells, and factor-variable labeling
$\underline{\mathtt{noh}}\mathtt{eader}$	suppress header table from above coefficient table
<u>not</u> able	suppress coefficient table
$\underline{\mathtt{coefl}}\mathtt{egend}$	display legend instead of statistics

indepvars may contain factor variables; see [U] 11.4.3 Factor variables.

depvars and indepvars may contain time-series operators; see [U] 11.4.4 Time-series varlists.

bootstrap, by, jackknife, mi estimate, rolling, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

noheader, notable, and coeflegend do not appear in the dialog box.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

# **Options**

noconstant suppresses the constant term (intercept) in the model.

Reporting

level(#) specifies the confidence level, as a percentage, for confidence intervals. The default is level(95) or as set by set level; see [U] 20.7 Specifying the width of confidence intervals.

corr displays the correlation matrix of the residuals between the equations.

display\_options: noci, nopvalues, noomitted, vsquish, noemptycells, baselevels,
allbaselevels, nofvlabel, fvwrap(#), fvwrapon(style), cformat(%fmt), pformat(%fmt),
sformat(%fmt), and nolstretch; see [R] estimation options.

The following options are available with mvreg but are not shown in the dialog box:

noheader suppresses display of the table reporting F statistics, R-squared, and root mean squared error above the coefficient table.

notable suppresses display of the coefficient table.

coeflegend; see [R] estimation options.

## Remarks and examples

Multivariate regression differs from multiple regression in that several dependent variables are jointly regressed on the same independent variables. Multivariate regression is related to Zellner's seemingly unrelated regression (see [R] sureg), but because the same set of independent variables is used for each dependent variable, the syntax is simpler, and the calculations are faster.

The individual coefficients and standard errors produced by mvreg are identical to those that would be produced by regress estimating each equation separately. The difference is that mvreg, being a joint estimator, also estimates the between-equation covariances, so you can test coefficients across equations and, in fact, the test syntax makes such tests more convenient.

## ▶ Example 1

Using the automobile data, we fit a multivariate regression for space variables (headroom, trunk, and turn) in terms of a set of other variables, including three performance variables (displacement, gear\_ratio, and mpg):

- . use http://www.stata-press.com/data/r14/auto (1978 Automobile Data)
- . mvreg headroom trunk turn = price mpg displ gear\_ratio length weight

mpg        0093774         .0260463         -0.36         0.720        061366         .0426112           displacement         .0031025         .0024999         1.24         0.219        0018873         .0080922           gear_ratio         .2108071         .3539588         0.60         0.553        4956976         .9173115           length         .015886         .012944         1.23         0.224        0099504         .0417223           weight        0000868         .0004724         -0.18         0.855        0010296         .0008561           _cons        4525117         2.170073         -0.21         0.835         -4.783995         3.878972           trunk         price         .0000445         .0001567         0.28         0.778        0002684         .0003573           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690885           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight        0015944         .	Equation	0bs	Parms	RMSE	"R-sq"	F	P
Tunk	headroom	74	7	.7390205	0.2996	4.777213	0.0004
Coef. Std. Err. t P> t  [95% Conf. Interval]	trunk	74	7	3.052314	0.5326	12.7265	0.0000
headroom  price	turn	74	7	2.132377	0.7844	40.62042	0.0000
price        0000528         .000038         -1.39         0.168        0001286         .0000228           mpg        0093774         .0260463         -0.36         0.720        061366         .0426112           displacement         .0031025         .0024999         1.24         0.219        0018873         .0080922           gear_ratio         .2108071         .3539588         0.60         0.553        4956976         .9173115           length         .015886         .012944         1.23         0.224        0099504         .0417223           weight        0000868         .0004724         -0.18         0.855        0010296         .0008561           _cons        4525117         2.170073         -0.21         0.835         -4.783995         3.878972           trunk          price         .0000445         .0001567         0.28         0.778        0002684         .0003573           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690885           length         .170		Coef.	Std. Err	:. t	P> t	[95% Conf	. Interval]
mpg        0093774         .0260463         -0.36         0.720        061366         .0426112           displacement         .0031025         .0024999         1.24         0.219        0018873         .0080922           gear_ratio         .2108071         .3539588         0.60         0.553        4956976         .9173115           length         .015886         .012944         1.23         0.224        0099504         .0417223           weight        0000868         .0004724         -0.18         0.855        0010296         .0008561           _cons        4525117         2.170073         -0.21         0.835         -4.783995         3.878972           trunk         price         .0000445         .0001567         0.28         0.778        0002684         .0003573           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690882           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight        0015944         .	headroom						
displacement         .0031025         .0024999         1.24         0.219        0018873         .0080922           gear_ratio         .2108071         .3539588         0.60         0.553        4956976         .9173119           length         .015886         .012944         1.23         0.224        0099504         .0417223           weight        0000868         .0004724         -0.18         0.855        0010296         .0008561           _cons        4525117         2.170073         -0.21         0.835         -4.783995         3.878972           trunk           price         .0000445         .0001567         0.28         0.778        0002684         .0003573           mpg        0220919         .1075767         -0.21         0.838        2368159         .1926322           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690885           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight	price	0000528	.000038	-1.39	0.168	0001286	.0000229
Gear_ratio   .2108071   .3539588   0.60   0.553  4956976   .9173119   .9	mpg	0093774	.0260463	-0.36	0.720	061366	.0426112
length weight	displacement	.0031025	.0024999	1.24	0.219	0018873	.0080922
weight _cons        0000868         .0004724         -0.18         0.855        0010296         .0008561           _cons        4525117         2.170073         -0.21         0.835         -4.783995         3.878972           trunk         price         .0000445         .0001567         0.28         0.778        0002684         .0003573           mpg        0220919         .1075767         -0.21         0.838        2368159         .1926322           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.69088           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight        0015944         .001951         -0.82         0.417        0054885         .0022997           _cons         -13.28253         8.962868         -1.48         0.143         -31.17249         4.607428           turn         price        0002647         .0001095         -2.42         0.018        0004833        0000462           mpg        04929	gear_ratio	.2108071	.3539588	0.60	0.553	4956976	.9173119
cons	length	.015886	.012944	1.23	0.224	0099504	.0417223
trunk  price	weight	0000868	.0004724	-0.18	0.855	0010296	.0008561
price         .0000445         .0001567         0.28         0.778        0002684         .0003573           mpg        0220919         .1075767         -0.21         0.838        2368159         .1926322           displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690885           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight        0015944         .001951         -0.82         0.417        0054885         .0022997           _cons         -13.28253         8.962868         -1.48         0.143         -31.17249         4.607429           turn         price        0002647         .0001095         -2.42         0.018        0004833        0000462           mpg        0492948         .0751542         -0.66         0.514        1993031         .1007136           displacement         .0036977         .0072132         0.51         0.610        0106999         .0180953           gear_ratio        1048432	_cons	4525117	2.170073	-0.21	0.835	-4.783995	3.878972
mpg	trunk						
displacement         .0032118         .0103251         0.31         0.757        0173971         .0238207           gear_ratio        2271321         1.461926         -0.16         0.877         -3.145149         2.690885           length         .170811         .0534615         3.20         0.002         .0641014         .2775206           weight        0015944         .001951         -0.82         0.417        0054885         .0022997           _cons         -13.28253         8.962868         -1.48         0.143         -31.17249         4.607426           turn         price        0002647         .0001095         -2.42         0.018        0004833        0000462           mpg        0492948         .0751542         -0.66         0.514        1993031         .1007136           displacement         .0036977         .0072132         0.51         0.610        0106999         .0180953           gear_ratio        1048432         1.021316         -0.10         0.919         -2.143399         1.933712           length         .072128         .0373487         1.93         0.058        0024204         .1466764           weight         .0027059 <td>price</td> <td>.0000445</td> <td>.0001567</td> <td>0.28</td> <td>0.778</td> <td>0002684</td> <td>.0003573</td>	price	.0000445	.0001567	0.28	0.778	0002684	.0003573
gear_ratio	mpg	0220919	.1075767	-0.21	0.838	2368159	.1926322
length weight	displacement	.0032118	.0103251	0.31	0.757	0173971	.0238207
weight _cons        0015944	gear_ratio	2271321	1.461926	-0.16	0.877	-3.145149	2.690885
cons	length	.170811	.0534615	3.20	0.002	.0641014	.2775206
turn  price0002647 .0001095 -2.42 0.01800048330000462  mpg0492948 .0751542 -0.66 0.5141993031 .1007136  displacement .0036977 .0072132 0.51 0.6100106999 .0180953  gear_ratio1048432 1.021316 -0.10 0.919 -2.143399 1.933712  length .072128 .0373487 1.93 0.0580024204 .1466764  weight .0027059 .001363 1.99 0.0510000145 .0054264	weight	0015944	.001951	-0.82	0.417	0054885	.0022997
price        0002647         .0001095         -2.42         0.018        0004833        0000462           mpg        0492948         .0751542         -0.66         0.514        1993031         .1007136           displacement         .0036977         .0072132         0.51         0.610        0106999         .0180953           gear_ratio        1048432         1.021316         -0.10         0.919         -2.143399         1.933712           length         .072128         .0373487         1.93         0.058        0024204         .1466764           weight         .0027059         .001363         1.99         0.051        0000145         .0054264	_cons	-13.28253	8.962868	3 -1.48	0.143	-31.17249	4.607429
mpg        0492948         .0751542         -0.66         0.514        1993031         .1007136           displacement         .0036977         .0072132         0.51         0.610        0106999         .0180953           gear_ratio        1048432         1.021316         -0.10         0.919         -2.143399         1.933712           length         .072128         .0373487         1.93         0.058        0024204         .1466764           weight         .0027059         .001363         1.99         0.051        0000145         .0054264	turn						
displacement     .0036977     .0072132     0.51     0.610    0106999     .0180953       gear_ratio    1048432     1.021316     -0.10     0.919     -2.143399     1.933712       length     .072128     .0373487     1.93     0.058    0024204     .1466764       weight     .0027059     .001363     1.99     0.051    0000145     .0054264	price	0002647	.0001095	-2.42	0.018	0004833	0000462
gear_ratio    1048432     1.021316     -0.10     0.919     -2.143399     1.933712       length     .072128     .0373487     1.93     0.058    0024204     .1466764       weight     .0027059     .001363     1.99     0.051    0000145     .0054264	mpg	0492948	.0751542	-0.66	0.514	1993031	.1007136
length weight .072128 .0373487 1.93 0.0580024204 .1466764 .0027059 .001363 1.99 0.0510000145 .0054264	displacement	.0036977	.0072132	0.51	0.610	0106999	.0180953
weight .0027059 .001363 1.99 0.0510000145 .0054264	gear_ratio	1048432	1.021316	-0.10	0.919	-2.143399	1.933712
9	length	.072128	.0373487	1.93	0.058	0024204	.1466764
_cons   20.19157 6.261549 3.22 0.002 7.693467 32.68968	weight	.0027059	.001363	1.99	0.051	0000145	.0054264
	_cons	20.19157	6.261549	3.22	0.002	7.693467	32.68968

We should have specified the corr option so that we would also see the correlations between the residuals of the equations. We can correct our omission because mvreg—like all estimation commands—typed without arguments redisplays results. The noheader and notable (read "notable") options suppress redisplaying the output we have already seen:

. mvreg, notable noheader corr Correlation matrix of residuals: headroom trunk turn 1.0000 headroom trunk 0.4986 1.0000 turn -0.1090 -0.0628 1.0000 Breusch-Pagan test of independence: chi2(3) = 19.566, Pr = 0.0002

The Breusch-Pagan test is significant, so the residuals of these three space variables are not independent of each other.

The three performance variables among our independent variables are mpg, displacement, and gear\_ratio. We can jointly test the significance of these three variables in all the equations by typing

```
. test mpg displacement gear_ratio
      [headroom]mpg = 0
 ( 2) [trunk]mpg = 0
 (3) [turn]mpg = 0
 (4) [headroom]displacement = 0
 (5) [trunk]displacement = 0
 (6) [turn]displacement = 0
 (7)
      [headroom]gear_ratio = 0
 (8)
      [trunk]gear_ratio = 0
 (9)
     [turn]gear_ratio = 0
      F( 9,
                67) =
           Prob > F =
                         0.9622
```

These three variables are not, as a group, significant. We might have suspected this from their individual significance in the individual regressions, but this multivariate test provides an overall assessment with one *p*-value.

We can also perform a test for the joint significance of all three equations:

```
. test [headroom]
 (output omitted)
. test [trunk], accum
 (output omitted)
. test [turn], accum
 (1)
       [headroom]price = 0
 (2)
       [headroom]mpg = 0
 (3)
       [headroom]displacement = 0
 (4)
       [headroom]gear_ratio = 0
 (5)
      [headroom]length = 0
 (6)
       [headroom]weight = 0
 (7)
       [trunk]price = 0
 (8)
      [trunk]mpg = 0
 (9)
      [trunk]displacement = 0
 (10) [trunk]gear_ratio = 0
 (11) [trunk]length = 0
 (12) [trunk] weight = 0
 (13) [turn]price = 0
 (14) [turn]mpg = 0
 (15) [turn]displacement = 0
 (16) [turn]gear_ratio = 0
 (17) [turn]length = 0
 (18) [turn] weight = 0
                67) =
      F( 18.
                         19.34
           Prob > F =
                        0.0000
```

The set of variables as a whole is strongly significant. We might have suspected this, too, from the individual equations. 1

#### □ Technical note

The mvreg command provides a good way to deal with multiple comparisons. If we wanted to assess the effect of length, we might be dissuaded from interpreting any of its coefficients except that in the trunk equation. [trunk]length—the coefficient on length in the trunk equation—has a p-value of 0.002, but in the other two equations, it has p-values of only 0.224 and 0.058.

A conservative statistician might argue that there are 18 tests of significance in mvreg's output (not counting those for the intercept), so p-values more than 0.05/18 = 0.0028 should be declared insignificant at the 5% level. A more aggressive but, in our opinion, reasonable approach would be to first note that the three equations are jointly significant, so we are justified in making some interpretation. Then we would work through the individual variables using test, possibly using 0.05/6 = 0.0083 (6 because there are six independent variables) for the 5% significance level. For instance, examining length:

```
. test length
 (1) [headroom]length = 0
 (2) [trunk]length = 0
 (3) [turn]length = 0
      F( 3.
                67) =
                         4.94
           Prob > F =
                         0.0037
```

The reported significance level of 0.0037 is less than 0.0083, so we will declare this variable significant. [trunk] length is certainly significant with its p-value of 0.002, but what about in the remaining two equations with p-values 0.224 and 0.058? We perform a joint test:

```
. test [headroom]length [turn]length
( 1) [headroom]length = 0
( 2) [turn]length = 0

F( 2, 67) = 2.91
Prob > F = 0.0613
```

At this point, reasonable statisticians could disagree. The 0.06 significance value suggests no interpretation, but these were the two least-significant values out of three, so we would expect the *p*-value to be a little high. Perhaps an equivocal statement is warranted: there seems to be an effect, but chance cannot be excluded.

### Stored results

mvreg stores the following in e():

```
number of observations
    e(N)
                          number of parameters in each equation
    e(k)
                          number of equations in e(b)
    e(k_eq)
    e(df_r)
                          residual degrees of freedom
    e(chi2)
                          Breusch-Pagan \chi^2 (corr only)
    e(df_chi2)
                          degrees of freedom for Breusch-Pagan \chi^2 (corr only)
    e(rank)
                          rank of e(V)
Macros
    e(cmd)
                          mvreg
    e(cmdline)
                          command as typed
    e(depvar)
                          names of dependent variables
                          names of equations
    e(eqnames)
    e(wtype)
                          weight type
                          weight expression
    e(wexp)
                          R-squared for each equation
    e(r2)
    e(rmse)
                          RMSE for each equation
    e(F)
                          F statistic for each equation
    e(p_F)
                          significance of F for each equation
    e(properties)
    e(estat_cmd)
                          program used to implement estat
    e(predict)
                          program used to implement predict
                          predictions allowed by margins
    e(marginsok)
                          predictions disallowed by margins
    e(marginsnotok)
                          default predict() specification for margins
    e(marginsdefault)
                          factor variables fvset as asbalanced
    e(asbalanced)
    e(asobserved)
                          factor variables fyset as asobserved
Matrices
                          coefficient vector
    e(b)
                          Σ matrix
    e(Sigma)
    e(V)
                          variance-covariance matrix of the estimators
Functions
    e(sample)
                          marks estimation sample
```

### Methods and formulas

Given q equations and p independent variables (including the constant), the parameter estimates are given by the  $p \times q$  matrix

 $\mathbf{B} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{X}'\mathbf{W}\mathbf{Y}$ 

where  $\mathbf{Y}$  is an  $n \times q$  matrix of dependent variables and  $\mathbf{X}$  is a  $n \times p$  matrix of independent variables.  $\mathbf{W}$  is a weighting matrix equal to  $\mathbf{I}$  if no weights are specified. If weights are specified, let  $\mathbf{v} : 1 \times n$  be the specified weights. If fweight frequency weights are specified,  $\mathbf{W} = \operatorname{diag}(\mathbf{v})$ . If aweight analytic weights are specified,  $\mathbf{W} = \operatorname{diag}\{\mathbf{v}/(\mathbf{1}'\mathbf{v})(\mathbf{1}'\mathbf{1})\}$ , meaning that the weights are normalized to sum to the number of observations.

The residual covariance matrix is

$$\mathbf{R} = {\mathbf{Y'WY} - \mathbf{B'(X'WX)B}}/(n-p)$$

The estimated covariance matrix of the estimates is  $\mathbf{R} \otimes (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}$ . These results are identical to those produced by sureg when the same list of independent variables is specified repeatedly; see [R] sureg.

The Breusch and Pagan (1980)  $\chi^2$  statistic—a Lagrange multiplier statistic—is given by

$$\lambda = n \sum_{i=1}^{q} \sum_{j=1}^{i-1} r_{ij}^2$$

where  $r_{ij}$  is the estimated correlation between the residuals of the equations and n is the number of observations. It is distributed as  $\chi^2$  with q(q-1)/2 degrees of freedom.

### Reference

Breusch, T. S., and A. R. Pagan. 1980. The Lagrange multiplier test and its applications to model specification in econometrics. *Review of Economic Studies* 47: 239–253.

## Also see

[MV] mvreg postestimation — Postestimation tools for mvreg

[MV] manova — Multivariate analysis of variance and covariance

[MI] estimation — Estimation commands for use with mi estimate

[R] **nlsur** — Estimation of nonlinear systems of equations

[R] reg3 — Three-stage estimation for systems of simultaneous equations

[R] regress — Linear regression

[R] regress postestimation — Postestimation tools for regress

[R] sureg — Zellner's seemingly unrelated regression

[SEM] intro 5 — Tour of models

[U] 20 Estimation and postestimation commands

## **Title**

mvreg postestimation — Postestimation tools for mvreg

Postestimation commands predict margins Also see

# **Postestimation commands**

The following postestimation commands are available after mvreg:

	Command	Description
	contrast	contrasts and ANOVA-style joint tests of estimates
	estat summarize	summary statistics for the estimation sample
	estat vce	variance-covariance matrix of the estimators (VCE)
	estimates	cataloging estimation results
*	forecast	dynamic forecasts and simulations
	hausman	Hausman's specification test
	lincom	point estimates, standard errors, testing, and inference for linear combinations of coefficients
	margins	marginal means, predictive margins, marginal effects, and average marginal effects
	marginsplot	graph the results from margins (profile plots, interaction plots, etc.)
	nlcom	point estimates, standard errors, testing, and inference for nonlinear combinations of coefficients
	predict	predictions, residuals, influence statistics, and other diagnostic measures
	predictnl	point estimates, standard errors, testing, and inference for generalized predictions
	pwcompare	pairwise comparisons of estimates
	test	Wald tests of simple and composite linear hypotheses
	testnl	Wald tests of nonlinear hypotheses

<sup>\*</sup> forecast is not appropriate with mi estimation results.

## predict

### **Description for predict**

predict creates a new variable containing predictions such as linear predictions, standard errors, residuals, and differences between the linear predictions.

### Menu for predict

Statistics > Postestimation

### Syntax for predict

predict	[type] newvar [if] [in] [, equation(eqno[, eqno]) statistic]	
statistic	Description	
Main		
хb	linear prediction; the default	
stdp	standard error of the linear prediction	
<u>r</u> esiduals	residuals	
<u>d</u> ifference <u>stdd</u> p	difference between the linear predictions of two equations standard error of the difference in linear predictions	

These statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample.

## **Options for predict**

Main

equation(eqno[ , eqno]) specifies the equation to which you are referring.

equation() is filled in with one *eqno* for the xb, stdp, and residuals options. equation(#1) would mean the calculation is to be made for the first equation, equation(#2) would mean the second, and so on. You could also refer to the equations by their names. equation(income) would refer to the equation named income and equation(hours), to the equation named hours.

If you do not specify equation(), results are the same as if you specified equation(#1).

difference and stddp refer to between-equation concepts. To use these options, you must specify two equations, for example, equation(#1,#2) or equation(income,hours). When two equations must be specified, equation() is required. With equation(#1,#2), difference computes the prediction of equation(#1) minus the prediction of equation(#2).

xb, the default, calculates the fitted values—the prediction of  $x_j b$  for the specified equation.

stdp calculates the standard error of the prediction for the specified equation (the standard error of the predicted expected value or mean for the observation's covariate pattern). The standard error of the prediction is also referred to as the standard error of the fitted value.

residuals calculates the residuals.

difference calculates the difference between the linear predictions of two equations in the system.

stddp is allowed only after you have previously fit a multiple-equation model. The standard error of the difference in linear predictions  $(\mathbf{x}_{1j}\mathbf{b} - \mathbf{x}_{2j}\mathbf{b})$  between equations 1 and 2 is calculated.

For more information on using predict after multiple-equation estimation commands, see [R] predict.

# margins

### **Description for margins**

margins estimates margins of responses for linear predictions, fitted values, and differences between the linear predictions.

### Menu for margins

Statistics > Postestimation

# Syntax for margins

```
margins [marginlist], \underline{predict(statistic ...)} [\underline{predict(statistic ...)} ...] [options]

statistic Description

default linear predictions for each equation x_i b, fitted values
```

default	linear predictions for each equation
xb	$\mathbf{x}_{j}\mathbf{b}$ , fitted values
$\underline{\mathtt{d}}\mathtt{ifference}$	difference between the linear predictions of two equations
$\underline{\mathtt{r}}\mathtt{esiduals}$	not allowed with margins
stdp	not allowed with margins
<u>stdd</u> p	not allowed with margins

xb defaults to the first equation.

Statistics not allowed with margins are functions of stochastic quantities other than e(b).

For the full syntax, see [R] margins.

margins [marginlist] [, options]

## Also see

[MV] **mvreg** — Multivariate regression

[U] 20 Estimation and postestimation commands

#### **Title**

**mvtest** — Multivariate tests

Description Syntax References Also see

# Description

mvtest performs multivariate tests on means, covariances, and correlations and tests of univariate, bivariate, and multivariate normality. The tests of means, covariances, and correlations assume multivariate normality (Mardia, Kent, and Bibby 1979). Both one-sample and multiple-sample tests are provided. All multiple-sample tests provided by mvtest assume independent samples.

Structural equation modeling provides a more general framework for estimating means, covariances, and correlations and testing for differences across groups; see [SEM] intro 5 and [SEM] example 16.

# **Syntax**

mvtest subcommand ... [, ...]

subcommand	Description	See
means	test means	[MV] mvtest means
covariances	test covariances	[MV] mvtest covariances
correlations	test correlations	[MV] mvtest correlations
normality	test multivariate normality	[MV] mvtest normality

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#### Also see

- [MV] canon Canonical correlations
- [MV] **hotelling** Hotelling's T-squared generalized means test
- [MV] manova Multivariate analysis of variance and covariance
- [R] correlate Correlations (covariances) of variables or coefficients
- [R] mean Estimate means
- [R] **sdtest** Variance-comparison tests
- [R] **sktest** Skewness and kurtosis test for normality
- [R] swilk Shapiro-Wilk and Shapiro-Francia tests for normality
- [R] **ttest** t tests (mean-comparison tests)
- [SEM] **intro 5** Tour of models
- [SEM] example 16 Correlation

#### Title

**mvtest correlations** — Multivariate tests of correlations

Description Quick start

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## Menu

Options for one-sample tests Methods and formulas

# **Description**

mvtest correlations performs one-sample and multiple-sample tests on correlations. These tests assume multivariate normality.

See [MV] mvtest for more multivariate tests.

### **Quick start**

Lawley's test that the correlations of variables v1, v2, v3, and v4 are equal mytest correlations v1 v2 v3 v4

Jennrich's test that the correlation matrix equals hypothesized matrix mymat mvtest correlations v1 v2 v3 v4, equals(mymat)

Jennrich's test for equal correlations with samples defined by catvar mvtest correlations v1 v2 v3 v4 v5, by(catvar)

### Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Multivariate test of means, covariances, and normality

# **Syntax**

Multiple-sample tests

mvtest correlations varlist [if] [in] [weight], by(groupvars) [multisample\_options]

One-sample tests

mvtest correlations varlist [if] [in] [weight] [, one-sample\_options]

multisample_options	Description
Model *by(groupvars) missing	compare subsamples with same values in <i>groupvars</i> treat missing values in <i>groupvars</i> as ordinary values

<sup>\*</sup> by (groupvars) is required.

one-sample_options	Description
Options	
compound	test that correlation matrix is compound symmetric (equal correlations); the default
$\underline{\mathbf{e}}\mathtt{quals}(C)$	test that correlation matrix equals matrix C

bootstrap, by, jackknife, rolling, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

# Options for multiple-sample tests

Model

by (groupvars) is required with the multiple-sample version of the test. Observations with the same values in groupvars form each sample. Observations with missing values in groupvars are ignored, unless the missing option is specified. A Wald test due to Jennrich (1970) is displayed.

missing specifies that missing values in groupvars are treated like ordinary values.

# Options for one-sample tests

Options

compound, the default, tests the hypothesis that the correlation matrix of the variables is compound symmetric, that is, that the correlations of all variables in *varlist* are the same. Lawley's (1963) chi-squared test is displayed.

equals (C) tests the hypothesis that the correlation matrix of *varlist* is C. The matrix C should be  $k \times k$ , symmetric, and positive definite. C is converted to a correlation matrix if needed. The row and column names of C are immaterial. A Wald test due to Jennrich (1970) is displayed.

# Remarks and examples

Remarks are presented under the following headings:

One-sample tests for correlation matrices A multiple-sample test for correlation matrices

### One-sample tests for correlation matrices

Both one-sample and multiple-sample tests of correlation matrices are provided with the mvtest correlations command. The one-sample tests include Lawley's (1963) test that the correlation matrix is compound symmetric (that is, all correlations are equal), and the Wald test proposed by Jennrich (1970) that the correlation matrix equals a given correlation matrix.

### Example 1

The gasoline-powered milk-truck dataset introduced in example 1 of [MV] mvtest means has price per mile for fuel, repair, and capital. We test if the correlations between these three variables are equal (that is, the correlation matrix is compound symmetric) using the compound option of mvtest correlations.

We reject the null hypothesis and conclude that there are probably differences in the correlations of the three cost variables.

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# Example 2

Using the equals () option of mvtest correlations, we test the hypothesis that fuel and repair costs have a correlation of 0.75, while the correlation between capital and these two variables is zero.

```
. matrix C = (1, 0.75, 0 \setminus 0.75, 1, 0 \setminus 0, 0, 1)
. matrix list C
symmetric C[3,3]
     c1
         c2 c3
r1
      1
    .75
r2
           1
                 1
      0
. mvtest correlations fuel repair capital, equals(C)
Test that correlation matrix equals specified pattern C
                                4.55
      Jennrich chi2(3) =
            Prob > chi2 =
                              0.2077
```

We fail to reject this null hypothesis.

### A multiple-sample test for correlation matrices

A multiple-sample test of equality of correlation matrices is provided by the mvtest correlations command with the by() option defining the multiple samples (groups).

### Example 3

Psychological test score data are introduced in example 2 of [MV] **mvtest covariances**. We test whether the correlation matrices for the four test scores are the same for males and females.

```
. use http://www.stata-press.com/data/r14/genderpsych
(Four Psychological Test Scores, Rencher and Christensen (2012))
. mvtest correlations y1 y2 y3 y4, by(gender)
Test of equality of correlation matrices across samples
    Jennrich chi2(6) = 5.01
    Prob > chi2 = 0.5422
```

We fail to reject the null hypothesis of equal correlation matrices for males and females.

4

### Stored results

```
mvtest correlations stores the following in r():
```

```
Scalars r(\text{chi2}) \chi^2 statistic r(\text{df}) degrees of freedom for \chi^2 test r(p\_\text{chi2}) significance

Macros r(\text{chi2type}) type of model \chi^2 test
```

## Methods and formulas

Methods and formulas are presented under the following headings:

```
One-sample tests for correlation matrices
A multiple-sample test for correlation matrices
```

## One-sample tests for correlation matrices

Let the sample consist of N i.i.d. observations from a k-variate multivariate normal distribution  $\text{MVN}_k(\mu, \Sigma)$ , with sample correlation matrix  $\mathbf{R}$ .

To test that a correlation matrix equals a given matrix,  $\mathbf{R}_0$ , mytest correlations computes a Wald test proposed by Jennrich (1970):

$$\chi^2_{\mathrm{ocf}} = \frac{1}{2} \mathrm{trace}(\mathbf{Z}\mathbf{Z}) - \mathrm{diagonal}(\mathbf{Z})' \left(\mathbf{I} + \mathbf{R}_0 \bullet \mathbf{R}_0^{-1}\right)^{-1} \mathrm{diagonal}(\mathbf{Z})$$

where  $\mathbf{Z} = \sqrt{N}\mathbf{R}_0^{-1}(\mathbf{R} - \mathbf{R}_0)$  and  $\bullet$  denotes the Hadamard product.  $\chi^2_{\text{ocf}}$  is asymptotically  $\chi^2$  distributed with k(k-1)/2 degrees of freedom.

To test that the correlation matrix is compound symmetric, that is, to test that all correlations are equal, the likelihood-ratio test is somewhat cumbersome. Lawley (1963) offers an asymptotically equivalent test that is computationally simple (Johnson and Wichern 2007, 457–458):

$$\chi_{\text{occ}}^{2} = \frac{N-1}{(1-\overline{R})^{2}} \left\{ \sum_{i=2}^{k} \sum_{j=1}^{i-1} (R_{ij} - \overline{R})^{2} - u \sum_{h=1}^{k} (\overline{R}_{h} - \overline{R})^{2} \right\}$$

where

$$\overline{R} = \frac{2}{k(k-1)} \sum_{i=2}^{k} \sum_{j=1}^{i-1} R_{ij}$$

$$\overline{R}_h = \frac{1}{k-1} \sum_{i=1; i \neq h}^{k} R_{ih}$$

$$u = \frac{(k-1)^2 \left\{ 1 - (1 - \overline{R})^2 \right\}}{k - (k-2)(1 - \overline{R})^2}$$

and  $R_{ij}$  denotes element (i,j) of the  $k \times k$  correlation matrix  $\mathbf{R}$ .  $\chi^2_{\rm occ}$  is asymptotically  $\chi^2$  distributed with (k-2)(k+1)/2 degrees of freedom. Aitkin, Nelson, and Reinfurt (1968) study the quality of this  $\chi^2$  approximation for k up to six and various correlations, and conclude that the approximation is adequate for N as small as 25.

### A multiple-sample test for correlation matrices

Let there be  $m \geq 2$  independent samples with the jth sample containing  $N_j$  i.i.d. observations from a k-variate multivariate normal distribution,  $MVN_k(\mu_j, \Sigma_j)$ , with sample correlation matrix  $\mathbf{R}_j$ , j = 1, ..., m. Let  $N = \sum_{i=1}^{m} N_{i}$ .

To test for the equality of correlation matrices across m independent samples, mytest correlations computes a Wald test proposed by Jennrich (1970):

$$\chi^2_{\mathrm{mc}} = \sum_{j=1}^m \left\{ \frac{1}{2} \mathrm{trace} \left( \mathbf{Z}_j^2 \right) - \mathrm{diagonal} \left( \mathbf{Z}_j \right)' \left( \mathbf{I} + \overline{\mathbf{R}} \bullet \overline{\mathbf{R}}^{-1} \right)^{-1} \mathrm{diagonal} \left( \mathbf{Z}_j \right) \right\}$$

where  $\overline{\mathbf{R}} = 1/N \sum_{j=1}^{m} N_j \mathbf{R}_j$ ,  $\mathbf{Z}_j = \sqrt{N_j} \overline{\mathbf{R}}^{-1} (\mathbf{R}_j - \overline{\mathbf{R}})$ , and  $\bullet$  denotes the Hadamard product.  $\chi^2_{\rm mc}$  is asymptotically  $\chi^2$  distributed with (m-1)k(k-1)/2 degrees of freedom.

## References

Aitkin, M. A., W. C. Nelson, and K. H. Reinfurt. 1968. Tests for correlation matrices. Biometrika 55: 327-334.

Jennrich, R. I. 1970. An asymptotic  $\chi^2$  test for the equality of two correlation matrices. Journal of the American Statistical Association 65: 904-912.

Johnson, R. A., and D. W. Wichern. 2007. Applied Multivariate Statistical Analysis. 6th ed. Englewood Cliffs, NJ: Prentice Hall.

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# Also see

[MV] canon — Canonical correlations

[R] correlate — Correlations (covariances) of variables or coefficients

### Title

#### **mvtest covariances** — Multivariate tests of covariances

Description Quick start

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Remarks and examples Stored results Methods and formulas

References Also see

# **Description**

mvtest covariances performs one-sample and multiple-sample multivariate tests on covariances. These tests assume multivariate normality.

See [MV] mvtest for other multivariate tests. See [R] sdtest for univariate tests of standard deviations.

Menu

### **Quick start**

Test that the covariance matrix of v1, v2, v3, and v4 is diagonal mytest covariances v1 v2 v3 v4

Test that the covariance matrix is spherical

mvtest covariances v1 v2 v3 v4, spherical

Test that the covariance matrix is compound symmetric

mvtest covariances v1 v2 v3 v4, compound

Test that the covariance matrix of the variables equals matrix mymat

mvtest covariances v1 v2 v3 v4, equals(mymat)

Test that the covariance matrix is block diagonal with v1, v2, and v3 as block 1, v4 as block 2, and v5 and v6 as block 3

```
mvtest cov v1 v2 v3 v4 v5 v6, block(v1 v2 v3 || v4 || v5 v6)
```

Box's M test that the covariance matrix of v1, v2, and v3 is the same across the groups defined by catvar

```
mvtest cov v1 v2 v3, by(catvar)
```

### Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Multivariate test of means, covariances, and normality

# **Syntax**

```
Multiple-sample tests
```

mvtest covariances varlist [if] [in] [weight], by(groupvars) [multisample\_options]

One-sample tests

mvtest covariances varlist [if] [in] [weight] [, one-sample\_options]

multisample\_options

Description

Decemintion

Model

\*by(groupvars)
missing

compare subsamples with same values in *groupvars* treat missing values in *groupvars* as ordinary values

one-sample_opπons	Description		
Options			
diagonal	test that covariance matrix is diagonal; the default		
spherical	test that covariance matrix is spherical		
compound	test that covariance matrix is compound symmetric		
$\underline{e}$ quals( $C$ )	test that covariance matrix equals matrix C		
* $\underline{\text{bl}}$ ock( $varlist_1$ [  ])	test that covariance matrix is block diagonal with blocks corresponding to varlist#		

<sup>\*</sup> The full specification is  $\underline{\mathtt{block}}(\mathit{varlist}_1 \ [\ ||\ \mathit{varlist}_2 \ [\ ||\ \dots]\ ]).$ 

bootstrap, by, jackknife, rolling, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

# Options for multiple-sample tests

Model

by (*groupvars*) is required with the multiple-sample version of the test. Observations with the same values in *groupvars* form a sample. Observations with missing values in *groupvars* are ignored, unless the missing option is specified.

A modified likelihood-ratio statistic testing the equality of covariance matrices for the multiple independent samples defined by by () is presented along with an F and chi-squared approximation due to Box (1949). This test is also known as Box's M test.

missing specifies that missing values in *groupvars* are treated like ordinary values.

<sup>\*</sup> by (groupvars) is required.

# Options for one-sample tests

Options

- diagonal, the default, tests the hypothesis that the covariance matrix is diagonal, that is, that the variables in *varlist* are independent. A likelihood-ratio test with first-order Bartlett correction is displayed.
- spherical tests the hypothesis that the covariance matrix is diagonal with constant diagonal values, that is, that the variables in varlist are homoskedastic and independent. A likelihood-ratio test with first-order Bartlett correction is displayed.
- compound tests the hypothesis that the covariance matrix is compound symmetric, that is, that the variables in *varlist* are homoskedastic and that every pair of two variables has the same covariance. A likelihood-ratio test with first-order Bartlett correction is displayed.
- equals (C) specifies that the hypothesized covariance matrix for the k variables in varlist is C. The matrix C must be  $k \times k$ , symmetric, and positive definite. The row and column names of C are ignored. A likelihood-ratio test with first-order Bartlett correction is displayed.
- $block(varlist_1 \mid || varlist_2 \mid || \dots ||)$  tests the hypothesis that the covariance matrix is block diagonal with blocks  $varlist_1$ ,  $varlist_2$ , etc. Variables in varlist not included in  $varlist_1$ ,  $varlist_2$ , etc., are treated as an additional block. With this pattern, variables in different blocks are independent, but no assumptions are made on the within-block covariance structure. A likelihood-ratio test with first-order Bartlett correction is displayed.

## Remarks and examples

Remarks are presented under the following headings:

One-sample tests for covariance matrices A multiple-sample test for covariance matrices

## One-sample tests for covariance matrices

One-sample and multiple-sample tests for covariance matrices are provided by the mvtest covariances command. One-sample tests include the test that the covariance matrix of varlist is diagonal, spherical, compound symmetric, block diagonal, or equal to a given matrix.

## Example 1

The gasoline-powered milk-truck dataset introduced in example 1 of [MV] mytest means has price per mile for fuel, repair, and capital. We test if the covariance matrix for these three variables has any special structure.

```
. use http://www.stata-press.com/data/r14/milktruck
(Milk transportation costs for 25 gasoline trucks (Johnson and Wichern 2007))
. mvtest covariances fuel repair capital, diagonal
Test that covariance matrix is diagonal
   Adjusted LR chi2(3) =
                             17.91
                            0.0005
           Prob > chi2 =
. mvtest covariances fuel repair capital, spherical
Test that covariance matrix is spherical
   Adjusted LR chi2(5) =
                             21 53
                            0.0006
           Prob > chi2 =
```

```
. mvtest covariances fuel repair capital, compound
Test that covariance matrix is compound symmetric
   Adjusted LR chi2(4) = 11.29
        Prob > chi2 = 0.0235
```

We reject the hypotheses that the covariance is diagonal, spherical, or compound symmetric.

We now test whether there is covariance between fuel and repair, with capital not covarying with these two variables. Thus we hypothesize a block diagonal structure of the form

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_{11}^2 & \sigma_{12} & 0\\ \sigma_{21} & \sigma_{22}^2 & 0\\ 0 & 0 & \sigma_{33}^2 \end{pmatrix}$$

for the covariance matrix. The block() option of mytest covariances provides the test:

```
. mvtest covariances fuel repair capital, block(fuel repair || capital)
Test that covariance matrix is block diagonal
   Adjusted LR chi2(2) = 3.52
        Prob > chi2 = 0.1722
```

We fail to reject the null hypothesis. The covariance matrix might have the block diagonal structure we hypothesized.

The same p-value could have been obtained from Stata's canonical correlation command:

```
. canon (fuel repair) (capital)
  (output omitted)
```

See [MV] canon.

Now, in addition to hypothesizing that the covariance is block diagonal, we specifically hypothesize that the variance for capital is 10, the variance of fuel is three times that of capital, the variance of repair is two times that of capital, and that there is no covariance between capital and the other two variables, while there is a covariance of 15 between fuel and repair. We test that hypothesis by using the equals() option.

We fail to reject the null hypothesis; the covariance might follow the structure hypothesized.

If each block comprises a single variable, the test of independent subvectors reduces to a test that the covariance matrix is diagonal. Thus the following two commands are equivalent:

1

```
mvtest covariances x1 x2 x3 x4 x5, block(x1 || x2 || x3 || x4 || x5) and  mvtest \ covariances \ x1 \ x2 \ x3 \ x4 \ x5, \ diagonal
```

### A multiple-sample test for covariance matrices

The by() option of mvtest covariances provides a modified likelihood-ratio statistic testing the equality of covariance matrices for the multiple independent samples defined by by(). This test is also known as Box's M test. There are both F and chi-squared approximations for the null distribution of the test.

#### Example 2

We illustrate the multiple-sample test of equality of covariance matrices by using four psychological test scores on 32 men and 32 women (Rencher and Christensen 2012; Beall 1945).

Both the F and the chi-squared approximations indicate that we cannot reject the null hypothesis that the covariance matrices for males and females are equal (Rencher and Christensen 2012, 269).

Equality of group covariance matrices is an assumption of multivariate analysis of variance (see [MV] manova) and linear discriminant analysis (see [MV] discrim lda). Box's M test, produced by mvtest covariances with the by() option, is often recommended for testing this assumption.

## Stored results

mvtest covariances stores the following in r():

```
Scalars
    r(chi2)
                   chi-squared
    r(df)
                   degrees of freedom for chi-squared test
    r(p_chi2)
                   significance
    r(F_Box)
                    F statistic for Box test (by() only)
    r(df_m_Box)
                   model degrees of freedom for Box test (by() only)
    r(df_r_Box)
                   residual degrees of freedom for Box test (by() only)
    r(p_F_Box)
                   significance of Box F test (by() only)
Macros
    r(chi2type) type of model chi-squared test
```

### Methods and formulas

When comparing the formulas in this section with those found in some multivariate texts, be aware of whether they define the sample covariance matrix with a divisor of N or N-1. We use N. The formulas for several of the statistics are presented differently depending on your choice of divisor (but are still equivalent).

Methods and formulas are presented under the following headings:

One-sample tests for covariance matrices A multiple-sample test for covariance matrices

## One-sample tests for covariance matrices

Let the sample consist of N i.i.d. observations,  $\mathbf{x}_i$ ,  $i=1,\ldots,N$ , from a k-variate multivariate normal distribution,  $\text{MVN}_k(\boldsymbol{\mu},\boldsymbol{\Sigma})$ , with sample mean  $\overline{\mathbf{x}}=1/N\sum_{i=1}^N\mathbf{x}_i$ , sample covariance matrix  $\mathbf{S}=1/N\sum_{i=1}^N(\mathbf{x}_i-\overline{\mathbf{x}})'$ , and sample correlation matrix  $\mathbf{R}$ .

To test that a covariance matrix equals a given matrix,  $H_0: \Sigma = \Sigma_0$ , mytest covariances computes a likelihood-ratio test with Bartlett correction (Rencher and Christensen 2012, 260–261):

$$\begin{split} \chi_{\text{ovf}}^2 &= (N-1) \left\{ 1 - \frac{1}{6(N-1)-1} \left( 2k + 1 - \frac{2}{k+1} \right) \right\} \\ &\times \left\{ \ln |\mathbf{\Sigma}_0| - \ln \left| \frac{N}{N-1} \mathbf{S} \right| + \operatorname{trace} \left( \frac{N}{N-1} \mathbf{S} \mathbf{\Sigma}_0^{-1} \right) - k \right\} \end{split}$$

which is approximately  $\chi^2$  distributed with k(k+1)/2 degrees of freedom.

To test for a spherical covariance matrix,  $H_0$ :  $\Sigma = \sigma^2 \mathbf{I}$ , mytest covariances computes a likelihood-ratio test with Bartlett correction (Rencher and Christensen 2012, 261-262):

$$\chi^2_{\rm ovs} = \left\{ (N-1) - \frac{2k^2 + k + 2}{6k} \right\} \left[ k \ln \left\{ \operatorname{trace} \left( \mathbf{S} \right) \right\} - \ln |\mathbf{S}| - k \ln(k) \right]$$

which is approximately  $\chi^2$  distributed with k(k+1)/2-1 degrees of freedom.

To test for a diagonal covariance matrix,  $H_0: \Sigma_{ij} = 0$  for  $i \neq j$ , mytest covariances computes a likelihood-ratio test with first-order Bartlett correction (Rencher and Christensen 2012, 275):

$$\chi_{\text{ovd}}^2 = -\left(N - 1 - \frac{2k + 5}{6}\right) \, \ln|\mathbf{R}|$$

which is approximately  $\chi^2$  distributed with k(k-1)/2 degrees of freedom.

To test for a compound-symmetric covariance matrix,  $H_0$ :  $\Sigma = \sigma^2 \{(1 - \rho)\mathbf{I} + \rho \mathbf{1}\mathbf{1}'\}$ , that is, a covariance matrix with common variance  $\sigma^2$  and common correlation  $\rho$ , mytest covariances computes a likelihood-ratio test with first-order Bartlett correction (Rencher and Christensen 2012, 263–264):

$$\begin{split} \chi_{\text{ovc}}^2 &= \left\{ N - 1 - \frac{k(k+1)^2(2k-3)}{6(k-1)(k^2+k-4)} \right\} \\ &\times \left[ k \ln\left(s^2\right) + (k-1)\ln(1-r) + \ln\{1 + (k-1)r\} - \ln|\mathbf{S}| \right] \end{split}$$

where

$$s^2 = \frac{1}{k} \sum_{j=1}^k s_{jj}$$
 and  $r = \frac{1}{k(k-1)s^2} \sum_{j=1}^k \sum_{h=1, h \neq j}^k s_{jh}$ 

where  $s_{jh}$  is the (j,h) element of S.  $\chi^2_{\text{ovc}}$  is approximately  $\chi^2$  distributed with k(k+1)/2-2 degrees of freedom.

To test that a covariance matrix is block diagonal with b diagonal blocks and with  $k_j$  variables in block j, mytest covariances computes a likelihood-ratio test with first-order Bartlett correction (Rencher and Christensen 2012, 271–272). Thus variables in different blocks are hypothesized to be independent.

$$\chi_{\text{ovb}}^2 = \left(N - 1 - \frac{2a_3 + 3a_2}{6a_2}\right) \left(\sum_{j=1}^b \ln |\mathbf{S}_j| - \ln |\mathbf{S}|\right)$$

where  $a_2 = k^2 - \sum_{j=1}^b k_j^2$ ,  $a_3 = k^3 - \sum_{j=1}^b k_j^3$ , and  $\mathbf{S}_j$  is the covariance matrix for the jth block.  $\chi^2_{\mathrm{ovb}}$  is approximately  $\chi^2$  distributed with  $a_2/2$  degrees of freedom.

### A multiple-sample test for covariance matrices

Let there be  $m \geq 2$  independent samples with the jth sample containing  $N_j$  i.i.d. observations,  $\mathbf{x}_{ji}, \ i = 1, \dots, N_j$ , from a k-variate multivariate normal distribution  $\text{MVN}_k(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$ . The observed jth sample mean is  $\overline{\mathbf{x}}_j = 1/N_j \sum_{i=1}^{N_j} \mathbf{x}_{ji}$  and covariance is  $\mathbf{S}_j = 1/N_j \sum_{i=1}^{N_j} (\mathbf{x}_{ji} - \overline{\mathbf{x}}_j)(\mathbf{x}_{ji} - \overline{\mathbf{x}}_j)'$ . Let  $N = \sum_{j=1}^m N_j$ .

To test the equality of covariance matrices in m independent samples,  $H_0: \Sigma_1 = \Sigma_2 = \cdots = \Sigma_m$ , mvtest covariances computes a modified likelihood-ratio statistic, which is an unbiased variant of the likelihood-ratio statistic (Rencher and Christensen 2012, 266–268):

$$-2\ln(M) = (N-m)\ln\left|\mathbf{S}_{\mathbf{pooled}}\right| - \sum_{j=1}^{m} \left\{ (N_j - 1)\ln\left|\frac{N_j}{N_j - 1}\mathbf{S}_j\right| \right\}$$

where  $\mathbf{S}_{pooled} = \sum_{j=1}^{m} (N_j \mathbf{S}_j)/(N-m)$ . Asymptotically,  $-2 \ln(M)$  is  $\chi^2$  distributed. Box (1949, 1950) derived more accurate  $\chi^2$  and F approximations (Rencher and Christensen 2012, 267–268).

Box's  $\chi^2$  approximation is given by

$$\chi_{\rm mv}^2 = -2(1 - c_1) \ln(M)$$

which is approximately  $\chi^2$  distributed with (m-1)k(k+1)/2 degrees of freedom.

Box's F approximation is given by

$$F_{\rm mv} = \begin{cases} -2b_1 \ln(M) & \text{if } c_2 > c_1^2 \\ \\ \frac{2a_2b_2 \ln(M)}{a_1 \left\{ 1 + 2b_2 \ln(M) \right\}} & \text{otherwise} \end{cases}$$

which is approximately F distributed with  $a_1$  and  $a_2$  degrees of freedom.

In the  $\chi^2$  and F approximations, we have

$$c_1 = \left\{ \sum_{j=1}^m (N_j - 1)^{-1} - (N - m)^{-1} \right\} \frac{2k^2 + 3k - 1}{6(k+1)(m-1)}$$

$$c_2 = \left\{ \sum_{j=1}^m (N_j - 1)^{-2} - (N - m)^{-2} \right\} \frac{(k-1)(k+2)}{6(m-1)}$$

$$a_1 = (m-1)k(k+1)/2$$
,  $a_2 = (a_1+2)/|c_2-c_1^2|$ ,  $b_1 = (1-c_1-a_1/a_2)/a_1$ , and  $b_2 = (1-c_1+2/a_2)/a_2$ .

#### References

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—. 1950. Problems in the analysis of growth and wear curves. Biometrics 6: 362–389.

Johnson, R. A., and D. W. Wichern. 2007. Applied Multivariate Statistical Analysis. 6th ed. Englewood Cliffs, NJ: Prentice Hall.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley.

## Also see

[MV] candisc — Canonical linear discriminant analysis

[MV] canon — Canonical correlations

[R] correlate — Correlations (covariances) of variables or coefficients

[MV] discrim Ida — Linear discriminant analysis

[MV] manova — Multivariate analysis of variance and covariance

[R] **sdtest** — Variance-comparison tests

#### Title

#### mvtest means — Multivariate tests of means

Description Quick start
Menu Syntax

Options for multiple-sample tests 
Options with one-sample tests

Remarks and examples Stored results Methods and formulas References

Also see

# **Description**

mvtest means performs one-sample and multiple-sample multivariate tests on means. These tests assume multivariate normality.

See [MV] mvtest for other multivariate tests.

### **Quick start**

Test that the means of v1, v2, and v3 are equal mytest means v1 v2 v3

Test that the means of v1, v2, and v3 are zero

mvtest means v1 v2 v3, zero

Test that the means vector equals the hypothesized vector myvec mvtest means v1 v2 v3, equals(myvec)

Test that the means of v1, v2, and v3 are the same across groups defined by catvar assuming homogeneous covariance matrices

mvtest means v1 v2 v3, by(catvar)

As above, but allow heterogeneous covariance matrices

mvtest means v1 v2 v3, by(catvar) heterogeneous

As above, but use a likelihood-ratio test instead of a Wald test

mvtest means v1 v2 v3, by(catvar) lr

#### Menu

Statistics > Multivariate analysis > MANOVA, multivariate regression, and related > Multivariate test of means, covariances, and normality

# **Syntax**

```
Multiple-sample tests
```

```
mvtest \underline{m}eans \ varlist \ [if] \ [in] \ [weight], \ by(groupvars) \ [multisample\_options]
```

One-sample tests

 $mvtest \underline{m}eans \ varlist \ [if] \ [in] \ [weight] \ [, one-sample\_options]$ 

$multis ample\_options$	Description
Model	
* by (groupvars)	compare subsamples with same values in groupvars
<u>miss</u> ing	treat missing values in groupvars as ordinary values
Options	
<u>hom</u> ogeneous	test for equal means with homogeneous covariance matrices across by-groups; the default
<u>het</u> erogeneous	James's test for equal means, allowing heterogeneous covariance matrices across by-groups
lr	likelihood-ratio test for equal means, allowing heterogeneous covariance matrices across by-groups
<pre>protect(spec)</pre>	run protection as a safeguard against local minimum with the group means as initial values; use only with 1r option

<sup>\*</sup> by (groupvars) is required.

a agranta antiona

one-sample_options	Description
Options	
<u>e</u> qual	test that variables in varlist have equal means; the default
<u>z</u> ero	test that means of varlist are all equal to 0
$\underline{\mathbf{e}}\mathtt{quals}(M)$	test that mean vector equals vector M
$\underline{1}$ inear( $V$ )	test that mean vector of $varlist$ satisfies linear hypothesis described by matrix $V$

bootstrap, by, jackknife, rolling, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

Description

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

# Options for multiple-sample tests

Model

by (groupvars) is required with the multiple-sample version of the test. Observations with the same values in groupvars form a sample. Observations with missing values in groupvars are ignored, unless the missing option is specified.

missing specifies that missing values in groupvars are treated like ordinary values.

homogeneous, the default, specifies the hypothesis that the mean vectors are the same across the bygroups, assuming homogeneous covariance matrices across the bygroups. homogeneous produces the four standard tests of multivariate means (Wilks's lambda, Pillai's trace, Lawley-Hotelling trace, and Roy's largest root).

heterogeneous removes the assumption that the covariance matrices are the same across the bygroups. This is the multivariate Behrens–Fisher problem. With two groups, the MNV test, an affine-invariant modification by Krishnamoorthy and Yu (2004) of the Nel–Van der Merwe (1986) test, is displayed. With more than two groups, the Wald test, with *p*-values adjusted as proposed by James (1954), is displayed.

1r removes the assumption that the covariance matrices are the same across the by-groups and specifies that a likelihood-ratio test be presented. The associated estimation problem may have multiple local optima, though this seems rare with two groups.

protect(spec) is a technical option accompanying 1r, specifying that the "common means" model is fit from different starting values to ascertain with some confidence whether a global optimum to the underlying estimation problem was reached. The Mardia–Kent–Bibby (1979) proposal for initialization of the common means is always used as well. If the different trials do not converge to the same solution, the "best" one is used to obtain the test, and a warning message is displayed.

protect(groups) specifies to fit the common means model using each of the group means as starting values for the common means.

protect(randobs, reps(#)) specifies to fit the common means model using # random observations as starting values for the common means.

protect(#) is a convenient shorthand for protect(randobs, reps(#)).

# Options with one-sample tests

∫ Options Ì

equal performs Hotelling's test of the hypothesis that the means of all variables in *varlist* are equal. zero performs Hotelling's test of the hypothesis that the means of all variables in *varlist* are 0.

equals (M) performs Hotelling's test that the vector of means of the k variables in *varlist* equals M. The matrix M must be a  $k \times 1$  or  $1 \times k$  vector. The row and column names of M are ignored.

linear (V) performs Hotelling's test that the means satisfy a user-specified set of linear constraints, represented by V. V must be a matrix vector with k or k+1 columns, where k is the number of variables in varlist. Let A be a matrix of the first k columns of V. Let k be the last column of k if k has k+1 columns and a column of 0s otherwise. The linear hypothesis test is that k times a column vector of the means of k representations and column names.

# Remarks and examples

Remarks are presented under the following headings:

One-sample tests for mean vectors Multiple-sample tests for mean vectors

### One-sample tests for mean vectors

One-sample and multiple-sample tests of means are available with the mvtest means command. One-sample tests include tests that the means of *varlist* are equal, the means of *varlist* equal a given vector, the means of *varlist* are zero, and linear combinations of the means of *varlist* equal a given vector.

We first explore the use of mvtest means for testing the one-sample hypothesis that the means of *varlist* are equal.

### Example 1

The cost on a per-mile basis of 25 gasoline trucks used for transporting milk are provided in three categories: fuel, repair, and capital (Johnson and Wichern 2007, 269).

. use http://www.stata-press.com/data/r14/milktruck (Milk transportation costs for 25 gasoline trucks (Johnson and Wichern 2007))

. summarize

Max	Min	Std. Dev.	Mean	Obs	Variable
29.11	4.24	5.382	12.56	25	fuel
17.44	1.35	4.631723	8.1612	25	repair
17.59	3.28	3.687688	10.5444	25	capital

Are the means of the three costs equal? The equal option of mytest means provides a way of testing this hypothesis.

. mvtest means fuel repair capital, equal

Test that all means are the same

Hotelling T2 = 35.25 Hotelling F(2,23) = 16.89 Prob > F = 0.0000

We reject the null hypothesis of equal means for fuel, repair, and capital costs.

4

Hotelling's T-squared statistic is a multivariate generalization of the univariate t statistic; see [R] **ttest**. A test of the bivariate hypothesis that the means of the repair and capital costs are equal could be obtained with

```
ttest repair == capital
```

or with

```
mvtest means repair capital, equal
```

The square of the t statistic from ttest equals the T-squared value from mvtest means. With ttest, you are limited to comparing the means of two variables; with mvtest means, you can simultaneously compare the means of two or more variables.

The equals() option of mytest means provides Hotelling's T-squared statistic for the test that the mean vector for *varlist* equals a given vector. This provides a multivariate generalization of the univariate t statistic obtained using the ttest varname == # syntax of [R] test.

We compare the measurements of the available and exchangeable soil calcium (y1 and y2) and turnip-green calcium (y3) at 10 locations in the South (Rencher and Christensen 2012, 66; Kramer and Jensen 1969) to the values 15.0, 6.0, and 2.85 respectively (Rencher and Christensen 2012, 133–134).

. use http://www.stata-press.com/data/r14/turnip (Calcium in soil and turnip greens, Rencher and Christensen (2012))

. summarize v\*

Variable	Obs	Mean	Std. Dev.	Min	Max
у1	10	28.1	11.85514	6	40
у2	10	7.18	8.499908	1.6	30
у3	10	3.089	.5001211	2.7	4.38

- . matrix Mstd = (15.0, 6.0, 2.85)
- . mvtest means y\* , equals(Mstd)

Test that means equal vector Mstd

Hotelling T2 = 24.56 Hotelling F(3,7) = 6.37 Prob > F = 0.0207

The calcium measurements from these 10 locations in the South do not appear to match the hypothesized values.

1

The zero option of mvtest means tests the hypothesis that the means of *varlist* are zero. The same result could be obtained by creating a column or row vector of the appropriate length filled with zeros and supplying that to the equals() option.

```
mvtest means y1 y2 y3, zero
```

would give the same test as

```
matrix Zero = 0,0,0
mvtest means y1 y2 y3, equals(Zero)
```

This same test against a zero-mean vector can be obtained with the hotelling command; see [MV] hotelling. For example,

```
hotelling y1 y2 y3
```

mytest means also tests that linear combinations of the means of varlist equal a given vector.

### Example 3

The linear() option of mvtest means can be used to obtain the same result as in example 1, testing that the fuel, repair, and capital costs are equal. We do this by constructing two appropriate linear combinations of our three variables and testing that the means of these two linear combinations are zero.

```
. use http://www.stata-press.com/data/r14/milktruck (Milk transportation costs for 25 gasoline trucks (Johnson and Wichern 2007)) . matrix C = 1, -1, 0 \setminus 0, 1, -1 . matrix list C C[2,3] c1 c2 c3 r1 1 -1 0 r2 0 1 -1
```

```
. mvtest means fuel repair capital, linear(C)  
Test that mean vector satisfies linear hypothesis C  
Hotelling T2 = 35.25  
Hotelling F(2,23) = 16.89  
Prob > F = 0.0000
```

We formed a matrix C that contrasted fuel to repair (the first row of C) and repair to capital (the second row of C). Note that we need not set the matrix row and column names of C. By default, the linear contrast was tested equal to a vector of zeros.

We could explicitly append an extra column of zeros in our matrix and obtain the same result.

```
. matrix Czero = C, (0 \setminus 0)
. matrix list Czero
Czero[2,4]
    c1 c2 c3 c4
    1 -1
r1
            0
                 Λ
        1
           -1
. mvtest means fuel repair capital, linear(Czero)
Test that mean vector satisfies linear hypothesis Czero
          Hotelling T2 =
                              35.25
     Hotelling F(2,23) =
                              16.89
              Prob > F =
                             0.0000
```

Values other than zeros could have been appended to  $\tt C$  to test if the linear combinations equal those other values.

Rencher and Christensen (2012, 152–154) discusses one-sample profile analysis. The linear() option of mytest means allows you to do this and other one-sample comparisons of interest.

## Multiple-sample tests for mean vectors

Multiple-sample tests of mean vectors are also supported by mvtest means. The groups defining the multiple samples are specified with the by() option. The test that is presented depends on whether homogeneity of variance is assumed and whether there are more than two groups. The homogeneity option, the default, provides four standard multivariate tests (Wilks's lambda, Pillai's trace, Lawley–Hotelling trace, and Roy's largest root) under the assumption that the group covariance matrices are equal. The remaining possibilities do not assume equal covariances for the groups. The heterogeneous option with two by-groups presents the affine-invariant modification by Krishnamoorthy and Yu (2004) of the test proposed by Nel and Van der Merwe (1986). The heterogeneous option with more than two by-groups presents a Wald test along with James's approximation to the *p*-value of the test. The lr option also removes the assumption of equal covariance matrices for the groups and produces a likelihood-ratio test for the equality of the group means.

## ▶ Example 4

In example 2 of [MV] manova, we introduce two variables measured on four groups of rabbits. The groups have differing sample sizes. mvtest means with the by() option can test the hypothesis that the means of the two variables are the same for the four groups of rabbits under the assumption that the groups have equal covariance matrices.

. use http://www.stata-press.com/data/r14/metabolic (Table 4.5 Metabolic Comparisons of Rabbits -- Rencher (1998))

. mvtest means y1 y2, by(group)

Test for equality of 4 group means, assuming homogeneity

	Statistic	F(df1,	df2)	= F	Prob>F
Wilks' lambda	0.1596	6.0	32.0	8.02	0.0000 e
Pillai's trace	1.2004	6.0	34.0	8.51	0.0000 a
Lawley-Hotelling trace	3.0096	6.0	30.0	7.52	0.0001 a
Roy's largest root	1.5986	3.0	17.0	9.06	0.0008 u

e = exact, a = approximate, u = upper bound on F

We reject the null hypothesis and conclude that the means are likely different between the four groups of rabbits.

The statistics reported above are the same as reported by manova y1 y2 = group in example 2 of [MV] manova. mvtest means y1 y2, by(group) homogeneous would also have produced the same results because homogeneous is the default when by() is specified.

### Example 5

Continuing with the rabbit data, restricting ourselves to examining only the first two groups of rabbits and continuing to assume equal covariance matrices, we obtain the following:

. mvtest means y1 y2 if group < 3, by(group)

Test for equality of 2 group means, assuming homogeneity

		F(df1,	df2)	= F	Prob>F
Wilks' lambda Pillai's trace	0.3536	2.0	11.0 11.0	10.05 10.05	0.0033 e
Lawley-Hotelling trace Roy's largest root	1.8279 1.8279	2.0	11.0 11.0	10.05	0.0033 e 0.0033 e

e = exact, a = approximate, u = upper bound on F

We reject the null hypothesis of equal means for the two groups of rabbits.

With only two groups, the four multivariate tests above are equivalent. Because there were only two groups, we could have also produced this same F test with hotelling y1 y2 if group < 3, by(group); see [MV] hotelling.

## ▶ Example 6

We now remove the assumption of equal covariance matrices for these two groups of rabbits and see if our conclusions change.

```
. mytest means y1 y2 if group < 3, by(group) heterogeneous Test for equality of 2 group means, allowing for heterogeneity  \begin{array}{ccc} \text{MNV F(2,9.5)} &=& 9.92 \\ \text{Prob} > \text{F} &=& 0.0047 \end{array}
```

Removing the assumption of equal covariance matrices still leads to rejection of the null hypothesis that the means for the two groups of rabbits are equal.

4

4

Because there were only two groups, an F statistic based on an affine-invariant modification by Krishnamoorthy and Yu (2004) of the test proposed by Nel and Van der Merwe (1986) was presented.

## Example 7

If we attempt to test all four groups of rabbits while removing the assumption of equal covariance matrices,

. mvtest means y1 y2, by(group) heterogeneous

we receive an error message indicating that we have a singular covariance matrix. This is because there are only two observations for the fourth group of rabbits.

If we omit the fourth group, we obtain

```
. mvtest means y1 y2 if group < 4, by(group) heterogeneous  
Test for equality of 3 group means, allowing for heterogeneity  
Wald chi2(4) = 34.08
Prob > chi2 = 0.0000 (chi-squared approximation)
Prob > chi2 = 0.0017 (James' approximation)
```

With more than two groups, a Wald chi-squared statistic is presented along with two p-values. The first p-value is the approximate one based on the  $\chi^2$  distribution with four degrees of freedom. The second, more accurate, p-value is based on James's (1954) approximation. Both p-values lead to rejection of the null hypothesis; the three groups of rabbits are unlikely to have equal means.

4

### ▶ Example 8

We can request a likelihood-ratio test instead of a Wald test by specifying the 1r option. Like heterogeneous, the 1r option does not assume that the group covariance matrices are equal.

```
. mvtest means y1 y2 if group < 4, by(group) lr 
 Test for equality of 3 group means, allowing for heterogeneity 
 LR chi2(4) = 21.32
 Prob > chi2 = 0.0003
```

The likelihood-ratio test also leads us to reject the null hypothesis of equal means for the three groups of rabbits.

4

The computation of the likelihood-ratio test requires fitting the multivariate normal distribution with common means while allowing for different covariance matrices. The iterative fitting process may converge to local solutions rather than to the global solution, invalidating the reported test (Buot, Hoşten, and Richards 2007). As a precaution, you may use the protect() option to request fitting from different starting values so that the test results are based on the best solution found, and you can check whether the likelihood surface has multiple optima.

#### Stored results

mvtest means without the by() option (that is, a one-sample means test) stores the following in r():

```
Scalars

r(T2) Hotelling T-squared

r(F) F statistic

r(df_m) model degrees of freedom

r(df_r) residual degrees of freedom

r(p_F) significance

Macros

r(Ftype) type of model F test
```

mvtest means with by() but without the lr or heterogeneous options (that is, a multiple-sample means test, assuming homogeneity) stores the following in r():

```
Scalars
r(F) F statistic
r(df_m) model degrees of freedom
r(df_r) residual degrees of freedom
r(p_F) significance

Macros
r(Ftype) type of model F test

Matrices
r(stat_m) MANOVA model tests
```

mvtest means with by() defining two groups and with the heterogeneous option (that is, a two-sample test of means, allowing for heterogeneity) stores the following in r():

```
Scalars
r(F) F statistic
r(df_m) model degrees of freedom
r(df_r) residual degrees of freedom
r(p_F) significance

Macros
r(Ftype) type of model F test
```

mvtest means with by() defining more than two groups and with the heterogeneous option (that is, a multiple-sample test of means, allowing for heterogeneity) stores the following in r():

```
\begin{array}{lll} \text{Scalars} & & & & & \\ & \textbf{r}(\texttt{chi2}) & & \chi^2 \text{ statistic} \\ & \textbf{r}(\texttt{df}) & & \text{degrees of freedom for } \chi^2 \text{ test} \\ & \textbf{r}(\texttt{p\_chi2}) & & \text{significance} \\ & \textbf{r}(\texttt{p\_chi2\_James}) & & \text{significance via James's approximation} \\ \\ \text{Macros} & & & & \\ & \textbf{r}(\texttt{chi2type}) & & \text{type of model } \chi^2 \text{ test} \\ \end{array}
```

mvtest means with the by() and lr options (that is, a likelihood-ratio multiple-sample test of means, allowing for heterogeneity) stores the following in r():

```
Scalars
                            \chi^2 statistic
    r(chi2)
                            degrees of freedom for \chi^2 test
    r(df)
                            significance
    r(p_chi2)
                            return code
    r(rc)
    r(uniq)
                            1/0 if protection runs yielded/did not yield same solution (protect() only)
                            number of protection runs (protect() only)
    r(nprotect)
Macros
                            type of model \chi^2 test
    r(chi2type)
Matrices
                            maximum likelihood estimate of means
    r(M)
```

### Methods and formulas

When comparing the formulas in this section with those found in some multivariate texts, be aware of whether they define the sample covariance matrix with a divisor of N or N-1. We use N. The formulas for several of the statistics are presented differently depending on your choice of divisor (but are still equivalent).

Methods and formulas are presented under the following headings:

One-sample tests for mean vectors Multiple-sample tests for mean vectors

## One-sample tests for mean vectors

Let the sample consist of N i.i.d. observations,  $\mathbf{x}_i$ ,  $i=1,\ldots,N$ , from a k-variate multivariate normal distribution,  $\text{MVN}_k(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ , with sample mean  $\overline{\mathbf{x}} = 1/N \sum_{i=1}^N \mathbf{x}_i$  and sample covariance matrix  $\mathbf{S} = 1/N \sum_{i=1}^N (\mathbf{x}_i - \overline{\mathbf{x}})'$ .

mvtest means with the equals () option tests that a mean vector equals a fixed vector,  $H_0: \mu = \mu_0$ , and produces a Hotelling T-squared statistic, which is equivalent to the likelihood-ratio test (Mardia, Kent, and Bibby 1979, 125–126)

$$T_{\text{omf}}^2 = (N-1)(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)' \mathbf{S}^{-1}(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)$$

Under the null hypothesis,

$$F_{\rm omf} = \frac{N - k}{(N - 1)k} T_{\rm omf}^2$$

is distributed F(k, N - k).

mytest means with the zero option tests that the mean vector equals  $\mathbf{0}$  and is obtained from  $T_{\mathrm{omf}}^2$  by setting  $\boldsymbol{\mu}_0 = \mathbf{0}$ . For this case, denote Hotelling's T-squared as  $T_{\mathrm{omz}}^2$  and the corresponding F statistic as  $F_{\mathrm{omz}}$ .

mytest means with the linear() option tests that the mean vector  $\mu$  satisfies a linear hypothesis,  $H_0: \mathbf{C}\mu = \mathbf{b}$ , and produces a Hotelling  $T^2$  test, which is equivalent to the likelihood-ratio test (Mardia, Kent, and Bibby 1979, 132-133)

$$T_{\text{omc}}^2 = (N-1)(\mathbf{C}\overline{\mathbf{x}} - \mathbf{b})'(\mathbf{C}\mathbf{S}\mathbf{C}')^{-1}(\mathbf{C}\overline{\mathbf{x}} - \mathbf{b})$$

Under the null hypothesis,

$$F_{\rm omc} = \frac{N - q}{(N - 1)q} T_{\rm omc}^2$$

is distributed F(q, N-q), where q is the rank of  $\mathbf{CSC}'$ , typically the number of rows of  $\mathbf{C}$ .

mytest means with the equal option tests that all means are equal and is obtained from  $T_{\rm omc}^2$  by setting  $\mathbf{C}=(\mathbf{I},-\mathbf{1})$  and  $\mathbf{b}=\mathbf{0}$ . For this case, denote Hotelling's  $T^2$  as  $T_{\rm ome}^2$  and the corresponding F statistic as  $F_{\rm ome}$ .

## Multiple-sample tests for mean vectors

Let there be  $m \geq 2$  independent samples with the jth sample containing  $N_j$  i.i.d. observations,  $\mathbf{x}_{ji}, i = 1, \dots, N_j$ , from a k-variate multivariate normal distribution,  $\text{MVN}_k(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$ . The observed jth sample mean is  $\overline{\mathbf{x}}_j = 1/N_j \sum_{i=1}^{N_j} \mathbf{x}_{ji}$  and covariance is  $\mathbf{S}_j = 1/N_j \sum_{i=1}^{N_j} (\mathbf{x}_{ji} - \overline{\mathbf{x}}_j)(\mathbf{x}_{ji} - \overline{\mathbf{x}}_j)'$ . Let  $N = \sum_{j=1}^m N_j$ .

The tests for the hypothesis that the mean vector is the same across m independent samples, obtained from mytest means with the by() option, come in four different flavors, depending on whether the additional assumption is made that the covariance matrix  $\mathbf{S}_j$  is the same over the m samples (the homogeneous and heterogeneous options) and on the number of samples (whether the by() option defines more than two groups). If equal covariance is not assumed, the problem is commonly referred to as the multivariate Behrens-Fisher problem.

When assuming equal covariance matrices for the by() groups (the homogeneous option, the default), mvtest means tests the equality of the group means by using manova to compute the classic quartet of test statistics: Wilks's lambda, Pillai's trace, Lawley-Hotelling trace, and Roy's largest root. See [MV] manova for details. For m=2 samples, the four tests are equivalent.

mvtest means has the heterogeneous and lr options, which remove the assumption of equal covariance matrices for the by() groups. The statistic produced with the heterogeneous option depends on whether there are m=2 groups or m>2 groups.

With the heterogeneous option and m=2 samples, the test for equal means is computed using the affine-invariant modification by Krishnamoorthy and Yu (2004) of the test proposed by Nel and Van der Merwe (1986):

$$T_{\text{mm2}}^2 = (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)' \widetilde{\mathbf{S}}^{-1} (\overline{\mathbf{x}}_1 - \overline{\mathbf{x}}_2)$$

where

$$F_{\text{mm2}} = \frac{v - k + 1}{vk} T_{\text{mm2}}^2$$

is approximately F(k, v - k + 1) distributed, and where  $\widetilde{\mathbf{S}}_j = \mathbf{S}_j/(N_j - 1)$ ,  $\widetilde{\mathbf{S}} = \widetilde{\mathbf{S}}_1 + \widetilde{\mathbf{S}}_2$ ,  $v = k(k+1)/(a_1 + a_2)$ , and

$$a_{j} = \left[ \operatorname{trace} \left\{ \left( \widetilde{\mathbf{S}}_{j} \widetilde{\mathbf{S}}^{-1} \right)^{2} \right\} + \operatorname{trace} \left( \widetilde{\mathbf{S}}_{j} \widetilde{\mathbf{S}}^{-1} \right)^{2} \right] / \left( N_{j} - 1 \right)$$

With the heterogeneous option and m>2 samples, mytest means computes the Wald test for equal means (Seber 1984, 445-447)

$$T_{\text{mmw}} = \sum_{j=1}^{m} (\overline{\mathbf{x}}_{j} - \overline{\overline{\mathbf{x}}})' \mathbf{W}_{j} (\overline{\mathbf{x}}_{j} - \overline{\overline{\mathbf{x}}})$$

where 
$$\mathbf{W}_j = {\{\mathbf{S}_j/(N_j-1)\}}^{-1}$$
,  $\mathbf{W} = \sum_{j=1}^m \mathbf{W}_j$ , and  $\overline{\overline{\mathbf{x}}} = \mathbf{W}^{-1} \sum_{j=1}^m \mathbf{W}_j \overline{\mathbf{x}}_j$ .

James (1954) showed that the upper  $\alpha$  quantile of  $T_{\rm mmw}$  under the null hypothesis can, to order  $N_i^{-1}$ , be obtained as  $\chi^2_{r,\alpha}(a+b\chi^2_{r,\alpha})$ , where  $\chi^2_{r,\alpha}$  is the upper  $\alpha$  quantile of a  $\chi^2$  with r=k(m-1) degrees of freedom, and

$$a = 1 + \frac{1}{2r} \sum_{j=1}^{m} \frac{\left\{ \operatorname{trace} \left( \mathbf{I} - \mathbf{W}^{-1} \mathbf{W}_{j} \right) \right\}^{2}}{N_{j} - 1}$$

$$b = \frac{1}{r(r+2)} \left[ \sum_{j=1}^{m} \frac{\operatorname{trace} \left\{ \left( \mathbf{I} - \mathbf{W}^{-1} \mathbf{W}_{j} \right)^{2} \right\}}{N_{j} - 1} + \frac{\left\{ \operatorname{trace} \left( \mathbf{I} - \mathbf{W}^{-1} \mathbf{W}_{j} \right) \right\}^{2}}{2(N_{j} - 1)} \right]$$

mvtest computes the p-value associated with the observed  $T_{\rm mmw}$  by inverting James's expansion with a scalar solver using Brent's (1973) algorithm.

With the lr option, mytest means provides a likelihood-ratio test for constant means across  $m \geq 2$  samples, without the assumption of constant covariances. To fit the null model with a common mean,  $\mu_c$ , an iterative procedure proposed by Mardia, Kent, and Bibby (1979, 142–143) is used. Let h denote the iteration. Let  $\hat{\Sigma}_j^{(0)} = \mathbf{S}_j$ , and  $\hat{\mu}_c^{(0)}$  be obtained using the second formula below, then iterate these two formulas starting with h=1 until convergence is achieved.

$$\widehat{\boldsymbol{\Sigma}}_{j}^{(h)} = \mathbf{S}_{j} + \left(\overline{\mathbf{x}}_{j} - \widehat{\boldsymbol{\mu}}_{c}^{(h-1)}\right) \left(\overline{\mathbf{x}}_{j} - \widehat{\boldsymbol{\mu}}_{c}^{(h-1)}\right)'$$

$$\widehat{\boldsymbol{\mu}}_{c}^{(h)} = \left\{\sum_{j=1}^{m} N_{j} \left(\widehat{\boldsymbol{\Sigma}}_{j}^{(h)}\right)^{-1}\right\}^{-1} \left\{\sum_{j=1}^{m} N_{j} \left(\widehat{\boldsymbol{\Sigma}}_{j}^{(h)}\right)^{-1} \overline{\mathbf{x}}_{j}\right\}$$

The likelihood-ratio chi-squared statistic

$$\chi^2_{\mathrm{mml}} = \sum_{j=1}^{m} N_j \ln \left\{ 1 + \left( \overline{\mathbf{x}}_j - \widehat{\boldsymbol{\mu}}_c^{(h)} \right)' \left( \widehat{\boldsymbol{\Sigma}}_j^{(h)} \right)^{-1} \left( \overline{\mathbf{x}}_j - \widehat{\boldsymbol{\mu}}_c^{(h)} \right) \right\}$$

is approximately  $\chi^2$  distributed with k(m-1) degrees of freedom.

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#### Also see

- [MV] **hotelling** Hotelling's T-squared generalized means test
- [MV] manova Multivariate analysis of variance and covariance
- [R] **mean** Estimate means
- [R] **ttest** t tests (mean-comparison tests)

#### Title

#### mvtest normality — Multivariate normality tests

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# **Description**

mvtest normality performs tests for univariate, bivariate, and multivariate normality. See [MV] mvtest for more multivariate tests.

### **Quick start**

Doornik-Hansen omnibus test for multivariate normality for v1, v2, v3, and v4 mvtest normality v1 v2 v3 v4

Also show Henze–Zirkler's consistent test, Mardia's multivariate kurtosis test, and Mardia's multivariate skewness test

Same as above

mvtest normality v1 v2 v3 v4, stats(all)

Also show Doornik-Hansen test for bivariate normality for each pair of variables mvtest normality v1 v2 v3 v4, stats(all) bivariate

As above, but show univariate normality tests from sktest instead of the bivariate tests mvtest normality v1 v2 v3 v4, stats(all) univariate

Show all multivariate, bivariate, and univariate tests of normality for v1, v2, v3, and v4 mvtest normality v1 v2 v3 v4, stats(all) bivariate univariate

#### Menu

 ${\it Statistics} > {\it Multivariate analysis} > {\it MANOVA}, \ {\it multivariate regression}, \ {\it and related} > {\it Multivariate test of means}, \ {\it covariances}, \ {\it and normality}$ 

# **Syntax**

mvtest <u>norm</u> ality	varlist [if] [in] [weight] [, options]		
options	Description		
Options			
<u>uni</u> variate	display tests for univariate normality (sktest)		
<u>bi</u> variate	display tests for bivariate normality (Doornik-Hansen)		
<pre>stats(stats)</pre>	statistics to be computed		
stats	Description		
<u>dh</u> ansen	Doornik-Hansen omnibus test; the default		
<u>hz</u> irkler	Henze-Zirkler's consistent test		
<u>ku</u> rtosis	Mardia's multivariate kurtosis test		
<u>sk</u> ewness	Mardia's multivariate skewness test		
all	all tests listed here		

bootstrap, by, jackknife, rolling, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

fweights are allowed; see [U] 11.1.6 weight.

# **Options**

Options

univariate specifies that tests for univariate normality be displayed, as obtained from sktest; see [R] sktest.

bivariate specifies that the Doornik-Hansen (2008) test for bivariate normality be displayed for each pair of variables.

stats (*stats*) specifies one or more test statistics for multivariate normality. Multiple *stats* are separated by white space. The following *stats* are available:

dhansen produces the Doornik-Hansen (2008) omnibus test.

hzirkler produces Henze-Zirkler's (1990) consistent test.

kurtosis produces the test based on Mardia's (1970) measure of multivariate kurtosis.

skewness produces the test based on Mardia's (1970) measure of multivariate skewness.

all is a convenient shorthand for stats(dhansen hzirkler kurtosis skewness).

## Remarks and examples

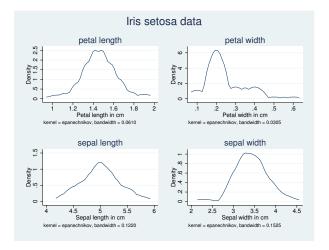
Univariate and multivariate tests of normality are provided by the mytest normality command.

### Example 1

The classic Fisher iris data from Anderson (1935) consists of four features measured on 50 samples from each of three iris species. The four features are the length and width of the sepal and petal. The three species are *Iris setosa*, *Iris versicolor*, and *Iris virginica*. We hypothesize that these features might be normally distributed within species, though they are likely not normally distributed across species. We will examine the *Iris setosa* data.

```
. use http://www.stata-press.com/data/r14/iris
(Iris data)
```

- . kdensity petlen if iris==1, name(petlen, replace) title(petal length)
- . kdensity petwid if iris==1, name(petwid, replace) title(petal width)
- . kdensity sepwid if iris==1, name(sepwid, replace) title(sepal width)
- . kdensity seplen if iris==1, name(seplen, replace) title(sepal length)
- . graph combine petlen petwid seplen sepwid, title("Iris setosa data")



We perform all multivariate, univariate, and bivariate tests of normality.

. mvtest norm pet\* sep\* if iris==1, bivariate univariate stats(all)
Test for univariate normality

Variable	Pr(Skewness)	Pr(Kurtosis)		joint ——— Prob>chi2
petlen	0.7403	0.1447	2.36	0.3074
petwid	0.0010	0.0442	12.03	0.0024
seplen	0.7084	0.8157	0.19	0.9075
sepwid	0.8978	0.1627	2.07	0.3553

Doornik-Hansen test for bivariate normality

Pair of variables		chi2	df	Prob>chi2
petlen	petwid seplen	17.47 5.76	4	0.0016 0.2177
	sepwid	8.50	4	0.0748
petwid	seplen sepwid	14.97 19.15	4 4	0.0048 0.0007
seplen	sepwid	5.92	4	0.2049

Test for multivariate normality

Mardia mSkewness =	3.079721	chi2(20) =	27.860	Prob>chi2 =	0.1128
Mardia mKurtosis =	26.53766	chi2(1) =	1.677	Prob>chi2 =	0.1953
Henze-Zirkler =	.9488453	chi2(1) =	2.707	Prob>chi2 =	0.0999
Doornik-Hansen		chi2(8) =	24.414	Prob>chi2 =	0.0020

From the univariate tests of normality, petwid does not appear to be normally distributed: p-values of 0.0010 for skewness, 0.0442 for kurtosis, and 0.0024 for the joint univariate test. The univariate tests of the other three variables do not lead to a rejection of the null hypothesis of normality.

The bivariate tests of normality show a rejection (at the 5% level) of the null hypothesis of bivariate normality for all pairs of variables that include petwid. Other pairings fail to reject the null hypothesis of bivariate normality.

Of the four multivariate normality tests, only the Doornik–Hansen test rejects the null hypothesis of multivariate normality, p-value of 0.0020.

The Doornik-Hansen (2008) test and Mardia's (1970) test for multivariate kurtosis take computing time roughly proportional to the number of observations. In contrast, the computing time of the test by Henze-Zirkler (1990) and Mardia's (1970) test for multivariate skewness are roughly proportional to the square of the number of observations.

1

#### Stored results

mvtest normality stores the following in r():

```
Scalars
                       significance of chi2_dh (stats(dhansen))
    r(p_dh)
    r(df_dh)
                       degrees of freedom of chi2_dh (stats(dhansen))
    r(chi2_dh)
                       Doornik-Hansen statistic (stats(dhansen))
                       rank of covariance matrix (stats(hzirkler))
    r(rank_hz)
                       two-sided significance of hz (stats(hzirkler))
    r(p_hz)
    r(z_hz)
                       normal variate associated with hz (stats(hzirkler))
    r(V_hz)
                       expected variance of log(hz) (stats(hzirkler))
    r(E_hz)
                       expected value of log(hz) (stats(hzirkler))
    r(hz)
                       Henze-Zirkler discrepancy statistic (stats(hzirkler))
    r(rank_mkurt)
                       rank of covariance matrix (stats(kurtosis))
    r(p_mkurt)
                       significance of Mardia mKurtosis test (stats(kurtosis))
    r(z_mkurt)
                       normal variate associated with Mardia mKurtosis (stats(kurtosis))
    r(chi2_mkurt)
                       chi-squared of Mardia mKurtosis (stats(kurtosis))
                       Mardia mKurtosis test statistic (stats(kurtosis))
    r(mkurt)
    r(rank_mskew)
                       rank for Mardia mSkewness test (stats(skewness))
    r(p_mskew)
                       significance of Mardia mSkewness test (stats(skewness))
    r(df_mskew)
                       degrees of freedom of Mardia mSkewness test (stats(skewness))
    r(chi2_mskew)
                       chi-squared of Mardia mSkewness test (stats(skewness))
    r(mskew)
                       Mardia mSkewness test statistic (stats(skewness))
Matrices
    r(U_dh)
                       matrix with the skewness and kurtosis of orthonormalized variables
                         (used in the Doornik-Hansen test): b1, b2, z(b1), and z(b2) (stats(dhansen))
    r(Btest)
                       bivariate test statistics (bivariate)
                       univariate test statistics (univariate)
    r(Utest)
```

## Methods and formulas

There are N independent k-variate observations,  $\mathbf{x}_i$ ,  $i=1,\ldots,N$ . Let  $\mathbf{X}$  denote the  $N\times k$  matrix of observations. We wish to test whether these observations are multivariate normal distributed,  $\text{MVN}_k(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ . The sample mean is  $\overline{\mathbf{x}} = 1/N \sum_i \mathbf{x}_i$ , and the sample covariance matrix is  $\mathbf{S} = 1/N \sum_i (\mathbf{x}_i - \overline{\mathbf{x}})(\mathbf{x}_i - \overline{\mathbf{x}})'$ .

Methods and formulas are presented under the following headings:

Mardia mSkewness and mKurtosis Henze–Zirkler Doornik–Hansen

#### Mardia mSkewness and mKurtosis

Mardia (1970) defined multivariate skewness,  $b_{1,k}$ , and kurtosis,  $b_{2,k}$ , as

$$b_{1,k} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} g_{ij}^3$$
 and  $b_{2,k} = \frac{1}{N} \sum_{i=1}^{N} g_{ii}^2$ 

where  $g_{ij} = (\mathbf{x}_i - \overline{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_j - \overline{\mathbf{x}})$ . The test statistic

$$z_1 = \frac{(k+1)(N+1)(N+3)}{6\{(N+1)(k+1) - 6\}} b_{1,k}$$

is approximately  $\chi^2$  distributed with k(k+1)(k+2)/6 degrees of freedom. The test statistic

$$z_2 = \frac{b_{2,k} - k(k+2)}{\sqrt{8k(k+2)/N}}$$

is approximately N(0,1) distributed. Also see Rencher and Christensen (2012, 108); Mardia, Kent, and Bibby (1979, 20–22); and Seber (1984, 148–149).

#### Henze-Zirkler

The Henze–Zirkler (1990) test, under the assumption that S is nonsingular, is

$$T = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \exp\left\{-\frac{\beta^{2}}{2} (\mathbf{x}_{i} - \mathbf{x}_{j})' \mathbf{S}^{-1} (\mathbf{x}_{i} - \mathbf{x}_{j})\right\}$$
$$-2(1+\beta^{2})^{-k/2} \sum_{i=1}^{N} \exp\left\{-\frac{\beta^{2}}{2(1+\beta^{2})} (\mathbf{x}_{i} - \overline{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x}_{i} - \overline{\mathbf{x}})\right\}$$
$$+ N(1+2\beta^{2})^{-k/2}$$

where

$$\beta = \frac{1}{\sqrt{2}} \left\{ \frac{N(2k+1)}{4} \right\}^{1/(k+4)}$$

As  $N \to \infty$ , the first two moments of T are given by

$$E(T) = 1 - (1 + 2\beta^2)^{-k/2} \left\{ 1 + \frac{k\beta^2}{1 + 2\beta^2} + \frac{k(k+2)\beta^4}{2(1+2\beta^2)^2} \right\}$$

$$\operatorname{Var}(T) = 2(1 + 4\beta^2)^{-k/2} + 2(1 + 2\beta^2)^{-k} \left\{ 1 + \frac{2k\beta^4}{(1+2\beta^2)^2} + \frac{3k(k+2)\beta^8}{4(1+2\beta^2)^4} \right\}$$

$$-4w^{-k/2} \left\{ 1 + \frac{3k\beta^4}{2w} + \frac{k(k+2)\beta^8}{2w^2} \right\}$$

where  $w = (1 + \beta^2)(1 + 3\beta^2)$ .

Henze–Zirkler suggest obtaining a p-value from the assumption, supported by a series of simulations, that T is approximately lognormal distributed. Thus let  $VZ = \ln\left\{1 + \text{Var}(T)/E(T)^2\right\}$  and  $EZ = \ln\left\{E(T)\right\} - VZ/2$ . The transformation  $Z = \left\{\ln(T) - EZ\right\}/\sqrt{VZ}$ . The p-value of Z is computed as  $p = 2\Phi(-|Z|)$ , where  $\Phi()$  is the cumulative normal distribution.

#### Doornik-Hansen

For the Doornik–Hansen (2008) test, the multivariate observations are transformed, then the univariate skewness and kurtosis for each transformed variable is computed, and then these are combined into an approximate  $\chi^2$  statistic.

Let V be a matrix with ith diagonal element equal to  $S_{ii}^{-1/2}$ , where  $S_{ii}$  is the ith diagonal element of S. C = VSV is then the correlation matrix. Let H be a matrix with columns equal to the eigenvectors of C, and let  $\Lambda$  be a diagonal matrix with the corresponding eigenvalues. Let  $\breve{X}$  be the centered version of X, that is,  $\bar{x}$  subtracted from each row. The data are then transformed using  $\dot{X} = \breve{X}VH\Lambda^{-1/2}H'$ .

The univariate skewness and kurtosis for each column of  $\dot{\mathbf{X}}$  is then computed. The general formula for univariate skewness is  $\sqrt{b_1} = m_3/m_2^{3/2}$  and kurtosis is  $b_2 = m_4/m_2^2$ , where  $m_p = 1/N \sum_{i=1}^N (x_i - \overline{x})^p$ . Let  $\dot{x}_i$  denote the ith observation from the selected column of  $\dot{\mathbf{X}}$ . Because by construction the mean of  $\dot{x}$  is zero and the variance  $m_2$  is one, the formulas simplify to  $\sqrt{b_1} = m_3$  and  $b_2 = m_4$ , where  $m_p = 1/N \sum_{i=1}^N \dot{x}_i^p$ .

The univariate skewness,  $\sqrt{b_1}$ , is transformed into an approximately normal variate,  $z_1$ , as in D'Agostino (1970):

$$z_1 = \delta \log \left( y + \sqrt{1 + y^2} \right)$$

where

$$y = \left\{ \frac{b_1(\omega^2 - 1)(N+1)(N+3)}{12(N-2)} \right\}^{1/2}$$
$$\delta = \left( \log \sqrt{\omega^2} \right)^{-1/2}$$
$$\omega^2 = -1 + \sqrt{2(\beta - 1)}$$
$$\beta = \frac{3(N^2 + 27N - 70)(N+1)(N+3)}{(N-2)(N+5)(N+7)(N+9)}$$

The univariate kurtosis,  $b_2$ , is transformed from a gamma variate into a  $\chi^2$ -variate and then into a standard normal variable,  $z_2$ , using the Wilson-Hilferty (1931) transform:

$$z_2 = \sqrt{9\alpha} \left\{ \left(\frac{\chi}{2\alpha}\right)^{1/3} - 1 + \frac{1}{9\alpha} \right\}$$

where

$$\chi = 2f(b_2 - 1 - b_1)$$

$$\alpha = a + b_1 c$$

$$f = \frac{(N+5)(N+7)(N^3 + 37N^2 + 11N - 313)}{12\delta}$$

$$c = \frac{(N-7)(N+5)(N+7)(N^2 + 2N - 5)}{6\delta}$$

$$a = \frac{(N-2)(N+5)(N+7)(N^2 + 27N - 70)}{6\delta}$$

$$\delta = (N-3)(N+1)(N^2 + 15N - 4)$$

The  $z_1$  and  $z_2$  associated with the columns of  $\dot{\mathbf{X}}$  are collected into vectors  $\mathbf{Z}_1$  and  $\mathbf{Z}_2$ . The statistic  $\mathbf{Z}_1'\mathbf{Z}_1+\mathbf{Z}_2'\mathbf{Z}_2$  is approximately  $\chi^2$  distributed with 2k degrees of freedom.

## **Acknowledgment**

An earlier implementation of the Doornik and Hansen (2008) test is the omninorm package of Baum and Cox (2007).

#### References

Anderson, E. 1935. The irises of the Gaspe Peninsula. Bulletin of the American Iris Society 59: 2-5.

Baum, C. F., and N. J. Cox. 2007. omninorm: Stata module to calculate omnibus test for univariate/multivariate normality. Boston College Department of Economics, Statistical Software Components S417501. http://ideas.repec.org/c/boc/bocode/s417501.html.

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### Also see

[R] sktest — Skewness and kurtosis test for normality

[R] swilk — Shapiro-Wilk and Shapiro-Francia tests for normality

#### **Title**

pca — Principal component analysis

Description Quick start

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References Also see

# **Description**

pca and pcamat display the eigenvalues and eigenvectors from the principal component analysis (PCA) eigen decomposition. The eigenvectors are returned in orthonormal form, that is, uncorrelated and normalized.

pca can be used to reduce the number of variables or to learn about the underlying structure of the data. pcamat provides the correlation or covariance matrix directly. For pca, the correlation or covariance matrix is computed from the variables in *varlist*.

#### **Quick start**

Principal component analysis of data

Principal component analysis of v1, v2, v3, and v4

pca v1 v2 v3 v4

As above, but retain only 2 components

pca v1 v2 v3 v4, components(2)

As above, but retain only those components with eigenvalues greater than or equal to 0.5 pca v1 v2 v3 v4, mineigen(.5)

Principal component analysis of covariance matrix instead of correlation matrix

pca v1 v2 v3 v4, covariance

Principal component analysis of a correlation matrix

Principal component analysis of matrix C representing the correlations from 1,000 observations pcamat C, n(1000)

As above, but retain only 4 components

pcamat C, n(1000) components(4)

#### Menu

#### pca

Statistics > Multivariate analysis > Factor and principal component analysis > Principal component analysis (PCA)

#### pcamat

Statistics > Multivariate analysis > Factor and principal component analysis > PCA of a correlation or covariance matrix

# **Syntax**

Principal component analysis of data

```
pca varlist [if] [in] [weight] [, options]
```

Principal component analysis of a correlation or covariance matrix

```
pcamat matname, n(#) [options pcamat_options]
```

matname is a  $k \times k$  symmetric matrix or a k(k+1)/2 long row or column vector containing the upper or lower triangle of the correlation or covariance matrix.

options	Description
Model 2	
<pre>components(#) mineigen(#) correlation covariance</pre>	retain maximum of # principal components; <a href="factors">factors</a> () is a synonym retain eigenvalues larger than #; default is 1e-5 perform PCA of the correlation matrix; the default perform PCA of the covariance matrix
vce( <u>nor</u> e) vce( <u>nor</u> mal)	do not compute VCE of the eigenvalues and vectors; the default compute VCE of the eigenvalues and vectors assuming multivariate normality
Reporting	
<u>l</u> evel(#)	set confidence level; default is level(95)
<u>bl</u> anks(#)	display loadings as blanks when $ loadings  < \#$
novce	suppress display of SEs even though calculated
* <u>me</u> ans	display summary statistics of variables
Advanced	
tol(#)	advanced option; see Options for details
ignore	advanced option; see Options for details
<u>norot</u> ated	display unrotated results, even if rotated results are available (replay only)

<sup>\*</sup> means is not allowed with pcamat.
norotated is not shown in the dialog box.

pcamat_options	Description
Model	
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{f}}\mathtt{ull})$	matname is a square symmetric matrix; the default
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{l}}\mathtt{ower})$	matname is a vector with the rowwise lower triangle (with diagonal)
$\underline{\mathtt{sh}}\mathtt{ape}(\underline{\mathtt{upper}})$	matname is a vector with the rowwise upper triangle (with diagonal)
$\underline{\mathtt{nam}}\mathtt{es}(\mathit{namelist})$	variable names; required if matname is triangular
forcepsd	modifies matname to be positive semidefinite
* n(#)	number of observations
$sds(matname_2)$	vector with standard deviations of variables
$means(matname_3)$	vector with means of variables

<sup>\*</sup> n() is required for pcamat.

bootstrap, by, jackknife, rolling, statsby, and xi are allowed with pca; see [U] 11.1.10 Prefix commands. However, bootstrap and jackknife results should be interpreted with caution; identification of the pca parameters involves data-dependent restrictions, possibly leading to badly biased and overdispersed estimates (Milan and Whittaker 1995).

Weights are not allowed with the bootstrap prefix; see [R] bootstrap. aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed with pca; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

# **Options**

Model 2

components(#) and mineigen(#) specify the maximum number of components (eigenvectors or
factors) to be retained. components() specifies the number directly, and mineigen() specifies it
indirectly, keeping all components with eigenvalues greater than the indicated value. The options
can be specified individually, together, or not at all. factors() is a synonym for components().

components(#) sets the maximum number of components (factors) to be retained. pca and pcamat always display the full set of eigenvalues but display eigenvectors only for retained components. Specifying a number larger than the number of variables in *varlist* is equivalent to specifying the number of variables in *varlist* and is the default.

mineigen(#) sets the minimum value of eigenvalues to be retained. The default is 1e-5 or the value of tol() if specified.

Specifying components() and mineigen() affects only the number of components to be displayed and stored in e(); it does not enforce the assumption that the other eigenvalues are 0. In particular, the standard errors reported when vce(normal) is specified do not depend on the number of retained components.

correlation and covariance specify that principal components be calculated for the correlation matrix and covariance matrix, respectively. The default is correlation. Unlike factor analysis, PCA is not scale invariant; the eigenvalues and eigenvectors of a covariance matrix differ from those of the associated correlation matrix. Usually, a PCA of a covariance matrix is meaningful only if the variables are expressed in the same units.

For pcamat, do not confuse the type of the matrix to be analyzed with the type of *matname*. Obviously, if *matname* is a correlation matrix and the option sds() is not specified, it is not possible to perform a PCA of the covariance matrix.

vce(none | normal) specifies whether standard errors are to be computed for the eigenvalues, the eigenvectors, and the (cumulative) percentage of explained variance (confirmatory PCA). These standard errors are obtained assuming multivariate normality of the data and are valid only for a PCA of a covariance matrix. Be cautious if applying these to correlation matrices.

Reporting

level(#) specifies the confidence level, as a percentage, for confidence intervals. The default is
level(95) or as set by set level; see [U] 20.7 Specifying the width of confidence intervals.
level() is allowed only with vce(normal).

blanks (#) shows blanks for loadings with absolute value smaller than #. This option is ignored when specified with vce(normal).

novce suppresses the display of standard errors, even though they are computed, and displays the PCA results in a matrix/table style. You can specify novce during estimation in combination with vce(normal). More likely, you will want to use novce during replay.

means displays summary statistics of the variables over the estimation sample. This option is not available with pcamat.

Advanced

- tol(#) is an advanced, rarely used option and is available only with vce(normal). An eigenvalue,  $ev_i$ , is classified as being close to zero if  $ev_i < tol \times max(ev)$ . Two eigenvalues,  $ev_1$  and  $ev_2$ , are "close" if  $abs(ev_1 - ev_2) < tol \times max(ev)$ . The default is tol(1e-5). See option ignore below and the technical note later in this entry.
- ignore is an advanced, rarely used option and is available only with vce(normal). It continues the computation of standard errors and tests, even if some eigenvalues are suspiciously close to zero or suspiciously close to other eigenvalues, violating crucial assumptions of the asymptotic theory used to estimate standard errors and tests. See the technical note later in this entry.

The following option is available with pca and pcamat but is not shown in the dialog box:

norotated displays the unrotated principal components, even if rotated components are available. This option may be specified only when replaying results.

## Options unique to pcamat

Model

shape (shape\_arg) specifies the shape (storage mode) for the covariance or correlation matrix matname. The following shapes are supported:

full specifies that the correlation or covariance structure of k variables is stored as a symmetric  $k \times k$  matrix. Specifying shape(full) is optional in this case.

lower specifies that the correlation or covariance structure of k variables is stored as a vector with k(k+1)/2 elements in rowwise lower-triangular order:

$$C_{11} C_{21} C_{22} C_{31} C_{32} C_{33} \dots C_{k1} C_{k2} \dots C_{kk}$$

upper specifies that the correlation or covariance structure of k variables is stored as a vector with k(k+1)/2 elements in rowwise upper-triangular order:

$$C_{11} \; C_{12} \; C_{13} \; \ldots \; C_{1k} \; C_{22} \; C_{23} \; \ldots C_{2k} \; \ldots \; C_{(k-1k-1)} \; C_{(k-1k)} \; C_{kk}$$

- names (namelist) specifies a list of k different names, which are used to document output and to label estimation results and are used as variable names by predict. By default, pcamat verifies that the row and column names of matname and the column or row names of matname2 and matname3 from the sds() and means() options are in agreement. Using the names() option turns off this check.
- forcepsd modifies the matrix matname to be positive semidefinite (psd) and so to be a proper covariance matrix. If matname is not positive semidefinite, it will have negative eigenvalues. By setting negative eigenvalues to 0 and reconstructing, we obtain the least-squares positive-semidefinite approximation to matname. This approximation is a singular covariance matrix.
- n(#) is required and specifies the number of observations.
- $sds(matname_2)$  specifies a  $k \times 1$  or  $1 \times k$  matrix with the standard deviations of the variables. The row or column names should match the variable names, unless the names() option is specified. sds() may be specified only if matname is a correlation matrix.

means ( $matname_3$ ) specifies a  $k \times 1$  or  $1 \times k$  matrix with the means of the variables. The row or column names should match the variable names, unless the names() option is specified. Specify means() if you have variables in your dataset and want to use predict after pcamat.

# Remarks and examples

Principal component analysis (PCA) is commonly thought of as a statistical technique for data reduction. It helps you reduce the number of variables in an analysis by describing a series of uncorrelated linear combinations of the variables that contain most of the variance. In addition to data reduction, the eigenvectors from a PCA are often inspected to learn more about the underlying structure of the data.

PCA originated with the work of Pearson (1901) and Hotelling (1933). For an introduction, see Rabe-Hesketh and Everitt (2007, chap. 14), van Belle, Fisher, Heagerty, and Lumley (2004), or Afifi, May, and Clark (2012). More advanced treatments are Mardia, Kent, and Bibby (1979, chap. 8), and Rencher and Christensen (2012, chap. 12). For monograph-sized treatments, including extensive discussions of the relationship between PCA and related approaches, see Jackson (2003) and Jolliffe (2002).

The objective of PCA is to find unit-length ( $\mathbf{L}'\mathbf{L} = \mathbf{I}$ ) linear combinations of the variables with the greatest variance. The first principal component has maximal overall variance. The second principal component has maximal variance among all unit-length linear combinations that are uncorrelated to the first principal component, etc. The last principal component has the smallest variance among all unit-length linear combinations of the variables. All principal components combined contain the same information as the original variables, but the important information is partitioned over the components in a particular way: the components are orthogonal, and earlier components contain more information than later components. PCA thus conceived is just a linear transformation of the data. It does not assume that the data satisfy a specific statistical model, though it does require that the data be interval-level data—otherwise taking linear combinations is meaningless.

PCA is scale dependent. The principal components of a covariance matrix and those of a correlation matrix are different. In applied research, PCA of a covariance matrix is useful only if the variables are expressed in commensurable units.

#### □ Technical note

Principal components have several useful properties. Some of these are geometric. Both the principal components and the principal scores are uncorrelated (orthogonal) among each other. The f leading principal components have maximal generalized variance among all f unit-length linear combinations.

It is also possible to interpret PCA as a fixed-effects factor analysis with homoskedastic residuals

$$y_{ij} = \mathbf{a}_i' \mathbf{b}_j + e_{ij}$$
  $i = 1, \dots, n$   $j = 1, \dots, p$ 

where  $y_{ij}$  are the elements of the matrix  $\mathbf{Y}$ ,  $\mathbf{a}_i$  (scores) and  $\mathbf{b}_j$  (loadings) are f-vectors of parameters, and  $e_{ij}$  are independent homoskedastic residuals. (In factor analysis, the scores  $\mathbf{a}_i$  are random rather than fixed, and the residuals are allowed to be heteroskedastic in j.) It follows that  $E(\mathbf{Y})$  is a matrix of rank f, with f typically substantially less than n or p. Thus we may think of PCA as a regression model with a restricted number but unknown independent variables. We may also say that the expected values of the rows (or columns) of  $\mathbf{Y}$  are in some unknown f-dimensional space.

For more information on these properties and for other characterizations of PCA, see Jackson (2003) and Jolliffe (2002).

#### Example 1: Principal component analysis of audiometric data

We consider a dataset of audiometric measurements on 100 males, age 39. The measurements are minimal discernible intensities at four different frequencies with the left and right ear (see Jackson 2003, 106). The variable lft1000 refers to the left ear at 1,000 Hz.

- . use http://www.stata-press.com/data/r14/audiometric (Audiometric measures)
- . correlate lft\* rght\*
  (obs=100)

	1ft500	lft1000	lft2000	lft4000	rght500	rght1000	rght2000
lft500	1.0000						
lft1000	0.7775	1.0000					
lft2000	0.4012	0.5366	1.0000				
lft4000	0.2554	0.2749	0.4250	1.0000			
rght500	0.6963	0.5515	0.2391	0.1790	1.0000		
rght1000	0.6416	0.7070	0.4460	0.2632	0.6634	1.0000	
rght2000	0.2372	0.3597	0.7011	0.3165	0.1589	0.4142	1.0000
rght4000	0.2041	0.2169	0.3262	0.7097	0.1321	0.2201	0.3746
	rght4000						
rght4000	1.0000						

As you may have expected, measurements on the same ear are more highly correlated than measurements on different ears. Also, measurements on different ears at the same frequency are more highly correlated than at different frequencies. Because the variables are in commensurable units, it would make theoretical sense to analyze the covariance matrix of these variables. However, the variances of the measures differ widely:

. summarize lft\* rght\*, sep(4)

Variable	Obs	Mean	Std. Dev.	Min	Max
1ft500	100	-2.8	6.408643	-10	15
1ft1000	100	5	7.571211	-10	20
1ft2000	100	2	10.94061	-10	45
1ft4000	100	21.35	19.61569	-10	70
rght500	100	-2.6	7.123726	-10	25
rght1000	100	7	6.396811	-10	20
rght2000	100	1.6	9.289942	-10	35
rght4000	100	21.35	19.33039	-10	75

In an analysis of the covariances, the higher frequency measures would dominate the results. There is no clinical reason for such an effect (see also Jackson [2003]). Therefore, we will analyze the correlation matrix

1.0000

```
. pca lft* rght*
```

Principal components/correlation Number of obs = 100
Number of comp. = 8
Trace = 8

Rotation: (unrotated = principal)

_					
	Component	Eigenvalue	Difference	Proportion	Cumulative
	Comp1	3.92901	2.31068	0.4911	0.4911
	Comp2	1.61832	.642997	0.2023	0.6934
	Comp3	.975325	.508543	0.1219	0.8153
	Comp4	.466782	.126692	0.0583	0.8737
	Comp5	.34009	.0241988	0.0425	0.9162
	Comp6	.315891	.11578	0.0395	0.9557
	Comp7	.200111	.0456375	0.0250	0.9807
	Comp8	.154474		0.0193	1.0000

Rho

Principal components (eigenvectors)

Variable	Comp1	Comp2	Comp3	Comp4	Comp5	Comp6
1ft500	0.4011	-0.3170	0.1582	-0.3278	0.0231	0.4459
1ft1000	0.4210	-0.2255	-0.0520	-0.4816	-0.3792	-0.0675
1ft2000	0.3664	0.2386	-0.4703	-0.2824	0.4392	-0.0638
1ft4000	0.2809	0.4742	0.4295	-0.1611	0.3503	-0.4169
rght500	0.3433	-0.3860	0.2593	0.4876	0.4975	0.1948
rght1000	0.4114	-0.2318	-0.0289	0.3723	-0.3513	-0.6136
rght2000	0.3115	0.3171	-0.5629	0.3914	-0.1108	0.2650
rght4000	0.2542	0.5135	0.4262	0.1591	-0.3960	0.3660

Variable	Comp7	Comp8	Unexplained
lft500	0.3293	-0.5463	0
lft1000	-0.0331	0.6227	0
lft2000	-0.5255	-0.1863	0
lft4000	0.4269	0.0839	0
rght500	-0.1594	0.3425	0
rght1000	-0.0837	-0.3614	0
rght2000	0.4778	0.1466	0
rght4000	-0.4139	-0.0508	0
=			

pca shows two panels. The first panel lists the eigenvalues of the correlation matrix, ordered from largest to smallest. The corresponding eigenvectors are listed in the second panel. These are the principal components and have unit length; the columnwise sum of the squares of the loadings is  $1(0.4011^2 + 0.4210^2 + \cdots + 0.2542^2 = 1)$ .

Remark: Literature and software that treat principal components in combination with factor analysis tend to display principal components normed to the associated eigenvalues rather than to 1. This normalization is available in the postestimation command estat loadings; see [MV] pca postestimation.

The eigenvalues add up to the sum of the variances of the variables in the analysis—the "total variance" of the variables. Because we are analyzing a correlation matrix, the variables are standardized to have unit variance, so the total variance is 8. The eigenvalues are the variances of the principal components. The first principal component has variance 3.93, explaining 49% (3.93/8) of the total variance. The second principal component has variance 1.62 or 20% (1.62/8) of the total variance. Principal components are uncorrelated. You may want to verify that; for instance,

$$0.4011(-0.3170) + 0.4210(-0.2255) + \cdots + 0.2542(0.5135) = 0$$

As a consequence, we may also say that the first two principal components explain the sum of the variances of the individual components, or 49+20=69% of the total variance. Had the components been correlated, they would have partly represented the same information, so the information contained in the combination would not have been equal to the sum of the information of the components. All eight principal components combined explain all variance in all variables; therefore, the unexplained variances listed in the second panel are all zero, and Rho = 1.00 as shown above the first panel.

More than 85% of the variance is contained in the first four principal components. We can list just these components with the option components (4).

Component	Eigenvalue	Difference	Proportion	Cumulative
Comp1	3.92901	2.31068	0.4911	0.4911
Comp2	1.61832	.642997	0.2023	0.6934
Comp3	.975325	.508543	0.1219	0.8153
Comp4	.466782	.126692	0.0583	0.8737
Comp5	.34009	.0241988	0.0425	0.9162
Comp6	.315891	.11578	0.0395	0.9557
Comp7	.200111	.0456375	0.0250	0.9807
Comp8	.154474	•	0.0193	1.0000

Principal components (eigenvectors)

_						,
	Variable	Comp1	Comp2	Comp3	Comp4	Unexplained
	lft500	0.4011	-0.3170	0.1582	-0.3278	.1308
	lft1000	0.4210	-0.2255	-0.0520	-0.4816	.1105
	lft2000	0.3664	0.2386	-0.4703	-0.2824	.1275
	lft4000	0.2809	0.4742	0.4295	-0.1611	.1342
	rght500	0.3433	-0.3860	0.2593	0.4876	.1194
	rght1000	0.4114	-0.2318	-0.0289	0.3723	.1825
	rght2000	0.3115	0.3171	-0.5629	0.3914	.07537
	rght4000	0.2542	0.5135	0.4262	0.1591	.1303
	-					ł

The first panel is not affected. The second panel now lists the first four principal components. These four components do not contain all information in the data, and therefore some of the variances in the variables are unaccounted for or unexplained. These equal the sums of squares of the loadings in the deleted components, weighted by the associated eigenvalues. The unexplained variances in all variables are of similar order. The average unexplained variance is equal to the overall unexplained variance of 13% (1 – 0.87).

Look more closely at the principal components. The first component has positive loadings of roughly equal size on all variables. It can be interpreted as overall sensitivity of a person's ears. The second principal component has positive loadings on the higher frequencies with both ears and negative loadings for the lower frequencies. Thus the second principal component distinguishes sensitivity for higher frequencies versus lower frequencies. The third principal component similarly differentiates sensitivity at medium frequencies from sensitivity at other frequencies. Finally, the fourth principal component has negative loadings on the left ear and positive loadings on the right ear; it differentiates the left and right ear.

We stated earlier that the first principal component had similar loadings on all eight variables. This can be tested if we are willing to assume that the data are multivariate normal distributed. For this case, pca can estimate the standard errors and related statistics. To conserve paper, we request only the results of the first two principal components and specify the option vce(normal).

. pca l\* r\*, comp(2) vce(normal) (with PCA/correlation, SEs and tests are approximate) 100 Principal components/correlation Number of obs Number of comp. 2 Trace 8 Rho = 0.6934 SEs assume multivariate normality SE(Rho) 0.0273 Std. Err. P>|z| [95% Conf. Interval] Coef. z Eigenvalues Comp1 3.929005 .5556453 7.07 0.000 2.839961 5.01805 7.07 Comp2 1.618322 .2288653 0.000 1.169754 2.066889 Comp1 1ft500 .4010948 .0429963 9.33 0.000 .3168236 .485366 .4209908 .0359372 11.71 0.000 .4914264 lft1000 .3505551 1ft2000 .3663748 .0463297 7.91 0.000 .2755702 .4571794 .2808559 4.48 0.000 .4036628 lft4000 .0626577 .1580491 6.50 0.000 rght500 .343251 .0528285 .2397091 .446793 rght1000 10.99 .4114209 .0374312 0.000 .3380571 .4847846 rght2000 .3115483 .0551475 5.65 0.000 .2034612 .4196354 rght4000 .2542212 .066068 3.85 0.000 .1247303 .3837121 Comp2 1ft500 -.3169638 .067871 -4.670.000 -.4499885 -.1839391 lft1000 -.225464.0669887 -3.370.001 -.3567595 -.0941686 2.21 1ft2000 .2385933 .1079073 0.027 .0270989 .4500877 4.90 1ft4000 .4741545 .0967918 0.000 .284446 .6638629 -4.81 rght500 -.3860197 .0803155 0.000 -.5434352-.2286042rght1000 -.2317725 .0674639 -3.440.001 -.3639994 -.0995456 rght2000 .317059 .1215412 2.61 0.009 .0788427 .5552752 rght4000 .0951842 .5135121 5.39 0.000 .3269544 .7000697 LR test for independence: chi2(28) 448.21 Prob > chi2 = 0.0000LR test for sphericity: chi2(35) 451.11 Prob > chi2 = 0.0000Explained variance by components Components Eigenvalue Proportion SE\_Prop Cumulative  $SE_Cum$ Bias Comp1 3.929005 0.4911 0.0394 0.4911 0.0394 .056663 Comp2 1.618322 0.2023 0.0271 0.6934 0.0273 .015812 0.0175 Comp3 -.014322 .9753248 0.1219 0.0178 0.8153 Comp4 .4667822 0.0583 0.0090 0.8737 0.0127 .007304 Comp5 .34009 0.0425 0.0066 0.9162 0.0092 .026307 0.0055 Comp6 .3158912 0.0395 0.0062 0.9557 -.057717 Comp7 0.0040 0.0031 .2001111 0.0250 0.9807 -.013961Comp8 .1544736 0.0193 0.0031 1.0000 0.0000 -.020087

Here pca acts like an estimation command. The output is organized in different equations. The first equation contains the eigenvalues. The second equation named, Comp1, is the first principal component, etc. pca reports, for instance, standard errors of the eigenvalues. Although testing the values of eigenvalues may, up to now, be rare in applied research, interpretation of results should take stability into consideration. It makes little sense to report the first eigenvalue as 3.929 if you see that the standard error is 0.56.

pca has also reported the standard errors of the principal components. It has also estimated the covariances.

```
. estat vce
 (output omitted)
```

Showing the large amount of information contained in the VCE matrix is not useful by itself. The fact that it has been estimated, however, enables us to test properties of the principal components. Does it make good sense to talk about the loadings of the first principal component being of the same size? We use testparm with two options; see [R] test. eq(Comp1) specifies that we are testing coefficients for equation Comp1, that is, the first principal component. equal specifies that instead of testing that the coefficients are zero, we want to test that the coefficients are equal to each other—a more sensible hypothesis because principal components are normalized to 1.

```
. testparm lft* rght*, equal eq(Comp1)
(1)
     - [Comp1]1ft500 + [Comp1]1ft1000 = 0
(2)
     - [Comp1]1ft500 + [Comp1]1ft2000 = 0
(3)
     - [Comp1]1ft500 + [Comp1]1ft4000 = 0
(4)
     - [Comp1]1ft500 + [Comp1]rght500 = 0
(5)
     - [Comp1]lft500 + [Comp1]rght1000 = 0
(6)
      - [Comp1]1ft500 + [Comp1]rght2000 = 0
     - [Comp1]lft500 + [Comp1]rght4000 = 0
          chi2(7) =
                         7.56
        Prob > chi2 =
                         0.3729
```

We cannot reject the null hypothesis of equal loadings, so our interpretation of the first component does not seem to conflict with the data.

pca also displays standard errors of the proportions of variance explained by the leading principal components. Again this information is useful primarily to indicate the strength of formulations of results rather than to test hypotheses about these statistics. The information is also useful to compare studies: if in one study the leading two principal components explain 70% of variance, whereas in a replicating study they explain 80%, are these differences significant given the sampling variation?

Because pca is an estimation command just like regress or xtlogit, you may replay the output by typing just pca. If you have used pca with the vce(normal) option, you may use the option novce at estimation or during replay to display the standard PCA output.

```
. pca, novce
                                                                              100
Principal components/correlation
                                                   Number of obs
                                                   Number of comp.
                                                                                2
                                                   Trace
                                                                                8
    Rotation: (unrotated = principal)
                                                                           0.6934
                                                  Rho
```

Eigenvalue	Difference	Proportion	Cumulative
3.92901	2.31068	0.4911	0.4911
1.61832	.642997	0.2023	0.6934
.975325	.508543	0.1219	0.8153
.466782	.126692	0.0583	0.8737
.34009	.0241988	0.0425	0.9162
.315891	.11578	0.0395	0.9557
.200111	.0456375	0.0250	0.9807
.154474	•	0.0193	1.0000
	3.92901 1.61832 .975325 .466782 .34009 .315891 .200111	3.92901 2.31068 1.61832 .642997 .975325 .508543 .466782 .126692 .34009 .0241988 .315891 .11578 .200111 .0456375	3.92901       2.31068       0.4911         1.61832       .642997       0.2023         .975325       .508543       0.1219         .466782       .126692       0.0583         .34009       .0241988       0.0425         .315891       .11578       0.0395         .200111       .0456375       0.0250

Principal components (eigenvectors)

Variable	Comp1	Comp2	Unexplained
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000 rght4000	0.4011 0.4210 0.3664 0.2809 0.3433 0.4114 0.3115	-0.3170 -0.2255 0.2386 0.4742 -0.3860 -0.2318 0.3171 0.5135	. 2053 . 2214 . 3805 . 3262 . 2959 . 248 . 456

4

### □ Technical note

Inference on the eigenvalues and eigenvectors of a covariance matrix is based on a series of assumptions:

- (A1) The variables are multivariate normal distributed.
- (A2) The variance–covariance matrix of the observations has all distinct and strictly positive eigenvalues.

Under assumptions A1 and A2, the eigenvalues and eigenvectors of the sample covariance matrix can be seen as maximum likelihood estimates for the population analogues that are asymptotically (multivariate) normally distributed (Anderson 1963; Jackson 2003). See Tyler (1981) for related results for elliptic distributions. Be cautious when interpreting because the asymptotic variances are rather sensitive to violations of assumption A1 (and A2). Wald tests of hypotheses that are in conflict with assumption A2 (for example, testing that the first and second eigenvalues are the same) produce incorrect *p*-values.

Because the statistical theory for a PCA of a correlation matrix is much more complicated, pca and pcamat compute standard errors and tests of a correlation matrix as if it were a covariance matrix. This practice is in line with the application of asymptotic theory in Jackson (2003). This will usually lead to some underestimation of standard errors, but we believe that this problem is smaller than the consequences of deviations from normality.

You may conduct tests for multivariate normality using the mvtest normality command (see [MV] mvtest normality):

```
. mvtest normality lft* rght*, stats(all)
Test for multivariate normality
    Mardia mSkewness =
                        14.52785
                                   chi2(120) =
                                                251.052
                                                          Prob>chi2 =
                                                                       0.0000
    Mardia mKurtosis = 94.53331
                                     chi2(1) =
                                                 33.003
                                                          Prob>chi2 =
                                                                       0.0000
    Henze-Zirkler
                    = 1.272529
                                     chi2(1) = 118.563
                                                          Prob>chi2 =
                                                                       0.0000
   Doornik-Hansen
                                                 95.318
                                                          Prob>chi2 =
                                                                       0.0000
                                    chi2(16) =
```

These tests cast serious doubt on the multivariate normality of the variables. We advise caution in interpreting the inference results. Time permitting, you may want to turn to bootstrap methods for inference on the principal components and eigenvalues, but you should be aware of some serious identification problems in using the bootstrap here (Milan and Whittaker 1995).

### Example 2: Analyzing the covariance instead of the correlation

We remarked before that the principal components of a correlation matrix are generally different from the principal components of a covariance matrix. pca defaults to performing the PCA of the correlation matrix. To obtain a PCA of the covariance matrix, specify the covariance option.

Component	Eigenvalue	Difference	Proportion	Cumulative
Comp1	706.795	527.076	0.6122	0.6122
Comp2	179.719	68.3524	0.1557	0.7679
Comp3	111.366	24.5162	0.0965	0.8643
Comp4	86.8501	57.4842	0.0752	0.9396
Comp5	29.366	9.53428	0.0254	0.9650
Comp6	19.8317	6.67383	0.0172	0.9822
Comp7	13.1578	5.74352	0.0114	0.9936
Comp8	7.41432		0.0064	1.0000

Principal components (eigenvectors)

Variable	Comp1	Comp2	Comp3	Comp4	Unexplained
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000	0.0835 0.1091 0.2223 0.6782 0.0662 0.0891	0.2936 0.3982 0.5578 -0.1163 0.2779 0.3119	-0.0105 0.0111 0.0558 -0.7116 -0.0226 0.0268	0.3837 0.3162 -0.4474 -0.0728 0.4951 0.2758	7.85 11.71 11.13 .4024 12.42 11.14
rght2000 rght4000	0.1707 0.6560	0.3745 -0.3403	0.2721 0.6441	-0.4496 0.1550	14.71 .4087
-02101000		1.0100			

As expected, the results are less clear. The total variance to be analyzed is 1,154.5; this is the sum of the variances of the eight variables, that is, the trace of the covariance matrix. The leading principal components now account for a larger fraction of the variance; this is often the case with covariance matrices where the variables have widely different variances. The principal components are somewhat harder to interpret; mainly the loadings are no longer of roughly comparable size.

## Example 3: PCA directly from a correlation matrix

Sometimes you do not have the original data but have only the correlation or covariance matrix. pcamat performs a PCA for such a matrix. To simplify presentation, we use the data on the left ear.

. correlate lft\*, cov
(obs=100)

	lft500	lft1000	lft2000	lft4000
lft500 lft1000 lft2000 lft4000	28.1313	57.3232 44.4444 40.8333		384 775

4

Suppose that we have the covariances of the variables but not the original data. correlate stores the covariances in r(C), so we can use that matrix and invoke pcamat with the options n(100), specifying the number of observations, and names(), providing the variable names.

```
. matrix Cfull = r(C)
```

. pcamat Cfull, comp(2) n(100) names(lft500 lft1000 lft2000 lft4000)

1101000 1102000 11040	00)	
Number of obs	=	100
Number of comp.	=	2
Trace	=	4
Rho	=	0.8169
	Number of obs Number of comp. Trace	Number of comp. = Trace =

Component	Eigenvalue	Difference	Proportion	Cumulative
Comp1 Comp2 Comp3 Comp4	2.37181 .895925 .529687 .202581	1.47588 .366238 .327106	0.5930 0.2240 0.1324 0.0506	0.5930 0.8169 0.9494 1.0000

#### Principal components (eigenvectors)

Variable	Comp1	Comp2	Unexplained
1ft500	0.5384	-0.4319	.1453
1ft1000	0.5730	-0.3499	.1116
1ft2000	0.4958	0.2955	.3387
1ft4000	0.3687	0.7770	.1367

If we had to type in the covariance matrix, to avoid excess typing peamat allows you to provide the covariance (or correlation) matrix with just the upper or lower triangular elements including the diagonal. (Thus, for correlations, you have to enter the 1s for the diagonal.) For example, we could enter the lower triangle of our covariance matrix row by row up to and including the diagonal as a one-row Stata matrix.

```
. matrix Clow = (41.0707, 37.7273, 57.3232, 28.1313, 44.4444, 
> 119.697, 32.101, 40.8333, 91.2121, 384.775)
```

The matrix Clow has one row and 10 columns. To make seeing the structure easier, we prefer to enter these numbers in the following way:

When using the lower or upper triangle stored in a row or column vector, it is not possible to define the variable names as row or column names of the matrix; the option names() is required. Moreover, we have to specify the option shape(lower) to inform pcamat that the vector contains the lower triangle, not the upper triangle.

```
. pcamat Clow, comp(2) shape(lower) n(100) names(lft500 lft1000 lft2000 lft4000) (output omitted)
```

### Stored results

Scalars

pca and pcamat without the vce(normal) option store the following in e():

```
e(N)
                           number of observations
    e(f)
                           number of retained components
    e(rho)
                           fraction of explained variance
    e(trace)
                           trace of e(C)
                           In of the determinant of e(C)
    e(lndet)
    e(cond)
                           condition number of e(C)
Macros
    e(cmd)
                           pca (even for pcamat)
    e(cmdline)
                           command as typed
    e(Ctype)
                           correlation or covariance
    e(wtype)
                           weight type
    e(wexp)
                           weight expression
    e(title)
                           title in output
    e(properties)
                           nob noV eigen
    e(rotate_cmd)
                           program used to implement rotate
    e(estat_cmd)
                           program used to implement estat
                           program used to implement predict
    e(predict)
    e(marginsnotok)
                           predictions disallowed by margins
Matrices
    e(C)
                           p \times p correlation or covariance matrix
    e(means)
                           1 \times p matrix of means
    e(sds)
                           1 \times p matrix of standard deviations
    e(Ev)
                           1 \times p matrix of eigenvalues (sorted)
    e(L)
                           p \times f matrix of eigenvectors = components
    e(Psi)
                           1 \times p matrix of unexplained variance
Functions
                           marks estimation sample
    e(sample)
pca and pcamat with the vce(normal) option store the above, as well as the following:
Scalars
```

```
variance of e(rho)
    e(v_rho)
    e(chi2_i)
                             \chi^2 statistic for test of independence
    e(df_i)
                             degrees of freedom for test of independence
    e(p_i)
                             significance of test of independence
    e(chi2_s)
                             \chi^2 statistic for test of sphericity
    e(df_s)
                             degrees of freedom for test of sphericity
    e(p_s)
                             significance of test of sphericity
    e(rank)
                             rank of e(V)
Macros
                             multivariate normality
    e(vce)
    e(properties)
Matrices
    e(b)
                             1 \times p + fp coefficient vector (all eigenvalues and retained eigenvectors)
    e(Ev_bias)
                             1 \times p matrix: bias of eigenvalues
    e(Ev_stats)
                             p \times 5 matrix with statistics on explained variance
    e(V)
                             variance-covariance matrix of the estimates e(b)
```

## Methods and formulas

Methods and formulas are presented under the following headings:

Notation Inference on eigenvalues and eigenvectors More general tests for multivariate normal distributions

### **Notation**

Let  ${\bf C}$  be the  $p \times p$  correlation or covariance matrix to be analyzed. The spectral or eigen decomposition of  ${\bf C}$  is

$$\mathbf{C} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}' = \sum_{i=1}^{p} \lambda_i \mathbf{v}_i \mathbf{v}_i'$$

$$\mathbf{v}_i' \mathbf{v}_j = \delta_{ij} \qquad \text{(that is, orthonormality)}$$

$$\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_p \ge 0$$

The eigenvectors  $\mathbf{v}_i$  are also known as the principal components. The direction (sign) of principal components is not defined. pca returns principal components signed so that  $\mathbf{1}'\mathbf{v}_i > 0$ . In PCA, "total variance" equals trace( $\mathbf{C}$ ) =  $\sum \lambda_i$ .

## Inference on eigenvalues and eigenvectors

The asymptotic distribution of the eigenvectors  $\widehat{\mathbf{v}}_i$  and eigenvalues  $\widehat{\lambda}_i$  of a covariance matrix  $\mathbf{S}$  for a sample from a multivariate normal distribution  $N(\mu, \Sigma)$  was derived by Girshick (1939); for more results, see also Anderson (1963) and Jackson (2003). Higher-order expansions are discussed in Lawley (1956). See Tyler (1981) for related results for elliptic distributions. The theory of the exact distribution is rather complicated (Muirhead 1982, chap. 9) and hard to implement. If we assume that eigenvalues of  $\Sigma$  are distinct and strictly positive, the eigenvalues and eigenvectors of  $\mathbf{S}$  are jointly asymptotically multivariate normal distributed with the following moments (up to order  $n^{-3}$ ):

$$\begin{split} E(\widehat{\lambda}_i) &= \lambda_i \left\{ 1 + \frac{1}{n} \sum_{j \neq i}^k \left( \frac{\lambda_j}{\lambda_i - \lambda_j} \right) \right\} + O(n^{-3}) \\ \operatorname{Var}(\widehat{\lambda}_i) &= \frac{2\lambda_i^2}{n} \left\{ 1 - \frac{1}{n} \sum_{j \neq i}^k \left( \frac{\lambda_j}{\lambda_i - \lambda_j} \right)^2 \right\} + O(n^{-3}) \\ \operatorname{Cov}(\widehat{\lambda}_i, \widehat{\lambda}_j) &= \frac{2}{n^2} \left( \frac{\lambda_i \lambda_j}{\lambda_i - \lambda_j} \right)^2 + O(n^{-3}) \\ \operatorname{Var}(\widehat{\mathbf{v}}_i) &= \frac{1}{n} \sum_{j \neq i}^k \frac{\lambda_i \lambda_j}{(\lambda_i - \lambda_j)^2} \mathbf{v}_j \mathbf{v}_j' \\ \operatorname{Cov}(\widehat{\mathbf{v}}_i, \widehat{\mathbf{v}}_j) &= -\frac{1}{n} \frac{\lambda_i \lambda_j}{(\lambda_i - \lambda_j)^2} \mathbf{v}_i \mathbf{v}_j' \end{split}$$

For the asymptotic theory of the cumulative proportion of variance explained, see Kshirsagar (1972, 454).

# More general tests for multivariate normal distributions

The likelihood-ratio  $\chi^2$  test of independence (Basilevsky 1994, 187) is

$$\chi^2 = -\left(n - \frac{2p+5}{6}\right) \ln\{\det(\mathbf{C})\}$$

with p(p-1)/2 degrees of freedom.

The likelihood-ratio  $\chi^2$  test of sphericity (Basilevsky 1994, 192) is

$$\chi^2 = -\left(n - \frac{2p^2 + p + 2}{6p}\right) \left[\ln\{\det(\widetilde{\mathbf{\Lambda}})\} - p\ln\left\{\frac{\mathrm{trace}(\widetilde{\mathbf{\Lambda}})}{p}\right\}\right]$$

with (p+2)(p-1)/2 degrees of freedom and with  $\widetilde{\Lambda}$  the eigenvalues of the correlation matrix.

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## Also see

- [MV] pca postestimation Postestimation tools for pca and pcamat
- [MV] alpha Compute interitem correlations (covariances) and Cronbach's alpha
- [MV] **biplot** Biplots
- [MV] canon Canonical correlations
- [MV] factor Factor analysis
- [D] **corr2data** Create dataset with specified correlation structure
- [R] tetrachoric Tetrachoric correlations for binary variables
- [U] 20 Estimation and postestimation commands

## **Title**

pca postestimation — Postestimation tools for pca and pcamat

Postestimation commands predict estat

Remarks and examples Stored results Methods and formulas

References Also see

## **Postestimation commands**

The following postestimation commands are of special interest after pca and pcamat:

Command	Description
estat anti	anti-image correlation and covariance matrices
estat kmo	Kaiser-Meyer-Olkin measure of sampling adequacy
estat loadings	component-loading matrix in one of several normalizations
estat residuals	matrix of correlation or covariance residuals
estat rotatecompare	compare rotated and unrotated components
estat smc	squared multiple correlations between each variable and the rest
*estat summarize	display summary statistics over the estimation sample
loadingplot	plot component loadings
rotate	rotate component loadings
scoreplot	plot score variables
screeplot	plot eigenvalues

 $<sup>^</sup>st$  estat summarize is not available after pcamat.

The following standard postestimation commands are also available:

Command	Description
†estat vce	variance–covariance matrix of the estimators (VCE)
estimates	cataloging estimation results
*lincom	point estimates, standard errors, testing, and inference for linear combinations of coefficients
*nlcom	point estimates, standard errors, testing, and inference for nonlinear combinations of coefficients
predict	score variables, predictions, and residuals
*predictnl	point estimates, standard errors, testing, and inference for generalized predictions
*test	Wald tests of simple and composite linear hypotheses
*testnl	Wald tests of nonlinear hypotheses

 $<sup>\</sup>dagger$  estat vce is available after pca and pcamat with the vce(normal) option.

<sup>\*</sup> lincom, nlcom, predictnl, test, and testnl are available only after pca with the vce(normal) option.

# predict

## Description for predict

predict creates new variables containing predictions such as scores, fitted values, raw residuals, and residual sums of squares.

### Menu for predict

Statistics > Postestimation

## Syntax for predict

$predict [type] {stub*   newvarlist} [if] [in] [, statistic options]$			
statistic	# of vars.	Description ( $k = \#$ of orig. vars.; $f = \#$ of components)	
Main			
<u>sc</u> ore	$1, \ldots, f$	scores based on the components; the default	
<u>f</u> it	k	fitted values using the retained components	
<u>res</u> idual	k	raw residuals from the fit using the retained components	
<u>q</u>	1	residual sums of squares	
options		Description	
Main			
<u>norot</u> ated		use unrotated results, even when rotated results are available	
center base		base scores on centered variables	
notable suppress table of scoring coefficients		suppress table of scoring coefficients	
<u>format</u> (% fmt) format for displaying the scoring coefficients			

## Options for predict

Note on pcamat: predict requires that variables with the correct names be available in memory. Apart from centered scores, means () should have been specified with pcamat. If you used pcamat because you have access only to the correlation or covariance matrix, you cannot use predict.

Main

score calculates the scores for components 1, ..., #, where # is the number of variables in newvarlist.

- fit calculates the fitted values, using the retained components, for each variable. The number of variables in *newvarlist* should equal the number of variables in the *varlist* of pca; see [MV] pca.
- residual calculates for each variable the raw residuals (residual = observed fitted), with the fitted values computed using the retained components.
- q calculates the Rao statistics (that is, the sums of squares of the omitted components) weighted by the respective eigenvalues. This equals the residual sums of squares between the original variables and the fitted values.

norotated uses unrotated results, even when rotated results are available.

center bases scores on centered variables. This option is relevant only for a PCA of a covariance matrix, in which the scores are based on uncentered variables by default. Scores for a PCA of a correlation matrix are always based on the standardized variables.

notable suppresses the table of scoring coefficients.

format (% fint) specifies the display format for scoring coefficients. The default is format (%8.4f).

### estat

## **Description for estat**

estat anti displays the anti-image correlation and anti-image covariance matrices. These are minus the partial covariance and minus the partial correlation of all pairs of variables, holding all other variables constant.

estat kmo displays the Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy. KMO takes values between 0 and 1, with small values indicating that overall the variables have too little in common to warrant a PCA. Historically, the following labels are given to values of KMO (Kaiser 1974):

0.00 to 0.49	unacceptable
0.50 to 0.59	miserable
0.60 to 0.69	mediocre
0.70 to 0.79	middling
0.80 to 0.89	meritorious
0.90 to 1.00	marvelous

estat loadings displays the component-loading matrix in one of several normalizations of the columns (eigenvectors).

estat residuals displays the difference between the observed correlation or covariance matrix and the fitted (reproduced) matrix using the retained factors.

estat rotatecompare displays the unrotated (principal) components next to the most recent rotated components.

estat smc displays the squared multiple correlations between each variable and all other variables. SMC is a theoretical lower bound for communality and thus an upper bound for the unexplained variance.

estat summarize displays summary statistics of the variables in the principal component analysis over the estimation sample. This subcommand is not available after pcamat.

### Menu for estat

Statistics > Postestimation

## Syntax for estat

```
Display the anti-image correlation and covariance matrices
  estat anti [, nocorr nocov <u>for</u>mat(%fmt)]
Display the Kaiser-Meyer-Olkin measure of sampling adequacy
  estat kmo [, novar format(%fmt)]
Display the component-loading matrix
  estat <u>loa</u>dings [, <u>cn</u>orm(<u>unit</u>|<u>eigen</u>|<u>i</u>nveigen) <u>for</u>mat(%fmt)]
Display the differences in matrices
  estat residuals [, obs fitted format(%fmt)]
Display the unrotated and rotated components
  estat rotatecompare [, format(%fmt)]
Display the squared multiple correlations
  estat smc [, format(%fmt)]
Display the summary statistics
  estat <u>summarize</u> [, <u>lab</u>els <u>nohea</u>der <u>noweights</u>]
```

## Options for estat

nocorr, an option used with estat anti, suppresses the display of the anti-image correlation matrix, that is, minus the partial correlation matrix of all pairs of variables, holding constant all other variables.

nocov, an option used with estat anti, suppresses the display of the anti-image covariance matrix, that is, minus the partial covariance matrix of all pairs of variables, holding constant all other variables.

format(%fmt) specifies the display format. The defaults differ between the subcommands.

novar, an option used with estat kmo, suppresses the Kaiser-Meyer-Olkin measures of sampling adequacy for the variables in the principal component analysis, displaying the overall KMO measure

cnorm(unit | eigen | inveigen), an option used with estat loadings, selects the normalization of the eigenvectors, the columns of the principal-component loading matrix. The following normalizations are available

```
ssq(column) = 1; the default
unit
eigen
              ssq(column) = eigenvalue
inveigen
              ssq(column) = 1/eigenvalue
```

with ssq(column) being the sum of squares of the elements in a column and eigenvalue, the eigenvalue associated with the column (eigenvector).

obs, an option used with estat residuals, displays the observed correlation or covariance matrix for which the PCA was performed.

fitted, an option used with estat residuals, displays the fitted (reconstructed) correlation or covariance matrix based on the retained components.

labels, noheader, and noweights are the same as for the generic estat summarize command; see [R] estat summarize.

## Remarks and examples

After computing the principal components and the associated eigenvalues, you have more issues to resolve. How many components do you want to retain? How well is the correlation or covariance matrix approximated by the retained components? How can you interpret the principal components? Is it possible to improve the interpretability by rotating the retained principal components? And, when these issues have been settled, the component scores are probably needed for later research.

The rest of this entry describes the specific tools available for these purposes.

Remarks are presented under the following headings:

Postestimation statistics
Plots of eigenvalues, component loadings, and scores
Rotating the components
How rotate interacts with pca
Predicting the component scores

In addition to these specific postestimation tools, general tools are available as well. pca is an estimation command, so it is possible to manage a series of PCA analyses with the estimates command; see [R] estimates. If you have specified the vce(normal) option, pca has stored the coefficients e(b) and the associated variance—covariance matrix e(V), and you can use standard Stata commands to test hypotheses about the principal components and eigenvalues ("confirmatory principal component analysis"), for instance, with the test, lincom, and testnl commands. We caution you to test only hypotheses that do not violate the assumptions of the theory underlying the derivation of the covariance matrix. In particular, all eigenvalues are assumed to be different and strictly positive. Thus it makes no sense to use test to test the hypothesis that the smallest four eigenvalues are equal (let alone that they are equal to zero.)

### Postestimation statistics

pca displays the principal components in unit normalization; the sum of squares of the principal loadings equals 1. This parallels the standard conventions in mathematics concerning eigenvectors. Some texts and some software use a different normalization. Some texts multiply the eigenvectors by the square root of the eigenvalues. In this normalization, the sum of the squared loadings equals the variance explained by that component. estat loadings can display the loadings in this normalization.

```
. use http://www.stata-press.com/data/r14/audiometric
(Audiometric measures)
. pca l* r*, comp(4)
  (output omitted)
```

. estat loadings, cnorm(eigen)

Principal component loadings (unrotated)

component normalization: sum of squares(column) = eigenvalue

	Comp1	Comp2	Comp3	Comp4
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000	.795 .8345 .7262 .5567 .6804	4032 2868 .3035 .6032 4911	.1562 05132 4645 .4242 .2561	2239 3291 193 1101 .3331
rght2000 rght4000	.6175 .5039	.4033 .6533	5559 .4209	. 2674 . 1087
-				

How close the retained principal components approximate the correlation matrix can be seen from the fitted (reconstructed) correlation matrix and from the residuals, that is, the difference between the observed and fitted correlations.

. estat residual, fit format(%7.3f)

Fitted correlation matrix

Variable	lft500	lft1000	lft2000	lft4000	rght500	rg~1000
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000 rght4000	0.869 0.845 0.426 0.290 0.704 0.706 0.182 0.179	0.890 0.606 0.306 0.586 0.683 0.340 0.176	0.872 0.412 0.162 0.467 0.778 0.348	0.866 0.155 0.236 0.322 0.841	0.881 0.777 0.169 0.166	0.818 0.469 0.234

Variable	rg~2000	rg~4000
rght2000 rght4000	0.925 0.370	0.870

Residual correlation matrix

Variable	lft500	lft1000	lft2000	lft4000	rght500	rg~1000
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000 rght4000	0.131 -0.067 -0.024 -0.035 -0.008 -0.064 0.056 0.025	0.110 -0.070 -0.031 -0.034 0.024 0.020 0.041	0.128 0.013 0.077 -0.021 -0.076 -0.022	0.134 0.024 0.027 -0.005 -0.131	0.119 -0.114 -0.010 -0.034	0.182 -0.054 -0.014

Variable	rg~2000	rg~4000
rght2000 rght4000	0.075 0.005	0.130

All off diagonal residuals are small, except perhaps the two measurements at the highest frequency.

estat also provides some of the standard methods for studying correlation matrices to assess whether the variables have strong linear relations with each other. In a sense, these methods could be seen as preestimation rather than as postestimation methods. The first method is the inspection of the squared multiple correlation (the regression  $\mathbb{R}^2$ ) of each variable on all other variables.

. estat smc
Squared multiple correlations of variables with all other variables

Variable	smc
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000 rght4000	0.7113 0.7167 0.6229 0.5597 0.5893 0.6441 0.5611 0.5409
•	l

The SMC measures help identify variables that cannot be explained well from the other variables. For such variables, you should reevaluate whether they should be included in the analysis. In our examples, none of the SMCs are so small as to warrant exclusion. Two other statistics are offered. First, we can inspect the anti-image correlation and covariance matrices, that is, the negative of correlations (covariances) of the variables partialing out all other variables. If many of these correlations or covariances are "high", the relationships between some of the variables have little to do with the other variables, indicating that it will not be possible to obtain a low-dimensional reduction of the data.

. estat anti, nocov format(%7.3f)
Anti-image correlation coefficients —— partialing out all other variables

Variable	lft500	lft1000	lft2000	lft4000	rght500	rg~1000
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000 rght4000	1.000 -0.561 -0.051 -0.014 -0.466 0.023 0.085 -0.047	1.000 -0.267 0.026 0.131 -0.389 0.068 -0.002	1.000 -0.285 0.064 0.043 -0.617 0.150	1.000 -0.017 -0.042 0.161 -0.675	1.000 -0.441 0.067 0.019	1.000 -0.248 0.023

Variable	rg~2000	rg~4000
rght2000 rght4000	1.000 -0.266	1.000

The Kaiser-Meyer-Olkin measure of sampling adequacy compares the correlations and the partial correlations between variables. If the partial correlations are relatively high compared to the correlations, the KMO measure is small, and a low-dimensional representation of the data is not possible.

. estat kmo Kaiser-Meyer-Olkin measure of sampling adequacy

Variable	kmo
lft500 lft1000 lft2000 lft4000 rght500 rght1000 rght2000 rght4000	0.7701 0.7767 0.7242 0.6449 0.7562 0.8168 0.6673 0.6214
Overall	0.7328

Using the Kaiser (1974) characterization of KMO values,

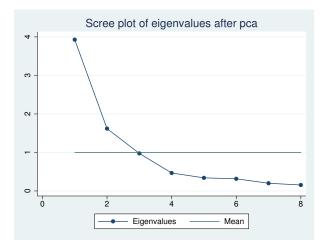
0.00 to 0.49	unacceptable
0.50 to 0.59	miserable
0.60 to 0.69	mediocre
0.70 to 0.79	middling
0.80 to 0.89	meritorious
0.90 to 1.00	marvelous

we declare our KMO value, 0.73, middling.

## Plots of eigenvalues, component loadings, and scores

After computing the principal components, we probably wish to determine how many components to keep. In factor analysis the question of the "true" number of factors is a complicated one. With PCA, it is a little more straightforward. We may set a percentage of variance we wish to account for, say, 90%, and retain just enough components to account for at least that much of the variance. Usually you will want to weigh the costs associated with using more components in later analyses against the benefits of the extra variance they account for. The relative magnitudes of the eigenvalues indicate the amount of variance they account for. A useful tool for visualizing the eigenvalues relative to one another, so that you can decide the number of components to retain, is the scree plot proposed by Cattell (1966); see [MV] screeplot.

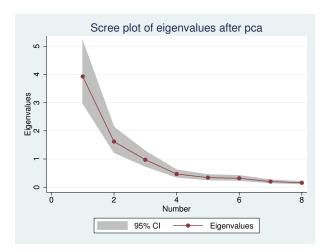
. screeplot, mean



Because we are analyzing a correlation matrix, the mean eigenvalue is 1. We wish to retain the components associated with the high part of the scree plot and drop the components associated with the lower flat part of the scree plot. The boundary between high and low is not clear here, but we would choose two or three components, although the fourth component had the nice interpretation of the left versus the right ear; see [MV] **pca**.

A problem in interpreting the scree plot is that no guidance is given with respect to its stability under sampling. How different could the plot be with different samples? The approximate variance of an eigenvalue  $\hat{\lambda}$  of a covariance matrix for multivariate normal distributed data is  $2\lambda^2/n$ . From this we can derive confidence intervals for the eigenvalues. These scree plot confidence intervals aid in the selection of important components.

. screeplot, ci
(caution is advised in interpreting an asymptotic theory-based confidence
interval of eigenvalues of a correlation matrix)

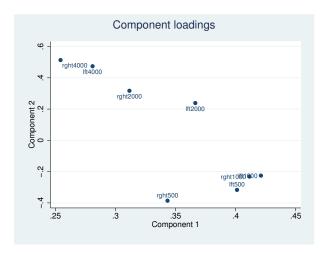


Despite our appreciation of the underlying interpretability of the fourth component, the evidence still points to retaining two or three principal components.

Plotting the components is sometimes useful in interpreting a PCA. We may look at the components from the perspective of the columns (variables) or the rows (observations). The associated plots are produced by the commands loadingplot (variables) and scoreplot (observations).

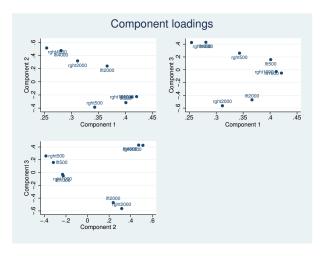
By default, the first two components are used to produce the loading plot.

. loadingplot



You may request more components, in which case each possible pair of requested components will be graphed. You can choose between a matrix or combined graph layout for the multiple graphs. Here we show the combined layout.

. loadingplot, comp(3) combined



Score plots approach the display of principal components from the perspective of the observations. scoreplot and loadingplot have most of their options in common; see [MV] scoreplot. Unlike loadingplot, which automatically uses the variable names as marker labels, with scoreplot you use the mlabel() graph option to provide meaningful marker labels. Score plots are especially helpful if the observations are well-known objects, such as countries, firms, or brands. The score plot may

help you visualize the principal components with your background knowledge of these objects. Score plots are sometimes useful for detecting outliers; see Jackson (2003).

### □ Technical note

In [MV] **pca**, we noted that PCA may also be interpreted as fixed-effects factor analysis; in that interpretation, the selection of the number of components to be retained is of comparable complexity as in factor analysis.

## Rotating the components

Rotating principal components is a disputed issue and one in which reasonable people may disagree. pca computes the principal components. Rotating the solution destroys some of the properties of principal components. In particular, the first rotated component no longer has maximal variance, the second rotated component no longer has maximal variance among those linear combinations uncorrelated to the first component, etc. If preserving the maximal variance property is very important to your interpretations, do not rotate.

On the other hand, when we rotate, say, the leading three principal components, the total variance explained by the three rotated components is equal to the variance explained by the three principal components. If you applied an orthogonal rotation, the rotated components are still uncorrelated. The only thing that has changed is that the explanation is distributed differently among the three rotated components. If the rotated components have a clearer interpretation, you may actually prefer to use them in your subsequent work.

After pca, a wide variety of rotations are available; see [MV] **rotate**. The default method of rotation is varimax, rotating the principal components to maximize the sum over the columns of the within-column variances.

### . rotate

Principal components/correlation	Number of obs	=	100
	Number of comp.	=	4
	Trace	=	8
Rotation: orthogonal varimax (Kaiser off)	Rho	=	0.8737

Component	Variance	Difference	Proportion	Cumulative
Comp1	2.11361	.400444	0.2642	0.2642
Comp2	1.71316	.118053	0.2141	0.4783
Comp3	1.59511	.0275517	0.1994	0.6777
Comp4	1.56756		0.1959	0.8737

### Rotated components

Variable	Comp1	Comp2	Comp3	Comp4	Unexplained
1ft500	0.5756	0.0265	-0.1733	0.1781	.1308
1ft1000	0.6789	-0.0289	-0.0227	-0.0223	.1105
1ft2000	0.3933	0.0213	0.5119	-0.2737	.1275
1ft4000	0.1231	0.6987	-0.0547	-0.0885	.1342
rght500	-0.0005	0.0158	-0.0380	0.7551	.1194
rght1000	0.0948	-0.0248	0.2289	0.5481	.1825
rght2000	-0.1173	-0.0021	0.8047	0.0795	.07537
rght4000	-0.1232	0.7134	0.0550	0.0899	

#### Component rotation matrix

	Comp1	Comp2	Comp3	Comp4
Comp1	0.6663	0.3784	0.4390	0.4692
Comp2	-0.3055	0.6998	0.4012	-0.5059
Comp3	-0.0657	0.6059	-0.7365	0.2936
Comp4	-0.6770	-0.0022	0.3224	0.6616

rotate now labels one of the columns of the first table as "Variance" instead of "Eigenvalue"; the rotated components have been ordered in decreasing order of variance. The variance explained by the four rotated components equals 87.37%, which is identical to the explained variance by the four leading principal components. But whereas the principal components have rather dispersed eigenvalues, the four rotated components all explain about the same fraction of the variance.

You may also choose to rotate only a few of the retained principal components. In contrast to most methods of factor analysis, the principal components are not affected by the number of retained components. However, the first two rotated components are different if you are rotating all four components or only the leading two or three principal components.

## . rotate, comp(3)

Principal components/correlation	Number of obs	=	100
	Number of comp.	=	4
	Trace	=	8
Rotation: orthogonal varimax (Kaiser off)	Rho	=	0.8737

Component	Variance	Difference	Proportion	Cumulative
Comp1 Comp2 Comp3 Comp4	2.99422 1.8258 1.70264 .466782	1.16842 .123163 1.23585	0.3743 0.2282 0.2128 0.0583	0.3743 0.6025 0.8153 0.8737

#### Rotated components

Variable	Comp1	Comp2	Comp3	Comp4	Unexplained
lft500	0.5326	-0.0457	0.0246	-0.3278	.1308
lft1000	0.4512	0.1618	-0.0320	-0.4816	.1105
lft2000	0.0484	0.6401	0.0174	-0.2824	.1275
lft4000	0.0247	0.0011	0.6983	-0.1611	.1342
rght500	0.5490	-0.1799	0.0163	0.4876	.1194
rght1000	0.4521	0.1368	-0.0259	0.3723	.1825
rght2000	-0.0596	0.7148	-0.0047	0.3914	.07537
rght4000	-0.0200	0.0059	0.7138	0.1591	.1303

### Component rotation matrix

	Comp1	Comp2	Comp3	Comp4
Comp1	0.7790	0.5033	0.3738	0.0000
Comp2	-0.5932	0.3987	0.6994	0.0000
Comp3	0.2030	-0.7666	0.6092	-0.0000
Comp4	0.0000	-0.0000	-0.0000	1.0000

The three-component varimax-rotated solution differs from the leading three components from the four component varimax-rotated solution. The fourth component is not affected by a rotation among the leading three component—it is still the fourth principal component. So, how interpretable are rotated components? We believe that for this example the original components had a much clearer interpretation than the rotated components. Notice how the clear symmetry in the treatment of left and right ears has been broken.

To add further to an already controversial method, we may use oblique rotation methods. An example is the oblique oblimin method.

100

. rotate, oblimin oblique

Principal components/correlation Number of obs = Number of comp. =

 ${\it Trace} = 8$  Rotation: oblique oblimin (Kaiser off) Rho = 0.8737

Component	Variance	Proportion	Rotated comp. are correlated
Comp1 Comp2	2.21066 1.71164	0.2763 0.2140	
Comp3	1.69708	0.2121	
Comp4	1.62592	0.2032	

#### Rotated components

Variable	Comp1	Comp2	Comp3	Comp4	Unexplained
1ft500 1ft1000 1ft2000 1ft4000 rght500 rght1000 rght2000	0.5834 0.6797 0.3840 0.1199 0.0261 0.1140 -0.1158	0.0259 -0.0292 0.0216 0.6988 0.0146 -0.0257	0.1994 0.0055 -0.2489 -0.0857 0.7561 0.5575	-0.1649 -0.0157 0.5127 -0.0545 -0.0283 0.2370 0.8048	.1308 .1105 .1275 .1342 .1194 .1825
rght4000	-0.1209	0.7134	0.0848	0.0549	.1303

#### Component rotation matrix

	Comp1	Comp2	Comp3	Comp4
Comp1	0.6836	0.3773	0.5053	0.4523
Comp2	-0.3250	0.7008	-0.5137	0.3916
Comp3	-0.0550	0.6054	0.2774	-0.7337
Comp4	-0.6557	-0.0029	0.6408	0.3238

The oblique rotation methods do not change the variance that is unexplained by the components. But this time, the rotated components are no longer uncorrelated. This makes measuring the importance of the rotated components more ambiguous, a problem that is similar to ambiguities in interpreting importance of correlated independent variables. In this oblique case, the sum of the variances of the rotated components equals 90.6% (0.2763 + 0.2140 + 0.2121 + 0.2032) of the total variance. This is larger than the 87.37% of variance explained by the four principal components. The oblique rotated components partly explain the same variance, and this shared variance is entering multiple times into the total.

### How rotate interacts with pca

rotate stores the rotated component loadings and associated statistics in e(), the estimation storage area, along with the regular pca estimation results. Replaying pca will display the rotated results again.

Other postestimation statistics also use the rotated results whenever this is meaningful. For instance, loadingplot would display the rotated loadings. These postestimation commands have an option norotated that specifies that the unrotated results, that is, the principal components, be used. Thus

. pca, norotated
 (output omitted)

displays the standard pca output for the unrotated (principal) solution, and

. loadingplot, norotated
 (output omitted)

produces the loading plot for the unrotated (principal) solution.

If you execute rotate again, the new rotate results are stored with the pca estimation, replacing the previous rotate results. Thus pca knows about at most one rotation.

To compare rotated and unrotated results, it is of course possible to replay the rotated results (pca) and unrotated results (pca, norotate) consecutively. You would especially seek to compare the loadings. Such a comparison is easier if the loadings are displayed in parallel. This feature is provided with the estat command rotatecompare.

. estat rotatecompare
Rotation matrix — oblique oblimin (Kaiser off)

Variable	Comp1	Comp2	Comp3	Comp4
Comp1	0.6836	0.3773	0.5053	0.4523
Comp2	-0.3250	0.7008	-0.5137	0.3916
Comp3	-0.0550	0.6054	0.2774	-0.7337
Comp4	-0.6557	-0.0029	0.6408	0.3238

#### Rotated component loadings

Variable	Comp1	Comp2	Comp3	Comp4
1ft500 1ft1000 1ft2000 1ft4000	0.5834 0.6797 0.3840 0.1199 0.0261	0.0259 -0.0292 0.0216 0.6988 0.0146	0.1994 0.0055 -0.2489 -0.0857 0.7561	-0.1649 -0.0157 0.5127 -0.0545 -0.0283
rght500 rght1000 rght2000 rght4000	0.0261 0.1140 -0.1158 -0.1209	-0.0257 -0.0022 0.7134	0.7561 0.5575 0.0892 0.0848	0.2370 0.8048 0.0549

Unrotated component loadings

Variable	Comp1	Comp2	Comp3	Comp4
1ft500	0.4011	-0.3170	0.1582	-0.3278
1ft1000	0.4210	-0.2255	-0.0520	-0.4816
1ft2000	0.3664	0.2386	-0.4703	-0.2824
1ft4000	0.2809	0.4742	0.4295	-0.1611
rght500	0.3433	-0.3860	0.2593	0.4876
rght1000	0.4114	-0.2318	-0.0289	0.3723
rght2000	0.3115	0.3171	-0.5629	0.3914
rght4000	0.2542	0.5135	0.4262	0.1591

Finally, sometimes you may want to remove rotation results permanently; for example, you decide to continue with the unrotated (principal) solution. Because all postestimation commands operate on the rotated solution by default, you would have to add the option norotated over and over again. Instead, you can remove the rotated solution with the command

. rotate, clear

### □ Technical note

pca results may be stored and restored with estimates, just like other estimation results. If you have stored PCA estimation results without rotated results, and later rotate the solution, the rotated results are not automatically stored as well. The pca would need to be stored again.

## Predicting the component scores

After deciding on the number of components and, possibly, the rotation of the components, you may want to estimate the component scores for all respondents. To estimate only the first component scores, which here is called pc1:

```
. predict pc1
(score assumed)
(3 components skipped)
Scoring coefficients
    sum of squares(column-loading) = 1
```

Variable	Comp1	Comp2	Comp3	Comp4
lft500	0.4011	-0.3170	0.1582	-0.3278
lft1000	0.4210	-0.2255	-0.0520	-0.4816
lft2000	0.3664	0.2386	-0.4703	-0.2824
lft4000	0.2809	0.4742	0.4295	-0.1611
rght500	0.3433	-0.3860	0.2593	0.4876
rght1000	0.4114	-0.2318	-0.0289	0.3723
rght2000	0.3115	0.3171	-0.5629	0.3914
rght4000	0.2542	0.5135	0.4262	0.1591

The table is informing you that pc1 could be obtained as a weighted sum of standardized variables,

- . egen  $std_lft500 = std(lft500)$
- . egen std\_lft1000 = std(lft1000)
- . egen std\_rght4000 = std(rght4000)
- . gen pc1 = 0.4011\*std\_lft500 + 0.4210\*std\_lft1000 + ... + 0.2542\*std\_rght4000

(egen's std() function converts a variable to its standardized form (mean 0, variance 1); see [D] egen.) The principal-component scores are in standardized units after a PCA of a correlation matrix and in the original units after a PCA of a covariance matrix.

It is possible to predict other statistics as well. For instance, the fitted values of the eight variables by the first four principal components are obtained as

```
. predict f_1-f_8, fit
```

The predicted values are in the units of the original variables, with the means substituted back in. If we had retained all eight components, the fitted values would have been identical to the observations.

#### □ Technical note

The fitted values are meaningful in the interpretation of PCA as rank-restricted multivariate regression. The component scores are the "x variables"; the component loadings are the regression coefficients. If the PCA was computed for a correlation matrix, you could think of the regression as being in standardized units. The fitted values are transformed from the standardized units back to the original units.

### □ Technical note

You may have observed that the scoring coefficients were equal to the component loadings. This holds true for the principal components in unit normalization and for the orthogonal rotations thereof; it does not hold for oblique rotations.

### Stored results

```
Let p be the number of variables and f, the number of factors.
```

predict, in addition to generating variables, also stores the following in r():

#### Matrices

r(scoef)  $p \times f$  matrix of scoring coefficients

estat anti stores the following in r():

#### Matrices

r(acov)  $p \times p$  anti-image covariance matrix r(acorr)  $p \times p$  anti-image correlation matrix

estat kmo stores the following in r():

#### Scalars

r(kmo) the Kaiser-Meyer-Olkin measure of sampling adequacy

Matrices

r(kmow) column vector of KMO measures for each variable

estat loadings stores the following in r():

#### Macros

r(cnorm) component normalization: eigen, inveigen, or unit

Matrices

r(A)  $p \times f$  matrix of normalized component loadings

estat residuals stores the following in r():

Matrices

r(fit)  $p \times p$  matrix of fitted values r(residual)  $p \times p$  matrix of residuals

estat smc stores the following in r():

Matrices

r(smc) vector of squared multiple correlations of variables with all other variables

See the returned results of estat summarize in [R] estat summarize and of estat vce in [R] estat vce (available when vce(normal) is specified with pca or pcamat).

rotate after pca and pcamat add to the existing e():

Scalars

e(r\_f) number of components in rotated solution

e(r\_fmin) rotation criterion value

Macros

e(r\_class) orthogonal or oblique

e(r\_criterion) rotation criterion e(r\_ctitle) title for rotation e(r\_normalization) kaiser or none

Matrices

e(r\_L) rotated loadings

e(r\_T) rotation

e(r\_Ev) explained variance by rotated components

The components in the rotated solution are in decreasing order of e(r\_Ev).

## Methods and formulas

estat anti computes and displays the anti-image covariance matrix  ${f C}$  and the anti-image correlation matrix  ${f A}$ 

$$\mathbf{C} = \{\operatorname{diag}(\mathbf{R})\}^{-1/2} \mathbf{R} \{\operatorname{diag}(\mathbf{R})\}^{-1/2}$$

$$\mathbf{A} = \{\text{diag}(\mathbf{R})\}^{-1} \; \mathbf{R} \; \{\text{diag}(\mathbf{R})\}^{-1}$$

where  $\mathbf{R}$  is the inverse of the correlation matrix.

estat kmo computes the "Kaiser-Meyer-Olkin measure of sampling adequacy" (KMO) and is defined as

$$\mathrm{KMO} = \frac{\sum_{\mathcal{S}} r_{ij}^2}{\sum_{\mathcal{S}} (a_{ij}^2 + r_{ij}^2)}$$

where  $S = (i, j; i \neq j)$ ;  $r_{ij}$  is the correlation of variables i and j; and  $a_{ij}$  is the anti-image correlation. The variable-wise measure KMO $_i$  is defined analogously as

$$\mathrm{KMO}_i = \frac{\sum_{\mathcal{P}} r_{ij}^2}{\sum_{\mathcal{P}} (a_{ij}^2 + r_{ij}^2)}$$

where  $\mathcal{P} = (j; i \neq j)$ .

estat loadings displays the component loadings in different normalizations (see Jackson [2003, 16–18]; he labels them as U, V, and W vectors). Let  $C = L\Lambda L'$  be the spectral or eigen decomposition of the analyzed correlation or covariance matrix C, with L the orthonormal eigenvectors of C, and  $\Lambda$  a diagonal matrix of eigenvalues. The principal components A, that is, the eigenvectors L, are displayed in one of the following normalizations:

Normalization of the component loadings affects the normalization of the component scores.

The standard errors of the components are available only in unit normalization, that is, as normalized eigenvectors.

estat residuals computes the fitted values F for the analyzed correlation or covariance matrix C as  $F = L\Lambda L'$  over the retained components, with L being the retained components in unit normalization and  $\Lambda$  being the associated eigenvalues. The residuals are simply C - F.

estat smc displays the squared multiple correlation coefficients  $SMC_i$  of each variable on the other variables in the analysis. These are conveniently computed from the inverse  $\mathbf{R}$  of the correlation matrix  $\mathbf{C}$ ,

$$SMC_i = 1 - \mathbf{R}_{ii}^{-1}$$

See [MV] rotate and [MV] rotatemat for details concerning the rotation methods and algorithms used.

The variance of the rotated loadings  $L_r$  is computed as  $L_{r'}CL_r$ .

To understand predict after pca and pcamat, think of PCA as a fixed-effects factor analysis with homoskedastic residuals

$$Z = AL' + E$$

 ${f L}$  contains the loadings, and  ${f A}$  contains the scores.  ${f Z}$  is the centered variables for a PCA of a covariance matrix and standardized variables for a PCA of a correlation matrix.  ${f A}$  is estimated by OLS regression of  ${f Z}$  on  ${f L}$ 

$$\widehat{\mathbf{A}} = \mathbf{Z}\mathbf{B}$$
  $\mathbf{B} = \mathbf{L}(\mathbf{L}'\mathbf{L})^{-}$ 

The columns of A are called the scores. The matrix B contains the scoring coefficients. The PCA-fitted values for Z are defined as the fitted values from this regression, or in matrix terms,

$$\widehat{\mathbf{Z}} = \mathbf{Z}\mathbf{P}_{\mathbf{L}} = \mathbf{Z}\mathbf{L}(\mathbf{L}'\mathbf{L})^{-}\mathbf{L}'$$

with  $\mathbf{P_L}$  the orthogonal projection on (the rowspace of)  $\mathbf{L}$ .

This formulation allows orthogonal as well as oblique loadings L as well as loadings in different normalizations.

The above formulation is in transformed units. predict transforms the fitted values back to the original units. The component scores are left in transformed units, with one exception. After a PCA of covariances, means are substituted back in unless the option centered is specified. The residuals are returned in the original units. The residual sums of squares (over the variables) and the normalized versions are in transformed units.

## References

Cattell, R. B. 1966. The scree test for the number of factors. Multivariate Behavioral Research 1: 245-276.

Jackson, J. E. 2003. A User's Guide to Principal Components. New York: Wiley.

Kaiser, H. F. 1974. An index of factor simplicity. Psychometrika 39: 31-36.

Also see References in [MV] pca.

## Also see

[MV] **pca** — Principal component analysis

[MV] rotate — Orthogonal and oblique rotations after factor and pca

[MV] scoreplot — Score and loading plots

[MV] **screeplot** — Scree plot

[U] 20 Estimation and postestimation commands

### Title

## procrustes — Procrustes transformation

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Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

procrustes performs the Procrustean analysis, a standard method of multidimensional scaling in which the goal is to transform the source varlist to be as close as possible to the target varlist. Closeness is measured by the residual sum of squares. The permitted transformations are any combination of dilation (uniform scaling), rotation and reflection (that is, orthogonal or oblique transformations), and translation. procrustes deals with complete cases only. procrustes assumes equal weights or scaling for the dimensions. Variables measured on different scales should be standardized before using procrustes.

### **Quick start**

```
Procrustes transform source variables x1 and x2 to be close to target variables y1 and y2 procrustes (y1 y2) (x1 x2)
```

```
Add a third source variable, x3, and target variable, y3 procrustes (y1 y2 y3) (x1 x2 x3)
```

As above, but allow an oblique instead of an orthogonal rotation

```
procrustes (y1 y2 y3) (x1 x2 x3), transform(oblique)
```

As above, but suppress dilation

```
procrustes (y1 y2 y3) (x1 x2 x3), transform(oblique) norho
```

### Menu

Statistics > Multivariate analysis > Procrustes transformations

# **Syntax**

```
procrustes (varlist_y) (varlist_x) [if] [in] [weight] [, options]
```

options	Description
Model	
<u>transform(or</u> thogonal)	orthogonal rotation and reflection transformation; the default
$\underline{\mathtt{tr}}\mathtt{ansform}(\underline{\mathtt{ob}}\mathtt{lique})$	oblique rotation transformation
<u>transform(unrestricted)</u>	unrestricted transformation
noconstant	suppress the constant
<u>norh</u> o	suppress the dilation factor $\rho$ (set $\rho = 1$ )
force	allow overlap and duplicates in $varlist_y$ and $varlist_x$ (advanced)
Reporting	
nofit	suppress table of fit statistics by target variable

bootstrap, by, jackknife, and statsby are allowed; see [U] 11.1.10 Prefix commands.

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

aweights are not allowed with the jackknife prefix; see [R] jackknife.

aweights and fweights are allowed; see [U] 11.1.6 weight.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

## **Options**

Model

transform(transform) specifies the transformation method. The following transformation methods are allowed:

orthogonal specifies that the linear transformation matrix A should be orthogonal, A'A = AA' = I. This is the default.

oblique specifies that the linear transformation matrix A should be oblique, diag(AA') = 1.

unrestricted applies no restrictions to **A**, making the procrustes transformation equivalent to multivariate regression with uncorrelated errors; see [MV] **mvreg**.

noconstant specifies that the translation component c is fixed at 0 (the 0 vector).

norho specifies that the dilation (scaling) constant  $\rho$  is fixed at 1. This option is not relevant with transform(unrestricted); here  $\rho$  is always fixed at 1.

force, an advanced option, allows overlap and duplicates in the target variables  $varlist_y$  and source variables  $varlist_x$ .

Reporting

nofit suppresses the table of fit statistics per target variable. This option may be specified during estimation and upon replay.

## Remarks and examples

Remarks are presented under the following headings:

Introduction to Procrustes methods Orthogonal Procrustes analysis Is an orthogonal Procrustes analysis symmetric? Other transformations

### Introduction to Procrustes methods

The name *Procrustes analysis* was applied to optimal matching of configurations by Hurley and Cattell (1962) and refers to Greek mythology. The following account follows Cox and Cox (2001, 123). Travelers from Eleusis to Athens were kindly invited by Damastes to spend the night at his place. Damastes, however, practiced a queer kind of hospitality. If guests would not fit the bed, Damastes would either stretch them to make them fit, or chop off extremities if they were too long. Therefore, he was given the nickname Procrustes—ancient Greek for "the stretcher". Theseus, a warrior, finally gave Procrustes some of his own medicine.

Procrustes methods have been applied in many areas. Gower and Dijksterhuis (2004) mention applications in psychometrics (for example, the matching of factor loading matrices), image analysis, market research, molecular biology, biometric identification, and shape analysis.

Formally, procrustes solves the minimization problem

Minimize 
$$|\mathbf{Y} - (\mathbf{1c'} + \boldsymbol{\rho} \mathbf{X} \mathbf{A})|$$

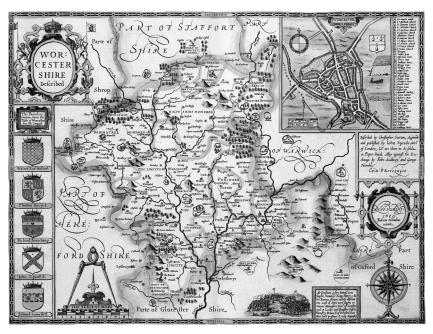
where  $\mathbf{c}$  is a row vector representing the translation,  $\boldsymbol{\rho}$  is the scalar "dilation factor",  $\mathbf{A}$  is the rotation and reflection matrix (orthogonal, oblique, or unrestricted), and |.| denotes the L2 norm. The goal is to transform the source  $\mathbf{X}$  to be as close as possible to the target  $\mathbf{Y}$ . The permitted Closeness is measured by the residual sum of squares.

Some of the early work on Procrustes analysis was done by Mosier (1939), Green (1952), Hurley and Cattell (1962), and Browne (1967); see Gower and Dijksterhuis (2004).

## **Orthogonal Procrustes analysis**

## Example 1

We illustrate procrustes with John Speed's historical 1610 map of the Worcestershire region in England, engraved and printed by Jodocus Hondius in Amsterdam in 1611–1612. Used with permission of Peen (2007).



We analyze the accuracy of this map. Cox and Cox (2001) present data on the locations of 20 towns and villages on this old map, as well as the locations on a modern map from the Landranger Series of Ordnance Survey Maps. The locations were measured relative to the lower-left corner of the maps. We list this small dataset, specifying the noobs option to prevent wrapping and sep(0) to suppress internal horizontal lines.

- . use http://www.stata-press.com/data/r14/speed\_survey
  (Data on Speed's Worcestershire map (1610))
- . list name lname speed\_x speed\_y survey\_x survey\_y, sep(0) noobs

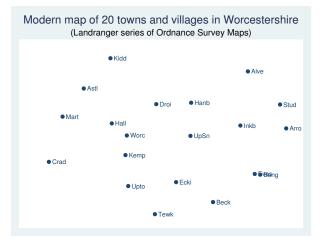
name	lname	speed_x	speed_y	survey_x	survey_y
Alve	Alvechurch	192	211	1027	725
Arro	Arrow	217	155	1083	565
Astl	Astley	88	180	787	677
Beck	Beckford	193	66	976	358
Beng	Bengeworth	220	99	1045	435
Crad	Cradley	79	93	736	471
Droi	Droitwich	136	171	893	633
Ecki	Eckington	169	81	922	414
Eves	Evesham	211	105	1037	437
Hall	Hallow	113	142	828	579
Hanb	Hanbury	162	180	944	637
Inkb	Inkberrow	188	156	1016	573
Kemp	Kempsey	128	108	848	490
Kidd	Kidderminster	104	220	826	762
Mart	Martley	78	145	756	598
Stud	Studley	212	185	1074	632
Tewk	Tewkesbury	163	40	891	324
UpSn	UpperSnodsbury	163	138	943	544
Upto	Upton	138	71	852	403
Worc	Worcester	125	132	850	545

You will probably conclude immediately that the scales of the two maps differ and that the coordinates are expressed with respect to different reference points; the lower-left corners of the maps correspond to different physical locations. Another distinction will not be so obvious—at least not by looking at these numbers: the orientations of the maps may well differ. We display as scatterplots Speed's data (speed\_x, speed\_y) and the modern survey data (survey\_x, survey\_y).

- . scatter speed\_y speed\_x, mlabel(name)
- > ytitle("") xtitle("") yscale(off) xscale(off) ylabel(,nogrid)
- > title(Historic map of 20 towns and villages in Worcestershire)
- > subtitle((Speed 1610))



- . scatter survey\_y survey\_x, mlabel(name)
- > ytitle("") xtitle("") yscale(off) xscale(off) ylabel(,nogrid)
- > title(Modern map of 20 towns and villages in Worcestershire)
- > subtitle((Landranger series of Ordnance Survey Maps))



To gauge the accuracy of the historic map, we must account for differences in scale, location, and orientation. Because the area depicted on the map is relatively small, we think that it is justified to ignore the curvature of the earth and approximate distances along the globe with Euclidean distances, and apply a Procrustes analysis,

$$survey\_map = transformation(speed\_map) + residual$$

choosing the transformation (from among the allowed transformations) to minimize the residual in terms of the residual sum of squares. The transformation should allow for, in mathematical terms,

translation, uniform scaling, and two-dimensional orthogonal rotation. The uniform scaling factor is often described as the dilation factor, a positive scalar. The transformation from source to target configuration can be written as

$$\left(\begin{array}{ll} \text{survey\_x} & \text{survey\_y} \end{array}\right) = \left(\begin{array}{cc} c_x & c_y \end{array}\right) + \rho \left(\begin{array}{cc} \text{speed\_x} & \text{speed\_y} \end{array}\right) \left(\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right) + \left(\begin{array}{cc} \text{res\_x} & \text{res\_y} \end{array}\right)$$

or simply as

 $survey\_map = translation + dilation \times speed\_map \times rotation + residual$ 

The matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

should satisfy the constraint that it represents an orthogonal rotation—it should maintain the lengths of vectors and the angles between vectors. We estimate the translation  $(c_x \quad c_y)$ , dilation factor  $\rho$ , and the rotation matrix  $\mathbf{A}$  with the procrustes command.

```
. procrustes (survey_x survey_y) (speed_x speed_y)
```

Procrustes analysis (orthogonal)

Number of observations	=	20
Model df (df_m)	=	4
Residual df (df_r)	=	36
SS(target)	=	495070
RSS(target)	=	1973.384
<pre>RMSE = root(RSS/df_r)</pre>	=	7.403797
Procrustes = RSS/SS	=	0.0040

Translation c

	survey_x	survey_y
_cons	503.8667	293.9878

Rotation & reflection matrix A (orthogonal)

	survey_x	survey_y
speed_x	.9841521	1773266
speed_y	.1773266	.9841521

Dilation factor

$$rho = 2.3556$$

Fit statistics by target variable

Statistics	survey_x	survey_y
SS	216310.2	278759.8
RSS	1081.36	892.0242
RMSE	7.750841	7.039666
Procrustes	.0049991	.0032
Corr_y_yhat	.9976669	.9985076

We can read the elements of the transformation from the output: the translation from the Speed map onto the survey map is (504, 294). The scale of the survey and Speed maps differ by a factor of 2.36. The orientations of the maps also differ somewhat; if the maps had been oriented the same, we would have expected the rotation to be an identity matrix. Note that  $.984^2 + .177^2 = 1$ , subject to rounding error—indeed the rotation is "norm preserving". A counterclockwise rotation in a plane over  $\theta$  can be written as

$$\begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}$$

See appendix B in Gower and Dijksterhuis (2004). Here  $\cos(\theta) = 0.984$ , so the difference in orientation of the two maps is  $\theta = 10.2$  degrees.

The other output produced by procrustes may be more familiar, procrustes estimated four parameters: the angle of rotation, two translation parameters, and the dilation factor  $\rho$ . SS(target) is the centered sum of squares of the survey data, and is meaningful mostly in relation to the residual sum of squares RSS(target). The Procrustes statistic, defined as RSS/SS, measures the size of the residuals relative to the variation in the target variables; it is equivalent to  $1-R^2$  in a regression analysis context. The smaller the Procrustes statistic, the closer the correspondence of Speed's map to the survey map. The number in this case, 0.004, is small indeed. Another way of looking at fit is via the square root of the mean squared residual error, RMSE, a measure for the average size of residuals.

The last output table describes how well the transformed Speed coordinates match the survey coordinates, separately for the horizontal (x) and the vertical (y) coordinates. In this case, we do not see disturbing differences between the coordinates. By definition, the overall Procrustes statistic and the overall RMSE are averages of the coordinate statistics. Because Procrustes analysis treats (weights) both coordinates the same and independently, analogous to the sphericity assumption in multivariate regression or MANOVA analysis, the comparable statistics for the different coordinates is reassuring.

This example is continued in [MV] **procrustes postestimation**, demonstrating how to generate fitted values and residual sum of squares with predict, how to produce a graph showing the target overlaid with the transformed source values with procoverlay, and how to produce various summaries and comparisons with estat.

A Procrustes analysis fits the transformation subject to the constraint that  $\mathbf{A}$  is orthogonal; for other constraints, see below. In two dimensions, there are actually two types of orthogonal matrices: rotations and reflections. Think of left and right hands. A rotation transforms a left hand into a left hand, never into a right hand; rotation preserves orientation. A reflection changes a left hand into a right hand; reflections invert orientation. In algebraic terms, an orthogonal matrix  $\mathbf{A}$  satisfies  $\det(\mathbf{A}) = \pm 1$ .  $\mathbf{A}$  is a rotation if  $\det(\mathbf{A}) = 1$ , and  $\mathbf{A}$  is a reflection if  $\det(\mathbf{A}) = -1$ . In more than

two dimensions, the classification of orthogonal transformations is more complicated.

## Example 2

In example 1, we treated the location, dilation, and orientation as estimable aspects of the transformation. It is possible to omit the location and dilation aspects—though, admittedly, from a casual inspection as well as the substantial understanding of the data, these aspects are crucial. For instance, we may omit the dilation factor—that is, assume  $\rho = 1$ —with the norho option.

4

```
. procrustes (survey_x survey_y) (speed_x speed_y), norho
```

Procrustes analysis (orthogonal)

Number of observations = 20
Model df (df\_m) = 3
Residual df (df\_r) = 495070
RSS(target) = 165278.1
RMSE = root(RSS/df\_r) = 66.83544
Procrustes = RSS/SS = 0.3338

Translation c

	survey_x	survey_y
_cons	741.4458	435.6215

Rotation & reflection matrix A (orthogonal)

	survey_x	survey_y
speed_x	.9841521	1773266
speed_y	.1773266	.9841521

Dilation factor

rho = 1.0000

Fit statistics by target variable

Statistics	survey_x	survey_y
SS	216310.2	278759.8
RSS	70385.78	94892.36
RMSE	61.68174	71.61925
Procrustes	.3253928	.340409
Corr_y_yhat	.9976669	.9985076

As expected, the optimal transformation without dilation implies a much weaker relation between the Speed and Survey maps; the Procrustes statistic has increased from 0.0040 to 0.3338. We conclude that we cannot adequately describe the correspondence between the maps if we ignore differences in scale.

4

## Is an orthogonal Procrustes analysis symmetric?

In examples 1 and 2, we transformed the Speed map to optimally match the modern Survey map. We could also have reversed the procedure, that is, transform the Survey map to match the Speed map.

### Example 3

Here we change the order of the Speed and Survey map in our call to procrustes from example 1.

. procrustes (speed\_x speed\_y) (survey\_x survey\_y)

Procrustes analysis (orthogonal)

Number of observations = 20
Model df (df\_m) = 4
Residual df (df\_r) = 36
SS(target) = 88862.75
RSS(target) = 354.2132
RMSE = root(RSS/df\_r) = 3.136759
Procrustes = RSS/SS = 0.0040

Translation c

	speed_x	speed_y
_cons	-187.0142	-159.5801

Rotation & reflection matrix A (orthogonal)

	speed_x	speed_y
survey_x	.9841521	.1773266
survey_y	1773266	.9841521

Dilation factor

rho = 0.4228

Fit statistics by target variable

speed_x	speed_y
41544.95	47317.8
218.3815	135.8317
3.483146	2.747036
.0052565	.0028706
.9975074	.9986641
	41544.95 218.3815 3.483146 .0052565

The implied transformations are similar but not identical. For instance, the product of estimated scale factors is  $2.3556 \times 0.4228 = 0.9959$ , which is close to 1 but not identical to 1—this is not due to roundoff error. Why do the results differ? Think about the analogy with regression analysis. The regression of Y on X and the regression of X on Y generally imply different relationships between the variables. In geometric terms, one minimizes the sum of squares of the "vertical" distances between the data point and the regression line, whereas the other minimizes the "horizontal" distances. The implied regression lines are the same if the variance in X and Y are the same. Even if this does not hold, the proportion of explained variance  $R^2$  in both regressions is the same. In Procrustes analysis, an analogous relationship holds between the analyses "Speed = transformed(Survey) + E" and "Survey = transformed(Speed) + E". Both analyses yield the same Procrustes statistic. The implied analyses are equivalent (that is, the implied transformation in one analysis is the mathematical inverse of the transformation in the other analysis) only if the Speed and Survey data are scaled so that the trace of the associated covariance matrices is the same.

#### Other transformations

A Procrustes analysis can also be applied with other classes of transformations. Browne (1967) analyzed Procrustes analyses with oblique rotations. Cramer (1974) and ten Berge and Nevels (1977) identified and solved some problems in Browne's solution (but still ignore the problem that the derived oblique rotations are not necessarily orientation preserving), procrustes supports oblique transformations, procrustes also allows dilation; see Methods and formulas.

### Example 4

Even though the orthogonal Procrustes analysis of example 1 demonstrated a similarity between the two configurations assuming an orthogonal transformation, we now investigate what happens with an oblique transformation.

. procrustes (survey\_x survey\_y) (speed\_x speed\_y), trans(oblique) Procrustes analysis (oblique) Number of observations = 20 Model df (df\_m) 5 Residual df (df\_r) 35 SS(target) 495070 RSS(target) 1967.854  $RMSE = root(RSS/df_r) =$ 7.498294 Procrustes = RSS/SS = 0.0040

Translation c

	survey_x	survey_y
_cons	503.0093	292.4346

Rotation & reflection matrix A (oblique)

	survey_x	survey_y
speed_x	.9835969	1737553
speed_y	.1803803	.9847889

Dilation factor

rho = 2.3562

Fit statistics by target variable

Statistics	survey_x	survey_y
SS	216310.2	278759.8
RSS	1080.677	887.1769
RMSE	7.858307	7.1201
Procrustes	.004996	.0031826
Corr_y_yhat	.9976685	.9985163

We see that the optimal oblique transformation is almost orthogonal; the columns of the oblique rotation and reflection matrix are almost perpendicular. The dilation factor and translation vector hardly differ from the orthogonal case shown in example 1. Finally, we see that the residual sum of squares decreased little, namely, from 1,973.4 to 1,967.9.

4

Procrustes analysis can be interpreted as multivariate regression Y = c + xB + e in which some nonlinear restriction is applied to the coefficients B. Procrustes analysis assumes  $\mathbf{B} = \rho \mathbf{A}$  with A assumed to be orthogonal or  $\bf A$  assumed to be oblique. The intercepts of the multivariate regression are, of course, the translation of the Procrustean transform. In contrast to multivariate regression, it is assumed that the distribution of the residuals  $\bf e$  is spherical; that is, all that is assumed is that  $var(\bf e)=\sigma^2 \bf I$ . This assumption affects standard errors, not the estimated coefficients. Multivariate regression serves as a useful baseline to gauge the extent to which the Procrustean analysis is appropriate. procrustes supports the transform(unrestricted) option and displays the fitted model in a format comparable to Procrustes analysis.

### Example 5

We demonstrate with Speed's map data.

. procrustes (survey\_x survey\_y) (speed\_x speed\_y), trans(unrestricted)

Procrustes analysis (unrestricted)

Number of observations	=	20
Model df (df_m)	=	6
Residual df (df_r)	=	34
SS(target)	=	495070
RSS(target)	=	1833.435
<pre>RMSE = root(RSS/df_r)</pre>	=	7.343334
Procrustes = RSS/SS	=	0.0037

Translation c

	survey_x	survey_y
_cons	510.8028	288.243

Rotation & reflection matrix A (unrestricted)

	survey_x	survey_y
speed_x	2.27584	4129564
speed_y	.4147244	2.355725

Fit statistics by target variable

Statistics	survey_x	survey_y
SS	216310.2	278759.8
RSS	1007.14	826.2953
RMSE	7.696981	6.971772
Procrustes	.004656	.0029642
Corr_y_yhat	.9976693	.9985168

Because we already saw that there is almost no room to improve on the orthogonal Procrustes transform with this particular dataset, dropping the restrictions on the coefficients hardly improves the fit. For instance, the residual sum of squares further decreases from 1,967.9 in the oblique case to 1,833.4 in the unrestricted case, with only a small reduction in the value of the Procrustes statistic.

### Stored results

procrustes stores the following in e():

```
Scalars
    e(N)
                           number of observations
    e(rho)
                           dilation factor
    e(P)
                           Procrustes statistic
    e(ss)
                           total sum of squares, summed over all y variables
    e(rss)
                           residual sum of squares, summed over all y variables
    e(rmse)
                           root mean squared error
                           root mean squared error (unadjusted for # of estimated parameters)
    e(urmse)
    e(df_m)
                           model degrees of freedom
    e(df_r)
                           residual degrees of freedom
                           number of y variables (target variables)
    e(ny)
Macros
    e(cmd)
                           procrustes
    e(cmdline)
                           command as typed
    e(ylist)
                           y variables (target variables)
    e(xlist)
                           x variables (source variables)
    e(transform)
                           orthogonal, oblique, or unrestricted
    e(uniqueA)
                           1 if rotation is unique, 0 otherwise
    e(wtype)
                           weight type
    e(wexp)
                           weight expression
    e(properties)
                           nob noV
    e(estat_cmd)
                           program used to implement estat
    e(predict)
                           program used to implement predict
    e(marginsnotok)
                           predictions disallowed by margins
Matrices
    e(c)
                           translation vector
    e(A)
                           orthogonal transformation matrix
    e(vstats)
                           matrix containing fit statistics
Functions
    e(sample)
                           marks estimation sample
```

# Methods and formulas

Methods and formulas are presented under the following headings:

Introduction
Orthogonal transformations
Oblique transformations
Unrestricted transformations
Reported statistics

#### Introduction

A Procrustes analysis is accomplished by solving a matrix minimization problem

Minimize 
$$|\mathbf{Y} - (\mathbf{1c'} + \boldsymbol{\rho} \mathbf{X} \mathbf{A})|$$

with respect to  $\bf A$ ,  $\bf c$ , and  $\rho$ .  $\bf A$  is a matrix representing a linear transformation,  $\rho>0$  is a scalar called the "dilation factor",  $\bf c$  is a translation (row-) vector, and |.| is the Frobenius (or L2) norm. Three classes of transformations are available in procrustes: orthogonal, oblique, and unrestricted. The orthogonal class consists of all orthonormal matrices  $\bf A$ , that is, all square matrices that satisfy  $\bf A'A=\bf I$ , representing orthogonal norm-preserving rotations and reflections. The oblique class comprises all normal matrices  $\bf A$ , characterized by  ${\rm diag}(\bf A'A)=\bf 1$ . Oblique transformations preserve the length of vectors but not the angles between vectors—orthogonal vectors will generally not remain orthogonal under oblique transformations. Finally, the unrestricted class consists of all conformable regular matrices  $\bf A$ .

Define  $\widetilde{Y}$  and  $\widetilde{X}$  as the centered Y and X, respectively, if a constant c is included in the analysis and as the uncentered Y and X otherwise.

The derivation of the optimal A obviously differs for the three classes of transformations.

### Orthogonal transformations

The solution for the orthonormal case can be expressed in terms of the singular value decomposition of  $\widetilde{\mathbf{Y}}'\widetilde{\mathbf{X}}$ .

$$\widetilde{\mathbf{Y}}'\widetilde{\mathbf{X}} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{V}'$$

where  $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}$ . Then

$$\hat{\mathbf{A}} = \mathbf{V}\mathbf{U}'$$

 $\widehat{\mathbf{A}}$  is the same whether or not scaling is required, that is, whether  $\rho$  is a free parameter or a fixed parameter. When  $\rho$  is a free parameter, the optimal  $\rho$  is

$$\widehat{\rho} = \frac{\operatorname{trace}(\widehat{\mathbf{A}}\widetilde{\mathbf{Y}}'\widetilde{\mathbf{X}})}{\operatorname{trace}(\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}})}$$

See ten Berge (1977) for a modern and elementary derivation; see Mardia, Kent, and Bibby (1979) for a derivation using matrix differential calculus.

# **Oblique transformations**

Improving on earlier studies by Browne (1967) and Cramer (1974), ten Berge and Nevels (1977) provide a full algorithm to compute the optimal oblique rotation without dilation, that is, with uniform scaling  $\rho=1$ . In contrast to the orthogonal case, the optimal oblique rotation  $\widehat{\mathbf{A}}$  depends on  $\rho$ . To the best of our knowledge, this case has not been treated in the literature (J. M. F. ten Berge, 2004, pers. comm.). However, an "alternating least squares" extension of the ten Berge and Nevels (1977) algorithm deals with this case.

For each iteration, step (a) follows ten Berge and Nevels (1977) for calculating  $\widetilde{\mathbf{Y}}$  and  $\widehat{\rho}\widetilde{\mathbf{X}}$ . In step (b) of an iteration,  $\rho$  is optimized, keeping  $\widehat{\mathbf{A}}$  fixed, with solution

$$\widehat{\rho} = \frac{\mathrm{trace}(\widehat{\mathbf{A}}\widetilde{\mathbf{Y}}'\widetilde{\mathbf{X}})}{\mathrm{trace}(\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}}\widehat{\mathbf{A}}\widehat{\mathbf{A}}')}$$

Iteration continues while the relative decrease in the residual sum of squares is large enough. This algorithm is ensured to yield a local optimum of the residual sum of squares as the RSS decreases both when updating the rotation  $\bf A$  and when updating the dilation factor  $\rho$ . Beware that the algorithm is not guaranteed to find the global minimum.

#### Unrestricted transformations

In the unrestricted solution, the dilation factor  $\rho$  is fixed at 1. The computation of the Procrustes transformation is obviously equivalent to the least-squares solution of multivariate regression

$$\widehat{\mathbf{A}} = (\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}'\widetilde{\mathbf{Y}}$$

Given  $\widehat{\mathbf{A}}$  and  $\widehat{\rho}$ , the optimal translation  $\widehat{\mathbf{c}}$  can be written as

$$\hat{\mathbf{c}} = \mathbf{Y}'\mathbf{1} - \widehat{\rho}\widehat{\mathbf{A}}\mathbf{X}$$

If the constant is suppressed, c is simply set to 0.

# Reported statistics

procrustes computes and displays the following statistics for each target variable separately and globally by adding the appropriate sums of squares over all target variables. The predicted values  $\hat{\mathbf{Y}}$  for  $\mathbf{Y}$  are defined as

$$\widehat{\mathbf{Y}} = \mathbf{1}\widehat{\mathbf{c}}' + \widehat{\rho}\mathbf{X}\widehat{\mathbf{A}}$$

The Procrustes statistic, P, is a scaled version of the squared distance of Y:

$$P = RSS/SS$$

where

$$\begin{aligned} \text{RSS} &= \text{trace}((\mathbf{Y} - \widehat{\mathbf{Y}})(\mathbf{Y} - \widehat{\mathbf{Y}})') \\ \text{SS} &= \text{trace}(\widetilde{\mathbf{Y}}'\widetilde{\mathbf{Y}}) \end{aligned}$$

Note that  $0 \le P \le 1$ , and a small value of P means that  $\mathbf{Y}$  is close to the transformed value of  $\mathbf{X}$ , that is, the  $\mathbf{X}$  and  $\mathbf{Y}$  configurations are similar. In the literature, this statistic is often denoted by  $R^2$ . It is easy to confuse this with the  $R^2$  statistic in a regression context, which is actually 1 - P.

A measure for the size of the residuals is the root mean squared error,

$$\text{RMSE} = \sqrt{\text{RSS}/\text{df}_{\rm r}}$$

Here  $df_r$  are  $Nn_y - df_m$ , with  $df_m = n_y n_x + n_y + 1 - k$ , and with N the number of observations,  $n_y$  and  $n_x$  the number of target variables and source variables, respectively, and k, the number of restrictions, defined as

orthogonal: 
$$k = n_x(n_x - 1)/2$$

oblique:  $k = n_y$  unrestricted: k = 1

procrustes computes RMSE(j) for target variable  $y_i$  as

$$\mathrm{RMSE}(j) = \sqrt{\mathrm{RSS}(j)/(\mathrm{df_r}/n_y)}$$

Finally, procrustes computes the Pearson correlation between  $y_j$  and  $\widehat{y_j}$ . For the unrestricted transformation, this is just the square root of the explained variance 1-P(j), where P(j) = RSS(j)/SS. For the orthogonal and oblique transformation, this relationship does not hold.

### References

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# Also see

[MV] **procrustes postestimation** — Postestimation tools for procrustes

[MV] ca — Simple correspondence analysis

[MV] **mvreg** — Multivariate regression

[MV] **pca** — Principal component analysis

[MV] rotate — Orthogonal and oblique rotations after factor and pca

[U] 20 Estimation and postestimation commands

# **Title**

procrustes	postestimation —	Postestimation	tools for	procrustes
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Postestimation commands	predict	estat	procoverlay
Remarks and examples	Stored results	Methods and formulas	References
Also see			

# **Postestimation commands**

The following postestimation commands are of special interest after procrustes:

Command	Description
estat compare	fit statistics for orthogonal, oblique, and unrestricted transformations
estat mvreg	display multivariate regression resembling unrestricted transformation
estat summarize	display summary statistics over the estimation sample
procoverlay	produce a Procrustes overlay graph

The following standard postestimation commands are also available:

Command	Description
*estimates predict	cataloging estimation results compute fitted values and residuals

<sup>\*</sup> All estimates subcommands except table and stats are available; see [R] estimates.

# predict

# **Description for predict**

predict creates new variables containing predictions such as fitted values, unstandardized residuals, and residual sum of squares.

### Menu for predict

Statistics > Postestimation

# Syntax for predict

predict	[type] {stub*   newvarlist} [if] [in], [statistic]
statistic	Description
Main fitted residuals q	fitted values $1 \mathbf{c}' + \rho \mathbf{X} \mathbf{A}$ ; the default (specify $\#_y$ vars) unstandardized residuals (specify $\#_y$ vars) residual sum of squares over the target variables (specify one var)

These statistics are available both in and out of sample; type predict ... if e(sample) ... if wanted only for the estimation sample.

# **Options for predict**

Main

fitted, the default, computes fitted values, that is, the least-squares approximations of the target (varlist<sub>u</sub>) variables. You must specify the same number of new variables as there are target variables.

residuals computes the raw (unstandardized) residuals for each target  $(varlist_y)$  variable. You must specify the same number of new variables as there are target variables.

q computes the residual sum of squares over all variables, that is, the squared Euclidean distance between the target and transformed source points. Specify one new variable.

#### estat

# **Description for estat**

estat compare displays a table with fit statistics of the three transformations provided by procrustes: orthogonal, oblique, and unrestricted. The two additional procrustes analyses are performed on the same sample as the original procrustes analysis and with the same options. F tests comparing the models are provided.

estat mvreg produces the mvreg (see [MV] mvreg) output related to the unrestricted Procrustes analysis (the transform(unrestricted) option of procrustes).

estat summarize displays summary statistics over the estimation sample of the target and source variables ( $varlist_y$  and  $varlist_x$ ).

#### Menu for estat

Statistics > Postestimation

# Syntax for estat

```
Table of fit statistics
estat compare [, detail]
```

Comparison of mvreg and procrustes output

```
estat mvreg [, mvreg_options]
```

Display summary statistics

```
estat <u>summarize</u> [, <u>lab</u>els <u>nohea</u>der <u>noweights</u>]
```

# **Options for estat**

detail, an option with estat compare, displays the standard procrustes output for the two additional transformations.

mvreg\_options, allowed with estat mvreg, are any of the options allowed by mvreg; see [MV] mvreg. The constant is already suppressed if the Procrustes analysis suppressed it.

labels, noheader, and noweights are the same as for the generic estat summarize command; see [R] estat summarize.

# Description for procoverlay

procoverlay displays a plot of the target variables overlaid with the fitted values derived from the source variables. If there are more than two target variables, multiple plots are shown in one graph.

# Menu for procoverlay

Statistics > Multivariate analysis > Procrustes overlay graph

procoverlay [if] [in] [. procoverlay\_options]

# Syntax for procoverlay

procoveriay [ <i>y</i> ] [ <i>m</i> ]	
procoverlay_options	Description
Main	
<u>auto</u> aspect	adjust aspect ratio on the basis of the data; default aspect ratio is 1
<pre>target_opts(target_opts)</pre>	affect the rendition of the target
<pre>source_opts(source_opts)</pre>	affect the rendition of the source
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by() documented in [G-3] twoway_options
Ву	
$\underline{\text{byo}}_{\text{pts}}(by\_option)$	affect the rendition of combined graphs
target_opts	Description
Main	
<u>nolab</u> el	removes the default observation label from the target
marker_options	change look of markers (color, size, etc.)
marker_label_options	change look or position of marker labels
source_opts	Description
Main	
<u>nolab</u> el	removes the default observation label from the source
marker_options	change look of markers (color, size, etc.)
marker_label_options	change look or position of marker labels

### Options for procoverlay

Main

autoaspect specifies that the aspect ratio be automatically adjusted based on the range of the data to be plotted. This option can make some procoverlay plots more readable. By default, procoverlay uses an aspect ratio of one, producing a square plot.

As an alternative to autoaspect, the  $twoway\_option$  aspectratio() can be used to override the default aspect ratio. procoverlay accepts the aspectratio() option as a suggestion only and will override it when necessary to produce plots with balanced axes, that is, where distance on the x axis equals distance on the y axis.

twoway\_options, such as xlabel(), xscale(), ylabel(), and yscale(), should be used with caution. These axis\_options are accepted but may have unintended side effects on the aspect ratio. See [G-3] twoway\_options.

targetopts(target\_opts) affects the rendition of the target plot. The following target\_opts are allowed:

nolabel removes the default target observation label from the graph.

marker\_options affect the rendition of markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] marker\_options.

marker\_label\_options specify if and how the markers are to be labeled; see [G-3] marker\_label\_options.

sourceopts(source\_opts) affects the rendition of the source plot. The following source\_opts are allowed:

nolabel removes the default source observation label from the graph.

*marker\_options* affect the rendition of markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] *marker\_options*.

marker\_label\_options specify if and how the markers are to be labeled; see [G-3] marker\_label\_options.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option). See autoaspect above for a warning against using options such as xlabel(), xscale(), ylabel(), and yscale().

Ву

byopts(*by\_option*) is documented in [G-3] *by\_option*. This option affects the appearance of the combined graph and is ignored, unless there are more than two target variables specified in procrustes.

# Remarks and examples

The examples in [MV] **procrustes** demonstrated a Procrustes transformation of a historical map, produced by John Speed in 1610, to a modern map. Here we demonstrate the use of procrustes postestimation tools in assessing the accuracy of Speed's map. Example 1 of [MV] **procrustes** performed the following analysis:

```
. use http://www.stata-press.com/data/r14/speed_survey
(Data on Speed's Worcestershire map (1610))
```

. procrustes (survey\_x survey\_y) (speed\_x speed\_y)
 (output omitted)

See example 1 of [MV] procrustes. The following examples are based on this procrustes analysis.

### ▶ Example 1: Predictions

Did John Speed get the coordinates of the towns right—up to the location, scale, and orientation of his map relative to the modern map? In example 1 of [MV] **procrustes**, we demonstrated how the optimal transformation from the historical coordinates to the modern (true) coordinates can be estimated by procrustes.

It is possible to "predict" the configuration of 20 cities on Speed's historical map, optimally transformed (rotated, dilated, and translated) to approximate the true configuration. predict with the fitted option expects the same number of variables as the number of target (dependent) variables (survey\_x and survey\_y).

```
. predict fitted_x fitted_y
(fitted assumed)
```

We omitted the fitted option because it is the default.

It is often useful to also compute the (squared) distance between the true location and the transformed location of the historical map. This can be seen as a quality measure—the larger the value, the more Speed erred in the location of the respective town.

. predict q, q

We now list the target data (survey\_x and survey\_y, the values from the modern map), the fitted values (fitted\_x and fitted\_y, produced by predict), and the squared distance between them (q, produced by predict with the q option).

liet	nama	SIITVEV	v	CHETTAT	77	fitted	v	fitted	77	α.	can(n)	noohe

name	survey_x	survey_y	fitted_x	fitted_y	q
Alve	1027	725	1037.117	702.9464	588.7149
Arro	1083	565	1071.682	562.6791	133.4802
Astl	787	677	783.0652	674.5216	21.62482
Beck	976	358	978.8665	366.3761	78.37637
Beng	1045	435	1055.245	431.6015	116.51
Crad	736	471	725.8594	476.5895	134.075
Droi	893	633	890.5839	633.6066	6.205747
Ecki	922	414	929.4932	411.1757	64.12465
Eves	1037	437	1036.887	449.2707	150.5827
Hall	828	579	825.1494	575.9836	17.22464
Hanb	944	637	954.6189	643.6107	156.4629
Inkb	1016	573	1004.869	577.1111	140.7917
Kemp	848	490	845.7215	490.8959	5.994327
Kidd	826	762	836.8665	760.5699	120.1264
Mart	756	598	745.2623	597.5585	115.4937
Stud	1074	632	1072.622	634.3164	7.264294
Tewk	891	324	898.4571	318.632	84.42448
UpSn	943	544	939.3932	545.8247	16.33858
Upto	852	403	853.449	400.9419	6.335171
Worc	850	545	848.7917	547.7881	9.233305

We see that Speed especially erred in the location of Alvechurch—it is off by no less than  $\sqrt{588} = 24$  miles, whereas the average error is about 8 miles. In a serious analysis of this dataset, we would check the data on Alvechurch, and, if we found it to be in order, consider whether we should actually drop Alvechurch from the analysis. In this illustration, we ignore this potential problem.

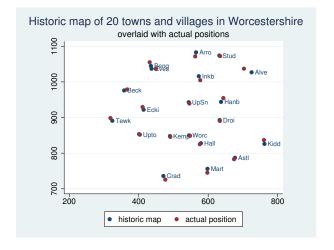
# Example 2: Procrustes overlay graph

Although the numerical information convinces us that Speed's map is generally accurate, a plot will convey this message more convincingly. procoverlay produces a plot that contains the target (survey) coordinates and the Procrustes-transformed historical coordinates. We could just type

. procoverlay

However, we decide to set several options to produce a presentation-quality graph. The suboption mlabel() of target() (or of source()) adds labels, identifying the towns. Because the target and source points are so close, there can be no confusing how they are matched. Displaying the labels twice in the plot is not helpful for this dataset. Therefore, we choose to label the target points, but not the source points using the nolabel suboption of source(). We preserve the equivalence of the x and y scale while using as much of the graphing region as possible with the autoaspect option. The span suboption of title() allows the long title to extend beyond the graph region if needed. We override the default legend by using the legend() option.

- . procoverlay, target(mlabel(name)) source(nolabel) autoaspect
- > title(Historic map of 20 towns and villages in Worcestershire, span)
- > subtitle(overlaid with actual positions)
- > legend(label(1 historic map) label(2 actual position))



# 4

# Example 3: estat

estat offers three specific facilities after procrustes. These can all be seen as convenience tools that accomplish simple analyses, ensuring that the same variables and the same observations are used as in the Procrustes analysis.

The variables involved in the Procrustes analysis can be summarized over the estimation sample, for instance, to gauge differences in scales and location of the target and source variables.

. estat summarize

Estimation sam	mple procrustes	Number of obs = 20				
Variable	Mean	Std. Dev.	Min	Max		
target survey_x survey_y	916.7 540.1	106.6993 121.1262	736 324	1083 762		
source speed_x speed_y	153.95 133.9	46.76084 49.90401	78 40	220 220		

From the summarization, the two maps have different origins and scale.

As pointed out in [MV] **procrustes**, orthogonal and oblique Procrustes analyses can be thought of as special cases of multivariate regression (see [MV] **mvreg**), subject to nonlinear restrictions on the coefficient matrix. Comparing the Procrustes statistics and the transformations for each of the three classes of transformations is helpful in selecting a transformation. The compare subcommand of estat provides summary information for the optimal transformations in each of the three classes.

. estat compare

Summary statistics for three transformations

	Procrustes	df_m	df_r	rmse
orthogonal	0.0040	4	36	7.403797
oblique	0.0040	5	35	7.498294
unrestricted	0.0037	6	34	7.343334

(F tests comparing the models suppressed)

The Procrustes statistic is ensured to decrease (not increase) from orthogonal to oblique to unrestricted because the associated classes of transformations are getting less restrictive. The model degrees of freedom ( $df_m$ ) of the three transformation classes are the dimension of the classes, that is, the number of "free parameters". For instance, with orthogonal transformations between two source and two target variables, there is 1 degree of freedom for the rotation (representing the rotation angle), 2 degrees of freedom for the translation, and 1 degree of freedom for dilation (uniform scaling), that is, four in total. The residual degrees of freedom ( $df_r$ ) are the number of observations (number of target variables times the number of observations) minus the model degrees of freedom. The root mean squared error RMSE, defined as

$$\mathrm{RMSE} = \sqrt{\frac{\mathrm{RSS}}{\mathrm{d}f_r}}$$

does not, unlike the Procrustes statistic, surely become smaller with the less restrictive models. In this example, in fact, the RMSE of the orthogonal transformation is smaller than that of the oblique transformation. This indicates that the additional degree of freedom allowing for skew rotations does not produce a closer fit. In this example, we see little reason to relax orthogonal transformations; very little is gained in terms of the Procrustes statistic (an illness-of-fit measure) or the RMSE. In this interpretation, we used our intuition to guide us whether a difference in fit is substantively and statistically meaningful—formal significance tests are not provided.

Finally, the unrestricted transformation can be estimated with procrustes ..., transform(unrestricted). This analysis is related to a multivariate regression with the target variables as the dependent variables and the source variables as the independent variables. Although the unrestricted Procrustes analysis assumes spherical (uncorrelated homoskedastic) residuals, this restrictive assumption is not made in multivariate regression as estimated by the mvreg command. The comparable multivariate regression over the same estimation sample can be viewed simply by typing

. estat mvreg

. obodo moros						
Multivariate :	regression, s	imilar to	"procrustes	, t	ransform(unres	stricted)"
Equation	Obs	Parms	RMSE	"R-sq"	F	P
survey_x	20	3	7.696981	0.9953	1817.102	0.0000
survey_y	20	3	6.971772	0.9970	2859.068	0.0000
	Coef.	Std. Er	r. t	P> t	[95% Conf.	Interval]
survey_x						
speed_x	2.27584	.0379369	59.99	0.000	2.1958	2.35588
speed_y	.4147244	.035547	5 11.67	0.000	.3397257	.489723
_cons	510.8028	8.065519	63.33	0.000	493.7861	527.8196
survey_y						
speed_x	4129564	.034362	-12.02	0.000	485455	3404579
speed_y	2.355725	.0321982	2 73.16	0.000	2.287793	2.423658
_cons	288.243	7.305587	7 39.46	0.000	272.8296	303.6564

This analysis is seen as postestimation after a Procrustes analysis, so it does not change the "last estimation results". We may still replay procrustes and use other procrustes postestimation commands.

#### Stored results

estat compare after procrustes stores the following in r():

Matrices

Procrustes statistics, degrees of freedom, and RMSEs r(cstat) F statistics, degrees of freedom, and p-values r(fstat)

estat mvreg does not return results.

estat summarize after procrustes stores the following in r():

Matrices

means, standard deviations, minimums, and maximums r(stats)

1

### Methods and formulas

The predicted values for the jth variable are defined as

$$\widehat{y}_j = \widehat{c}_j + \widehat{\rho} \mathbf{X} \ \widehat{\mathbf{A}}[.,j]$$

The residual for  $y_j$  is simply  $y_j - \hat{y}_j$ . The "rowwise" quality q of the approximation is defined as the residual sum of squares:

$$q = \sum_{j} (y_j - \widehat{y}_j)^2$$

The entries of the summary table produced by estat compare are described in Methods and formulas of [MV] procrustes. The F tests produced by estat compare are similar to standard nested model tests in linear models.

# References

See References in [MV] procrustes.

## Also see

[MV] **procrustes** — Procrustes transformation

[MV] mvreg — Multivariate regression

[U] 20 Estimation and postestimation commands

### Title

rotate — Orthogonal and oblique rotations after factor and pca

Description Quick start Menu Syntax

Options Remarks and examples Stored results Methods and formulas

References Also see

# Description

rotate performs a rotation of the loading matrix after factor, factormat, pca, or pcamat; see [MV] **factor** and [MV] **pca**. Many rotation criteria (such as varimax and oblimin) are available that can be applied with respect to the orthogonal and oblique class of rotations.

rotate, clear removes the rotation results from the estimation results.

If you want to rotate a given matrix, see [MV] rotatemat.

If you want a Procrustes rotation, which rotates variables optimally toward other variables, see [MV] **procrustes**.

### **Quick start**

Orthogonal varimax rotation of loading matrix after pca or factor rotate

As above, but apply the minimum entropy rotation criterion rotate, entropy

As above, but apply oblique quartimin rotation criterion rotate, oblique quartimin

As above, but rotate the Kaiser normalized matrix rotate, oblique quartimin normalize

#### Menu

Statistics > Multivariate analysis > Factor and principal component analysis > Postestimation > Rotate loadings

# **Syntax**

```
\underline{\mathtt{rot}}\mathtt{ate}\ ig[\ ,\ \mathit{options}\ ig]
rotate, clear
```

options	Description
Main	
<u>ortho</u> gonal	restrict to orthogonal rotations; the default, except with promax()
oblique	allow oblique rotations
rotation_methods	rotation criterion
$\underline{\mathtt{norm}}\mathtt{alize}$	rotate Kaiser normalized matrix
$\underline{\mathbf{f}}$ actors(#)	rotate # factors or components; default is to rotate all
<pre>components(#)</pre>	synonym for factors()
Reporting	
<u>bl</u> anks(#)	display loadings as blanks when  loading  < #; default is blanks(0)
<u>det</u> ail	show rotatemat output; seldom used
<pre>format(%fmt)</pre>	display format for matrices; default is format(%9.5f)
<u>noload</u> ing	suppress display of rotated loadings
<u>norota</u> tion	suppress display of rotation matrix
Optimization	
optimize_options	control the maximization process; seldom used
rotation_methods	Description
* <u>v</u> arimax	varimax (orthogonal only); the default
* <u>v</u> arimax vgpf	varimax (orthogonal only); the default varimax via the GPF algorithm (orthogonal only)
_	
vgpf	varimax via the GPF algorithm (orthogonal only)
vgpf quartimax	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only)
vgpf quartimax equamax	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only)
vgpf quartimax equamax parsimax	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only)
vgpf quartimax equamax parsimax entropy	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only)
vgpf quartimax equamax parsimax entropy tandem1	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only)
vgpf quartimax equamax parsimax entropy tandem1 tandem2	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only)
vgpf quartimax equamax parsimax entropy tandem1 tandem2 *promax[(#)]	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only) promax power # (implies oblique); default is promax(3)
vgpf quartimax equamax parsimax entropy tandem1 tandem2 *promax[(#)] oblimin[(#)]	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only) promax power # (implies oblique); default is promax(3) oblimin with $\gamma = \#$ ; default is oblimin(0)
vgpf quartimax equamax parsimax entropy tandem1 tandem2 *promax[(#)] oblimin[(#)] cf(#)	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only) promax power # (implies oblique); default is promax(3) oblimin with $\gamma = \#$ ; default is oblimin(0) Crawford-Ferguson family with $\kappa = \#$ , $0 \le \# \le 1$
vgpf quartimax equamax parsimax entropy tandem1 tandem2  *promax[(#)] oblimin[(#)] cf(#) bentler oblimax quartimin	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only) promax power # (implies oblique); default is promax(3) oblimin with $\gamma = \#$ ; default is oblimin(0) Crawford-Ferguson family with $\kappa = \#$ , $0 \le \# \le 1$ Bentler's invariant pattern simplicity
vgpf quartimax equamax parsimax entropy tandem1 tandem2  *promax[(#)] oblimin[(#)] cf(#) bentler oblimax	varimax via the GPF algorithm (orthogonal only) quartimax (orthogonal only) equamax (orthogonal only) parsimax (orthogonal only) minimum entropy (orthogonal only) Comrey's tandem 1 principle (orthogonal only) Comrey's tandem 2 principle (orthogonal only) promax power # (implies oblique); default is promax(3) oblimin with $\gamma = \#$ ; default is oblimin(0) Crawford-Ferguson family with $\kappa = \#$ , $0 \le \# \le 1$ Bentler's invariant pattern simplicity oblimax

<sup>\*</sup> varimax and promax ignore all optimize\_options.

# **Options**

Main

orthogonal specifies that an orthogonal rotation be applied. This is the default.

See Rotation criteria below for details on the rotation\_methods available with orthogonal.

oblique specifies that an oblique rotation be applied. This often yields more interpretable factors with a simpler structure than that obtained with an orthogonal rotation. In many applications (for example, after factor and pca) the factors before rotation are orthogonal (uncorrelated), whereas the oblique rotated factors are correlated.

See Rotation criteria below for details on the rotation\_methods available with oblique.

clear specifies that rotation results be cleared (removed) from the last estimation command. clear may not be combined with any other option.

rotate stores its results within the e() results of pca and factor, overwriting any previous rotation results. Postestimation commands such as predict operate on the last rotated results, if any, instead of the unrotated results, and allow you to specify norotated to use the unrotated results. The clear option of rotate allows you to remove the rotation results from e(), thus freeing you from having to specify norotated for the postestimation commands.

normalize requests that the rotation be applied to the Kaiser normalization (Horst 1965) of the matrix **A**, so that the rowwise sums of squares equal 1. Kaiser normalization applies to the rotated columns only (see the factors() option below).

factors (#), and synonym components (#), specifies the number of factors or components (columns of the loading matrix) to be rotated, counted "from the left", that is, with the lowest column index. The other columns are left unrotated. All columns are rotated by default.

Reporting

blanks (#) shows blanks for loadings with absolute values smaller than #.

detail displays the rotatemat output; seldom used.

format (% fmt) specifies the display format for matrices. The default is format (%9.5f).

noloading suppresses the display of the rotated loadings.

norotation suppresses the display of the optimal rotation matrix.

Optimization

optimize\_options are seldom used; see [MV] rotatemat.

#### Rotation criteria

In the descriptions below, the matrix to be rotated is denoted as A, p denotes the number of rows of A, and f denotes the number of columns of A (factors or components). If A is a loading matrix from factor or pca, p is the number of variables, and f is the number of factors or components.

### Criteria suitable only for orthogonal rotations

varimax and vgpf apply the orthogonal varimax rotation (Kaiser 1958). varimax maximizes the variance of the squared loadings within factors (columns of A). It is equivalent to cf(I/p) and to oblimin(1). varimax, the most popular rotation, is implemented with a dedicated fast algorithm and ignores all *optimize\_options*. Specify vgpf to switch to the general GPF algorithm used for the other criteria.

- quartimax uses the quartimax criterion (Harman 1976). quartimax maximizes the variance of the squared loadings within the variables (rows of A). For orthogonal rotations, quartimax is equivalent to cf(0) and to oblimax.
- equamax specifies the orthogonal equamax rotation. equamax maximizes a weighted sum of the varimax and quartimax criteria, reflecting a concern for simple structure within variables (rows of  $\mathbf{A}$ ) as well as within factors (columns of  $\mathbf{A}$ ). equamax is equivalent to oblimin(p/2) and cf(#), where # = f/(2p).
- parsimax specifies the orthogonal parsimax rotation parsimax is equivalent to cf(#), where #=(f-1)/(p+f-2).
- entropy applies the minimum entropy rotation criterion (Jennrich 2004).
- tandem1 specifies that the first principle of Comrey's tandem be applied. According to Comrey (1967), this principle should be used to judge which "small" factors should be dropped.
- tandem2 specifies that the second principle of Comrey's tandem be applied. According to Comrey (1967), tandem2 should be used for "polishing".

#### Criteria suitable only for oblique rotations

promax[(#)] specifies the oblique promax rotation. The optional argument specifies the promax power. Not specifying the argument is equivalent to specifying promax(3). Values smaller than 4 are recommended, but the choice is yours. Larger promax powers simplify the loadings (generate numbers closer to zero and one) but at the cost of additional correlation between factors. Choosing a value is a matter of trial and error, but most sources find values in excess of 4 undesirable in practice. The power must be greater than 1 but is not restricted to integers.

Promax rotation is an oblique rotation method that was developed before the "analytical methods" (based on criterion optimization) became computationally feasible. Promax rotation comprises an oblique Procrustean rotation of the original loadings  $\bf A$  toward the elementwise #-power of the orthogonal varimax rotation of  $\bf A$ .

### Criteria suitable for orthogonal and oblique rotations

oblimin [(#)] specifies that the oblimin criterion with  $\gamma = \#$  be used. When restricted to orthogonal transformations, the oblimin() family is equivalent to the orthomax criterion function. Special cases of oblimin() include

$\gamma$	Special case				
0	quartimax / quartimin				
1/2	biquartimax / biquartimin				
1	varimax / covarimin				
p/2	equamax				
$p = \text{number of rows of } \mathbf{A}.$					

- $\gamma$  defaults to zero. Jennrich (1979) recommends  $\gamma \leq 0$  for oblique rotations. For  $\gamma > 0$ , it is possible that optimal oblique rotations do not exist; the iterative procedure used to compute the solution will wander off to a degenerate solution.
- cf(#) specifies that a criterion from the Crawford-Ferguson (1970) family be used with  $\kappa = \#$ . cf( $\kappa$ ) can be seen as  $(1 \kappa) \text{cf}_1(\mathbf{A}) + (\kappa) \text{cf}_2(\mathbf{A})$ , where cf<sub>1</sub>( $\mathbf{A}$ ) is a measure of row parsimony and cf<sub>2</sub>( $\mathbf{A}$ ) is a measure of column parsimony. cf<sub>1</sub>( $\mathbf{A}$ ) attains its greatest lower bound when no row of  $\mathbf{A}$  has more than one nonzero element, whereas cf<sub>2</sub>( $\mathbf{A}$ ) reaches zero if no column of  $\mathbf{A}$  has more than one nonzero element.

For orthogonal rotations, the Crawford-Ferguson family is equivalent to the oblimin() family. For orthogonal rotations, special cases include the following:

$\kappa$	Special case
$0 \ 1/p$	quartimax / quartimin varimax / covarimin
f/(2p) (f-1)/(p+f-2) 1	equamax parsimax factor parsimony
p = number of rows o f = number of column	

bentler specifies that the "invariant pattern simplicity" criterion (Bentler 1977) be used.

oblimax specifies the oblimax criterion. oblimax maximizes the number of high and low loadings. oblimax is equivalent to quartimax for orthogonal rotations.

quartimin specifies that the quartimin criterion be used. For orthogonal rotations, quartimin is equivalent to quartimax.

target(Tg) specifies that **A** be rotated as near as possible to the conformable matrix Tg. Nearness is expressed by the Frobenius matrix norm.

partial  $(Tg\ W)$  specifies that **A** be rotated as near as possible to the conformable matrix Tg. Nearness is expressed by a weighted (by W) Frobenius matrix norm. W should be nonnegative and usually is zero—one valued, with ones identifying the target values to be reproduced as closely as possible by the factor loadings, whereas zeros identify loadings to remain unrestricted.

# Remarks and examples

Remarks are presented under the following headings:

Orthogonal rotations Oblique rotations Other types of rotation

In this entry, we focus primarily on the rotation of factor loading matrices in factor analysis. rotate may also be used after pca, with the same syntax. We advise caution in the interpretation of rotated loadings in principal component analysis because some of the optimality properties of principal components are not preserved under rotation. See [MV] pca postestimation for more discussion of this point.

# Orthogonal rotations

The interpretation of a factor analytical solution is not always easy—an understatement, many will agree. This is due partly to the standard way in which the inherent indeterminacy of factor analysis is resolved. Orthogonal transformations of the common factors and the associated factor loadings are possible without affecting the reconstructed (fitted) correlation matrix and preserving the property that common factors are uncorrelated. This gives considerable freedom in selecting an orthogonal rotation to facilitate the interpretation of the factor loadings. Thurstone (1935) offered criteria for a "simple structure" required for a psychologically meaningful factor solution. These informal criteria for interpretation were then formalized into formal rotation criteria, for example, Harman (1976) and Gorsuch (1983).

### Example 1: Orthogonal varimax rotation

We illustrate rotate by using a factor analysis of the correlation matrix of eight physical variables (height, arm span, length of forearm, length of lower leg, weight, bitrochanteric diameter, chest girth, and chest width) of 305 girls.

```
. matrix input R = (1000)
                           846
                                 805
                                      859
                                           473
                                                 398
                                                      301
                                                           382 \
                      846 1000
                                 881
                                      826
                                           376
                                                 326
                                                      277
                                                           415 \
>
                      805
                           881 1000
                                      801
                                           380
                                                 319
                                                      237
                                                           345 \
>
                      859
                           826
                                 801 1000
                                           436
                                                 329
                                                      327
                                                           365 \
                      473
                           376
                                 380
                                      436 1000
                                                 762
                                                      730
                                                           629 \
                      398
                           326
                                 319
                                      329
                                           762 1000
                                                      583
                                                           577 \
                      301
                           277
                                 237
                                      327
                                           730
                                                 583 1000
                                                           539 \
                      382
                           415
                                 345
                                      365
                                           629
                                                 577
                                                      539 1000)
. matrix R = R/1000
  matrix colnames R = height
                                arm_span
                                          fore_arm
                                                     lower_leg
                       weight
                               bitrod
                                          ch_girth
                                          fore_arm
. matrix rownames R = height
                                arm_span
                       weight bitrod
                                          ch_girth ch_width
. matlist R, border format(%7.3f)
```

	height	arm_s~n	fore_~m	lower~g	weight	bitrod	ch_gi~h	ch_wi~h
height	1.000							
arm_span	0.846	1.000						
fore_arm	0.805	0.881	1.000					
lower_leg	0.859	0.826	0.801	1.000				
weight	0.473	0.376	0.380	0.436	1.000			
bitrod	0.398	0.326	0.319	0.329	0.762	1.000		
ch_girth	0.301	0.277	0.237	0.327	0.730	0.583	1.000	
ch_width	0.382	0.415	0.345	0.365	0.629	0.577	0.539	1.000

We extract two common factors with the iterated principal-factor method. See the description of factormat in [MV] factor for details on running a factor analysis on a Stata matrix rather than on a dataset.

```
. factormat R, n(305) fac(2) ipf (obs=305)
```

Factor analysis/correlation Number of obs = 305
Method: iterated principal factors Retained factors = 2
Rotation: (unrotated) Number of params = 15

Factor	Eigenvalue	Difference	Proportion	Cumulative
Factor1	4.44901	2.93878	0.7466	0.7466
Factor2	1.51023	1.40850	0.2534	1.0000
Factor3	0.10173	0.04705	0.0171	1.0171
Factor4	0.05468	0.03944	0.0092	1.0263
Factor5	0.01524	0.05228	0.0026	1.0288
Factor6	-0.03703	0.02321	-0.0062	1.0226
Factor7	-0.06025	0.01415	-0.0101	1.0125
Factor8	-0.07440		-0.0125	1.0000

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000

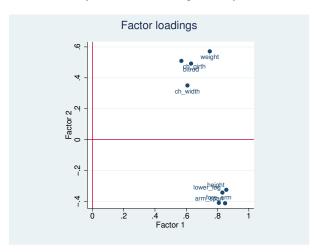
2

Variable Factor1 Factor2 Uniqueness height 0.8560 -0.32440.1620 arm\_span 0.8482 -0.4115 0.1112 0.8082 -0.4090 0.1795 fore\_arm 0.8309 -0.3424 lower\_leg 0.1923 0.7503 weight 0.5712 0.1108 0.6307 0.4922 0.3600 bitrod ch\_girth 0.5687 0.5096 0.4169 ch\_width 0.6074 0.3507 0.5081

Factor loadings (pattern matrix) and unique variances

The default factor solution is rather poor from the perspective of a "simple structure", namely, that variables should have high loadings on few (one) factors and factors should ideally have only low and high values. A plot of the loadings is illuminating.

. loadingplot, xlab(0(.2)1) ylab(-.4(.2).6) aspect(1) yline(0) xline(0)



There are two groups of variables. We would like to see one group of variables close to one axis and the other group of variables close to the other axis. Turning the plot by about 45 degrees counterclockwise should make this possible and offer a much "simpler" structure. This is what the rotate command accomplishes.

#### . rotate

305 Factor analysis/correlation Number of obs Method: iterated principal factors Retained factors = Rotation: orthogonal varimax (Kaiser off) Number of params = 15

Factor	Variance	Difference	Proportion	Cumulative	
Factor1	3.39957	0.83989	0.5705	0.5705	
Factor2	2.55968		0.4295	1.0000	

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000

Variable	Factor1	Factor2	Uniqueness
height	0.8802	0.2514	0.1620
arm_span	0.9260	0.1770	0.1112
fore_arm	0.8924	0.1550	0.1795
lower_leg	0.8708	0.2220	0.1923
weight	0.2603	0.9064	0.1108
bitrod	0.2116	0.7715	0.3600
ch_girth	0.1515	0.7484	0.4169
ch_width	0.2774	0.6442	0.5081

Rotated factor loadings (pattern matrix) and unique variances

Factor rotation matrix

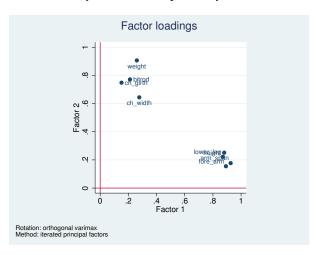
	Factor1	Factor2
Factor1	0.8018	0.5976
Factor2	-0.5976	0.8018

See [MV] factor for the interpretation of the first panel. Here we will focus on the second and third panel. The rotated factor loadings satisfy

$$\begin{aligned} & \text{Factor1}_{\text{rotated}} = 0.8018 \times \text{Factor1}_{\text{unrotated}} - 0.5976 \times \text{Factor2}_{\text{unrotated}} \\ & \text{Factor2}_{\text{rotated}} = 0.5976 \times \text{Factor1}_{\text{unrotated}} + 0.8018 \times \text{Factor2}_{\text{unrotated}} \end{aligned}$$

The uniqueness—the variance of the specific factors—is not affected, because we are changing only the coordinates in common factor space. The purpose of rotation is to make factor loadings easier to interpret. The first factor loads high on the first four variables and low on the last four variables; for the second factor, the roles are reversed. This is really a simple structure according to Thurstone's criteria. This is clear in the plot of the factor loadings.

. loadingplot, xlab(0(.2)1) ylab(0(.2)1) aspect(1) yline(0) xline(0)



rotate provides several different rotations. You may make your intention clearer by typing the command as

. rotate, orthogonal varimax (output omitted)

4

rotate defaults to orthogonal (angle and length preserving) rotations of the axes; thus, orthogonal may be omitted. The default rotation method is varimax, probably the most popular method. We warn that the varimax rotation is not appropriate if you expect a general factor contributing to all variables (see also Gorsuch 1983, chap. 9). In such a case you could, for instance, consider a quartimax rotation.

# Example 2: Orthogonal varimax rotation with normalization

rotate has performed what is known as "raw varimax", rotating the axes to maximize the sum of the variance of the squared loadings in the columns—the variance in a column is large if it comprises small and large (in the absolute sense) values. In rotating the axes, rows with large initial loadings—that is, with high communalities—have more influence than rows with only small values. Kaiser suggested that in the computation of the optimal rotation, all rows should have the same weight. This is usually known as the Kaiser normalization and sometimes known as the Horst normalization (Horst 1965). The option normalize applies this normalization method for rotation.

#### . rotate, normalize

Factor analysis/correlation	Number of obs =	305
Method: iterated principal factors	Retained factors =	2
Rotation: orthogonal varimax (Kaiser on)	Number of params =	15

Factor	Variance	Difference	Proportion	Cumulative
Factor1	3.31500	0.67075	0.5563	0.5563
Factor2	2.64425		0.4437	1.0000

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height arm_span fore_arm lower_leg weight bitrod ch_girth ch_width	0.8724	0.2775	0.1620
	0.9203	0.2045	0.1112
	0.8874	0.1815	0.1795
	0.8638	0.2478	0.1923
	0.2332	0.9137	0.1108
	0.1885	0.7775	0.3600
	0.1292	0.7526	0.4169
	0.2581	0.6522	0.5081

#### Factor rotation matrix

	Factor1	Factor2
Factor1	0.7837	0.6212
Factor2	-0.6212	0.7837

Here the raw and normalized varimax rotated loadings are not much different.

1

In the first example, loadingplot after rotate showed the rotated loadings, not the unrotated loadings. How can this be? Remember that Stata estimation commands store their results in e(), which we can list using ereturn list.

```
. ereturn list
scalars:
                  e(f) = 2
                  e(N) = 305
               e(df_m) = 15
               e(df_r) = 13
             e(chi2_i) = 2092.68137837692
               e(df_i) = 28
                e(p_i) = 0
              e(evsum) = 5.95922412962743
                e(r_f) = 2
macros:
    e(r_normalization) : "kaiser"
            e(r_class) : "orthogonal"
        e(r_criterion) : "varimax"
           e(r_ctitle) : "varimax"
            e(cmdline): "factormat R, n(305) fac(2) ipf"
                e(cmd) : "factor"
       e(marginsnotok) : "_ALL"
         e(properties) : "nob noV eigen"
              e(title): "Factor analysis"
            e(predict) : "factor_p"
          e(estat_cmd) : "factor_estat"
         e(rotate_cmd) : "factor_rotate"
           e(rngstate): "XAA1055b80bcee95e83ca9e2d41adfb0f0806ad6e5dec1468.."
            e(factors) : "factors(2)"
             e(mtitle): "iterated principal factors"
             e(method) : "ipf"
         e(matrixname) : "R"
matrices:
               e(r Ev) : 1 \times 2
              e(r_Phi) : 2 x 2
                e(r_T): 2 x 2
                e(r_L) : 8 \times 2
                  e(C): 8 x 8
                e(Phi) : 2 x 2
                  e(L) : 8 x 2
                e(Psi) : 1 x 8
                 e(Ev) : 1 \times 8
functions:
             e(sample)
```

When you replay an estimation command, it simply knows where to look, so that it can redisplay the output. rotate does something that few other postestimation commands are allowed to do: it adds information to the estimation results computed by factor or pca. But to avoid confusion, it writes in e() fields with the prefix  $r_{-}$ . For instance, the matrix  $e(r_{-}L)$  contains the rotated loadings.

If you replay factor after rotate, factor will display the rotated results. And this is what all factor and pca postestimation commands do. For instance, if you predict after rotate, predict will use the rotated results. Of course, it is still possible to operate on the unrotated results. factor, norotated replays the unrotated results. predict with the norotated option computes the factor scores for the unrotated results.

rotate stores information only about the most recent rotation, overwriting any information from the previous rotation. If you need the previous results again, run rotate with the respective options again; you do not need to run factor again. It is also possible to use estimates store to store estimation results for different rotations, which you may later restore and replay at will. See [R] estimates store for details.

If you no longer need the rotation results, you may type

. rotate, clear

to clean up the rotation result and return the factor results back to their pristine state (as if rotate had never been called).

### Example 3: Orthogonal quartimax and orthogonal oblimin rotations

rotate provides many more orthogonal rotations. Previously we stated that the varimax rotation can be thought of as the rotation that maximizes the varimax criterion, namely, the variance of the squared loadings summed over the columns. A column of loadings with a high variance tends to contain a series of large values and a series of low values, achieving the simplicity aim of factor analytic interpretation. The other types of rotation simply maximize other concepts of simplicity. For instance, the quartimax rotation aims at rowwise simplicity—preferably, the loadings within variables fall into a grouping of a few large ones and a few small ones, using again the variance in squared loadings as the criterion to be maximized.

#### . rotate, quartimax normalize

Factor analysis/correlation	Number of obs =	305
Method: iterated principal factors	Retained factors =	2
Rotation: orthogonal quartimax (Kaiser on)	Number of params =	15

Factor	Variance	Difference	Proportion	Cumulative
Factor1	3.32371	0.68818	0.5577	0.5577
Factor2	2.63553		0.4423	1.0000

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height arm_span fore_arm lower_leg weight bitrod ch_girth ch width	0.8732 0.9210 0.8880 0.8646 0.2360 0.1909 0.1315 0.2601	0.2749 0.2017 0.1788 0.2452 0.9130 0.7769 0.7522 0.6514	0.1620 0.1112 0.1795 0.1923 0.1108 0.3600 0.4169 0.5081

#### Factor rotation matrix

	Factor1	Factor2
Factor1	0.7855	0.6188
Factor2	-0.6188	0.7855

Here the quartimax and the varimax rotated results are rather similar. This need not be the case—varimax focuses on simplicity within columns (factors) and quartimax within rows (variables). It is possible to compromise, rotating to strive for a weighted sum of row simplicity and column simplicity. This is known as the orthogonal oblimin criterion; in the orthogonal case, oblimin() is equivalent to the Crawford–Ferguson (option cf()) family and to the orthomax family. These are parameterized families of criteria with, for instance, the following special cases:

oblimin(0) quartimax rotation oblimin(0.5) biquartimax rotation oblimin(1) varimax rotation

. rotate, oblimin(0.5) normalize

Factor analysis/correlation Number of obs = 305
Method: iterated principal factors Retained factors = 2
Rotation: orthogonal oblimin (Kaiser on) Number of params = 15

Factor	Variance	Difference	Proportion	Cumulative
Factor1	3.31854	0.67783	0.5569	0.5569
Factor2	2.64071		0.4431	1.0000

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height arm_span fore_arm lower_leg weight bitrod ch_girth ch_width	0.8727	0.2764	0.1620
	0.9206	0.2033	0.1112
	0.8877	0.1804	0.1795
	0.8642	0.2468	0.1923
	0.2343	0.9134	0.1108
	0.1895	0.7772	0.3600
	0.1301	0.7525	0.4169
	0.2589	0.6518	0.5081

Factor rotation matrix

	Factor1	Factor2
Factor1	0.7844	0.6202
Factor2	-0.6202	0.7844

Because the varimax and orthomax rotation are relatively close, the factor loadings resulting from an optimal rotation of a compromise criterion are close as well.

The orthogonal quartimax rotation may be obtained in different ways, namely, directly or by the appropriate member of the oblimin() or cf() families:

- . rotate, quartimax
   (output omitted)
- . rotate, oblimin(0)
   (output omitted)
- . rotate, cf(0)
   (output omitted)

#### □ Technical note

The orthogonal varimax rotation also belongs to the oblimin and Crawford-Ferguson families.

- . rotate, varimax
   (output omitted)
- . rotate, oblimin(1)
   (output omitted)
- . rotate, cf(0.125)
   (output omitted)

4

(The 0.125 = 1/8 above is 1 divided by the number of variables.) All three produce the orthogonal varimax rotation. (There is actually a fourth way, namely rotate, vgpf.) There is, however, a subtle difference in algorithms used. The varimax rotation as specified by the varimax option (which is also the default) is computed by the classic algorithm of cycling through rotations of two factors at a time. The other ways use the general "gradient projection" algorithm proposed by Jennrich; see [MV] rotatemat for more information.

### **Oblique rotations**

In addition to orthogonal rotations, oblique rotations are also available.

### Example 4: Oblique oblimin rotation

The rotation methods that we have discussed so far are all orthogonal: the angles between the axes are unchanged, so the rotated factors are uncorrelated.

Returning to our original factor analysis,

. factormat R, n(305) fac(2) ipf
 (output omitted)

we examine the correlation matrix of the common factors.

. estat common

Correlation matrix of the common factors

Factors	Factor1	Factor2
Factor1 Factor2	1 0	1

and see that they are uncorrelated.

The indeterminacy in the factor analytic model, however, allows us to consider other transformations of the common factors, namely, oblique rotations. These are rotations of the axes that preserve the norms of the rows of the loadings but not the angles between the axes or the angles between the rows. There are advantages and disadvantages of oblique rotations. See, for instance, Gorsuch (1983, chap. 9). In many substantive theories, there seems little reason to impose the restriction that the common factors be uncorrelated. The additional freedom in choosing the axes generally leads to more easily interpretable factors, sometimes to a great extent. However, although most researchers are willing to accept mildly correlated factors, they would prefer to use fewer of such factors.

rotate provides an extensive menu of oblique rotations; with a few exceptions, criteria suitable for orthogonal rotations are also suitable for oblique rotation. Again oblique rotation can be conceived of as maximizing some "simplicity" criterion. We illustrate with the oblimin oblique rotation.

. rotate, oblimin oblique normalize

Factor analysis/correlation Number of obs = 305
Method: iterated principal factors Retained factors = 2
Rotation: oblique oblimin (Kaiser on) Number of params = 15

Factor	Variance	Proportion	Rotated factors are correlated
Factor1	3.95010	0.6629	
Factor2	3.35832	0.5635	

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height arm_span	0.8831 0.9560	0.0648 -0.0288	0.1620 0.1112
fore_arm	0.9262	-0.0450	0.1795
lower_leg	0.8819	0.0344	0.1923
weight	0.0047	0.9408	0.1108
bitrod	-0.0069	0.8032	0.3600
ch_girth	-0.0653	0.7923	0.4169
ch_width	0.1042	0.6462	0.5081

Factor rotation matrix

	Factor1	Factor2
Factor1	0.9112	0.7930
Factor2	-0.4120	0.6092

The oblique rotation yields a much "simpler" structure in the Thurstone (1935) sense than that of the orthogonal rotations. This time, the common factors are moderately correlated.

. estat common

Correlation matrix of the oblimin(0) rotated common factors

Factors	Factor1	Factor2
Factor1 Factor2	1 .4716	1

1

## □ Technical note

The numerical maximization of a simplicity criterion with respect to the class of orthogonal or oblique rotations proceeds in a stepwise method, making small improvements from an initial guess, until no more small improvements are possible. Such a procedure is not guaranteed to converge to the global optimum but to a local optimum instead. In practice, we experience few such problems. To some extent, this is because we have a reasonable starting value using the unrotated factors or loadings. As a safeguard, Stata starts the improvement from multiple initial positions chosen at random from the classes of orthonormal and normal rotation matrices. If the maximization procedure converges to the same criterion value at each trial, we may be reasonably certain that we have found the global optimum. Let us illustrate.

```
. set seed 123
```

. rotate, oblimin oblique normalize protect(10)

1 : min criterion .0181657 Trial 2 : min criterion .0181657 Trial 3 : min criterion .0181657 4 : min criterion Trial .0181657 5 : min criterion .0181657 Trial 6 : min criterion .0181657 7 : min criterion Trial .0181657 Trial 8 : min criterion .0181657 Trial 9 : min criterion 458260.7 Trial 10: min criterion .0181657

Factor analysis/correlation

Method: iterated principal factors
Rotation: oblique oblimin (Kaiser on)

Number of obs	=	305
Retained factors	=	2
Number of params	=	15

Factor	Variance	Proportion	Rotated factors are correlated
Factor1	3.95010	0.6629	
Factor2	3.35832	0.5635	

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height arm_span fore_arm lower_leg weight bitrod ch_girth	0.8831 0.9560 0.9262 0.8819 0.0047 -0.0069	0.0648 -0.0288 -0.0450 0.0344 0.9408 0.8032 0.7923	0.1620 0.1112 0.1795 0.1923 0.1108 0.3600 0.4169
ch_width	0.1042	0.6462	0.5081

#### Factor rotation matrix

	Factor1	Factor2
Factor1	0.9112	0.7930
Factor2	-0.4120	0.6092

Here three of the random trials converged to distinct rotations from the rest. Specifying options log and trace would demonstrate that in these cases, the initial configurations were so far off that no improvements could be found. In a real application, we would probably rerun rotate with more trials, say, protect(50), for more reassurance.

#### □ Technical note

There is another but almost trivial source of nonuniqueness. All simplicity criteria supported by rotate and rotatemat are invariant with respect to permutations of the rows and of the columns. Also, the signs of rotated loadings are undefined. rotatemat, the computational engine of rotate, makes sure that all columns have a positive orientation, that is, have a positive sum. rotate, after factor and pca, also sorts the columns into decreasing order of explained variance.

# Other types of rotation

rotate supports a few rotation methods that do not fit into the scheme of "simplicity maximization". The first is known as the target rotation, which seeks to rotate the factor loading matrix to approximate as much as possible a target matrix of the same size as the factor loading matrix.

### Example 5: Rotation toward a target matrix

We continue with our same example. If we had expected a factor loading structure in which the first group of four variables would load especially high on the first factor and the second group of four variables on the second factor, we could have set up the following target matrix.

- . matrix W =  $(1,0 \setminus 1,0 \setminus 1,0 \setminus 0,1 \setminus 0,1 \setminus 0,1 \setminus 0,1)$
- . matrix list W

```
W[8,2]
        c2
    c1
     1
         Ω
r1
r2
     1
         Λ
r3
     1
         0
r4
     1
r5
     0
         1
r6
     0
         1
r7
     0
         1
r8
     0
```

It is also possible to request an orthogonal or oblique rotation toward the target W.

. rotate, target(W) normalize

Factor analysis/correlation Number of obs = 305
Method: iterated principal factors Retained factors = 2
Rotation: orthogonal target (Kaiser on) Number of params = 15

Factor	Variance	Difference	Proportion	Cumulative
Factor1	3.30616	0.65307	0.5548	0.5548
Factor2	2.65309		0.4452	1.0000

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

Variable	Factor1	Factor2	Uniqueness
height	0.8715	0.2802	0.1620
arm_span	0.9197	0.2073	0.1112
fore_arm	0.8869	0.1843	0.1795
lower_leg	0.8631	0.2505	0.1923
weight	0.2304	0.9144	0.1108
bitrod	0.1861	0.7780	0.3600
ch_girth	0.1268	0.7530	0.4169
ch_width	0.2561	0.6530	0.5081

Factor rotation matrix

	Factor1	Factor2
Factor1	0.7817	0.6236
Factor2	-0.6236	0.7817

1

With this target matrix, the result is not far different from the varimax and other orthogonal rotations.

# Example 6: Oblique promax rotation

For our last example, we return to the early days of factor analysis, the time before fast computing. Analytical methods for orthogonal rotation, such as varimax, were developed relatively early. Analogous methods for oblique rotations proved more complicated. Hendrickson and White (1964) proposed a computationally simple method to obtain an oblique rotation that comprises an oblique Procrustes rotation of the factor loadings toward a signed power of the varimax rotation of the factor loadings. The promax method has one parameter, the power to which the varimax loadings are raised. Larger promax powers simplify the factor loadings (that is, generate more zeros and ones) at the cost of more correlation between the common factors. Generally, we recommend that you keep the power in the range (1,4] and not restricted to integers. Specifying promax is equivalent to promax(3).

#### . rotate, promax normalize

Factor analysis/correlation	Number of obs =	305
Method: iterated principal factors	Retained factors =	2
Rotation: oblique promax (Kaiser on)	Number of params =	15

Factor	Variance	Proportion	Rotated factors are correlated
Factor1	3.92727	0.6590	
Factor2	3.31295	0.5559	

LR test: independent vs. saturated: chi2(28) = 2092.68 Prob>chi2 = 0.0000 Rotated factor loadings (pattern matrix) and unique variances

height arm_span         0.8797         0.0744         0.1620           arm_span         0.9505         -0.0176         0.1112           fore_arm         0.9205         -0.0340         0.1795           lower_leg         0.8780         0.0443         0.1923           weight         0.0214         0.9332         0.1108           bitrod         0.0074         0.7966         0.3600           ch_girth         -0.0509         0.7851         0.4169           ch_width         0.1152         0.6422         0.5081	Variable	Factor1	Factor2	Uniqueness
	arm_span fore_arm lower_leg weight bitrod ch_girth	0.9505 0.9205 0.8780 0.0214 0.0074 -0.0509	-0.0176 -0.0340 0.0443 0.9332 0.7966 0.7851	0.1112 0.1795 0.1923 0.1108 0.3600 0.4169

#### Factor rotation matrix

	Factor1	Factor2
Factor1	0.9069	0.7832
Factor2	-0.4214	0.6218

In this simple two-factor example, the promax solution is similar to the oblique oblimin solution.

4

### Stored results

rotate adds stored results named e(r\_name) to the stored results that were already defined by factor or pca.

rotate adds to the following results:

```
number of factors/components in rotated solution
    e(r_f)
    e(r_fmin)
                          rotation criterion value
Macros
    e(r_class)
                          orthogonal or oblique
    e(r_criterion)
                          rotation criterion
                          title for rotation
    e(r_ctitle)
    e(r_normalization) kaiser or none
Matrices
    e(r_L)
                          rotated loadings
    e(r_T)
                          rotation
    e(r_Phi)
                          correlations between common factors (after factor only)
    e(r_Ev)
                          explained variance by common factors (factor) or rotated components (pca)
```

The factors/components in the rotated solution are in decreasing order of e(r\_Ev).

#### □ Technical note

The rest of this section contains information of interest to programmers who want to provide rotate support to other estimation commands. Similar to other postestimation commands, such as estat and predict, rotate invokes a handler command. The name of this command is extracted from the field e(rotate\_cmd). The estimation command *cmd* should set this field appropriately. For instance, pca sets the macro e(rotate\_cmd) to pca\_rotate. The command pca\_rotate implements rotation after pca and pcamat, using rotatemat as the computational engine. pca\_rotate does not display output itself; it relies on pca to do so.

For consistent behavior for end users and programmers alike, we recommend that the estimation command *cmd*, the driver commands, and other postestimation commands adhere to the following guidelines:

#### **Driver command**

- The rotate driver command for *cmd* should be named *cmd*\_rotate.
- cmd\_rotate should be an e-class command, that is, returning in e().
- Make sure that cmd\_rotate is invoked after the correct estimation command (for example, if "'e(cmd)'" != "pca" ...).
- Allow at least the option <u>detail</u> and any option available to rotatemat.
- Extract from e() the matrix you want to rotate; invoke rotatemat on the matrix; and run this command quietly (that is, suppress all output) unless the option detail was specified.
- Extract the r() objects returned by rotatemat; see Methods and formulas of [MV] rotatemat
  for details.
- Compute derived results needed for your estimator.
- Store in e() fields (macros, scalars, matrices) named r\_name, adding to the existing e() fields.
   Store the macros returned by rotatemat under the same named prefixed with r\_. In particular, the macro e(r\_criterion) should be set to the name of the rotation criterion returned by rotatemat

macro e(r\_criterion) should be set to the name of the rotation criterion returned by rotatemat as r(criterion). Other commands can check this field to find out whether rotation results are available.

We suggest that only the most recent rotation results be stored, overwriting any existing e(r\_\*) results. The programmer command \_rotate\_clear clears any existing r\_\* fields from e().

• Display the rotation results by replaying cmd.

#### Estimation command cmd

- In cmd, define e(rotate\_cmd) to cmd\_rotate.
- cmd should be able to display the rotated results and should default to do so if rotated results are
  available. Include an option noROTated to display the unrotated results.
- You may use the programmer command \_rotate\_text to obtain a standard descriptive text for the rotation method.

#### Other postestimation commands

- Other postestimation commands after cmd should operate on the rotated results whenever they are
  appropriate and available, unless the option noROTated specifies otherwise.
- Mention that you operate on the unrotated results only if rotated results are available, but the user
  or you as the programmer decided not to use them.

### Methods and formulas

See Methods and formulas of [MV] rotatemat.

Henry Felix Kaiser (1927–1992) was born in Morristown, New Jersey, and educated in California, where he earned degrees at Berkeley in between periods of naval service during and after World War II. A specialist in psychological and educational statistics and measurement, Kaiser worked at the Universities of Illinois and Wisconsin before returning to Berkeley in 1968. He made several contributions to factor analysis, including varimax rotation (the subject of his PhD) and a measure for assessing sampling adequacy. Kaiser is remembered as an eccentric who spray-painted his shoes in unusual colors and listed ES (Eagle Scout) as his highest degree.

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Also see References in [MV] rotatemat.

### Also see

- [MV] **factor** Factor analysis
- [MV] factor postestimation Postestimation tools for factor and factormat
- [MV] **pca** Principal component analysis
- [MV] pca postestimation Postestimation tools for pca and pcamat
- [MV] **procrustes** Procrustes transformation
- [MV] rotatemat Orthogonal and oblique rotations of a Stata matrix

#### **Title**

**rotatemat** — Orthogonal and oblique rotations of a Stata matrix

Description Menu Syntax Options
Remarks and examples Stored results Methods and formulas References

Also see

### Description

rotatemat applies a linear transformation to the specified matrix so that the result minimizes a criterion function over all matrices in a class of feasible transformations. Two classes are supported: orthogonal (orthonormal) and oblique. A wide variety of criterion functions are available, representing different ways to measure the "simplicity" of a matrix. Most of these criteria can be applied with both orthogonal and oblique rotations.

This entry describes the computation engine for orthogonal and oblique transformations of Stata matrices. This command may be used directly on any Stata matrix.

If you are interested in rotation after factor, factormat, pca, or pcamat, see [MV] factor postestimation, [MV] pca postestimation, and the general description of rotate as a postestimation facility in [MV] rotate.

#### Menu

Statistics > Multivariate analysis > Orthogonal and oblique rotations of a matrix

### **Syntax**

rotatemat *matrix\_L* [, *options*] Description options Main restrict to orthogonal rotations; the default, except with promax() orthogonal allow oblique rotations oblique rotation criterion rotation\_methods rotate Kaiser normalized matrix normalize Reporting format(% fmt) display format for matrices; default is format(%9.5f) blanks(#) display loadings as blanks when |loading| < #; default is blanks(0) nodisplay suppress all output except log and trace noloading suppress display of rotated loadings suppress display of rotation matrix norotation matname(string) descriptive label of the matrix to be rotated colnames(string) descriptive name for columns of the matrix to be rotated Optimization optimize\_options control the optimization process; seldom used rotation\_methods Description varimax varimax (orthogonal only); the default varimax via the GPF algorithm (orthogonal only) vgpf quartimax (orthogonal only) quartimax equamax equamax (orthogonal only) parsimax (orthogonal only) parsimax minimum entropy (orthogonal only) entropy Comrey's tandem 1 principle (orthogonal only) tandem1 tandem2 Comrey's tandem 2 principle (orthogonal only) \*promax[(#)] promax power # (implies oblique); default is promax(3) oblimin (#) oblimin with  $\gamma = \#$ ; default is oblimin(0) cf(#) Crawford-Ferguson family with  $\kappa = \#$ , 0 < # < 1bentler Bentler's invariant pattern simplicity oblimax oblimax

 $\frac{\text{quartimin}}{\text{target}(T_g)}$ 

partial(Tg W)

quartimin

rotate toward matrix Tg

rotate toward matrix Tg, weighted by matrix W

<sup>\*</sup> varimax and promax ignore all optimize\_options.

### **Options**

Main

orthogonal specifies that an orthogonal rotation be applied. This is the default.

See Rotation criteria below for details on the rotation\_methods available with orthogonal.

oblique specifies that an oblique rotation be applied. This often yields more interpretable factors with a simpler structure than that obtained with an orthogonal rotation. In many applications (for example, after factor and pca), the factors before rotation are orthogonal (uncorrelated), whereas the oblique rotated factors are correlated.

See Rotation criteria below for details on the rotation\_methods available with oblique.

normalize requests that the rotation be applied to the Kaiser normalization (Horst 1965) of the matrix A so that the rowwise sums of squares equal 1.

Reporting

format (% fint) specifies the display format for matrices. The default is format (%9.5f).

blanks(#) specifies that small values of the rotated matrix—that is, those elements of  $\mathbf{A}(\mathbf{T}')^{-1}$  that are less than # in absolute value—are displayed as spaces.

nodisplay suppresses all output except the log and trace.

noloading suppresses the display of the rotated loadings.

norotation suppresses the display of the optimal rotation matrix.

matname(string) is a rarely used output option; it specifies a descriptive label of the matrix to be rotated.

colnames(string) is a rarely used output option; it specifies a descriptive name to refer to the columns of the matrix to be rotated. For instance, colnames(components) specifies that the output label the columns as "components". The default is "factors".

Optimization

optimize\_options control the iterative optimization process. These options are seldom used.

iterate(#) is a rarely used option; it specifies the maximum number of iterations. The default is iterate(1000).

log specifies that an iteration log be displayed.

trace is a rarely used option; it specifies that the rotation be displayed at each iteration.

tolerance(#) is one of three criteria for declaring convergence and is rarely used. The tolerance() convergence criterion is satisfied when the relative change in the rotation matrix T from one iteration to the next is less than or equal to #. The default is tolerance(1e-6).

gtolerance(#) is one of three criteria for declaring convergence and is rarely used. The gtolerance() convergence criterion is satisfied when the Frobenius norm of the gradient of the criterion function c() projected on the manifold of orthogonal matrices or of normal matrices is less than or equal to #. The default is gtolerance(1e-6).

ltolerance(#) is one of three criteria for declaring convergence and is rarely used. The ltolerance() convergence criterion is satisfied when the relative change in the minimization criterion c() from one iteration to the next is less than or equal to #. The default is ltolerance(1e-6).

- protect(#) requests that # optimizations with random starting values be performed and that
   the best of the solutions be reported. The output also indicates whether all starting values
   converged to the same solution. When specified with a large number, such as protect(50),
   this provides reasonable assurance that the solution found is the global maximum and not just
   a local maximum. If trace is also specified, the rotation matrix and rotation criterion value of
   each optimization will be reported.
- maxstep(#) is a rarely used option; it specifies the maximum number of step-size halvings. The default is maxstep(20).
- init(matname) is a rarely used option; it specifies the initial rotation matrix. matname should be square and regular (nonsingular) and have the same number of columns as the matrix matrix\_L to be rotated. It should be orthogonal ( $\mathbf{T}'\mathbf{T} = \mathbf{T}\mathbf{T}' = \mathbf{I}$ ) or normal (diag( $\mathbf{T}'\mathbf{T}$ ) = 1), depending on whether orthogonal or oblique rotations are performed. init() cannot be combined with random. If neither init() nor random is specified, the identity matrix is used as the initial rotation.
- random is a rarely used option; it specifies that a random orthogonal or random normal matrix be used as the initial rotation matrix. random cannot be combined with init(). If neither init() nor random is specified, the identity matrix is used as the initial rotation.

#### **Rotation criteria**

In the descriptions below, the matrix to be rotated is denoted as A, p denotes the number of rows of A, and f denotes the number of columns of A (factors or components). If A is a loading matrix from factor or pca, p is the number of variables and f is the number of factors or components.

### Criteria suitable only for orthogonal rotations

- varimax and vgpf apply the orthogonal varimax rotation (Kaiser 1958). varimax maximizes the variance of the squared loadings within factors (columns of A). It is equivalent to cf(I/p) and to oblimin(1). varimax, the most popular rotation, is implemented with a dedicated fast algorithm and ignores all *optimize\_options*. Specify vgpf to switch to the general GPF algorithm used for the other criteria.
- quartimax uses the quartimax criterion (Harman 1976). quartimax maximizes the variance of the squared loadings within the variables (rows of A). For orthogonal rotations, quartimax is equivalent to cf(0) and to oblimax.
- equamax specifies the orthogonal equamax rotation, equamax maximizes a weighted sum of the varimax and quartimax criteria, reflecting a concern for simple structure within variables (rows of  $\mathbf{A}$ ) as well as within factors (columns of  $\mathbf{A}$ ), equamax is equivalent to oblimin(p/2) and cf (#), where # = f/(2p).
- parsimax specifies the orthogonal parsimax rotation parsimax is equivalent to cf(#), where #=(f-1)/(p+f-2).
- entropy applies the minimum entropy rotation criterion (Jennrich 2004).
- tandem1 specifies that the first principle of Comrey's tandem be applied. According to Comrey (1967), this principle should be used to judge which "small" factors be dropped.
- tandem2 specifies that the second principle of Comrey's tandem be applied. According to Comrey (1967), tandem2 should be used for "polishing".

#### Criteria suitable only for oblique rotations

promax[(#)] specifies the oblique promax rotation. The optional argument specifies the promax power. Not specifying the argument is equivalent to specifying promax(3). Values less than 4 are recommended, but the choice is yours. Larger promax powers simplify the loadings (generate numbers closer to zero and one) but at the cost of additional correlation between factors. Choosing a value is a matter of trial and error, but most sources find values in excess of 4 undesirable in practice. The power must be greater than 1 but is not restricted to integers.

Promax rotation is an oblique rotation method that was developed before the "analytical methods" (based on criterion optimization) became computationally feasible. Promax rotation comprises an oblique Procrustean rotation of the original loadings  $\bf A$  toward the elementwise #-power of the orthogonal varimax rotation of  $\bf A$ .

#### Criteria suitable for orthogonal and oblique rotations

oblimin [(#)] specifies that the oblimin criterion with  $\gamma = \#$  be used. When restricted to orthogonal transformations, the oblimin() family is equivalent to the orthomax criterion function. Special cases of oblimin() include

$\gamma$	Special case		
0	quartimax / quartimin		
1/2	biquartimax / biquartimin		
1	varimax / covarimin		
p/2	equamax		
$p = \text{number of rows of } \mathbf{A}.$			

 $\gamma$  defaults to zero. Jennrich (1979) recommends  $\gamma \leq 0$  for oblique rotations. For  $\gamma > 0$ , it is possible that optimal oblique rotations do not exist; the iterative procedure used to compute the solution will wander off to a degenerate solution.

cf(#) specifies that a criterion from the Crawford-Ferguson (1970) family be used with  $\kappa = \#$ . cf( $\kappa$ ) can be seen as  $(1-\kappa)$ cf<sub>1</sub>( $\mathbf{A}$ ) + ( $\kappa$ )cf<sub>2</sub>( $\mathbf{A}$ ), where cf<sub>1</sub>( $\mathbf{A}$ ) is a measure of row parsimony and cf<sub>2</sub>( $\mathbf{A}$ ) is a measure of column parsimony. cf<sub>1</sub>( $\mathbf{A}$ ) attains its greatest lower bound when no row of  $\mathbf{A}$  has more than one nonzero element, whereas cf<sub>2</sub>( $\mathbf{A}$ ) reaches zero if no column of  $\mathbf{A}$  has more than one nonzero element.

For orthogonal rotations, the Crawford-Ferguson family is equivalent to the oblimin() family. For orthogonal rotations, special cases include the following:

$\kappa$	Special case
0	quartimax / quartimin
1/p	varimax / covarimin
f/(2p)	equamax
(f-1)/(p+f-2)	parsimax
1	factor parsimony
p = number of rows  q	of A.
f = number of colum	ns of A.

bentler specifies that the "invariant pattern simplicity" criterion (Bentler 1977) be used.

oblimax specifies the oblimax criterion, which maximizes the number of high and low loadings. oblimax is equivalent to quartimax for orthogonal rotations.

- quartimin specifies that the quartimin criterion be used. For orthogonal rotations, quartimin is equivalent to quartimax.
- target (Tg) specifies that **A** be rotated as near as possible to the conformable matrix Tg. Nearness is expressed by the Frobenius matrix norm.
- partial  $(Tg\ W)$  specifies that A be rotated as near as possible to the conformable matrix Tg. Nearness is expressed by a weighted (by W) Frobenius matrix norm. W should be nonnegative and usually is zero—one valued, with ones identifying the target values to be reproduced as closely as possible by the factor loadings, whereas zeros identify loadings to remain unrestricted.

### Remarks and examples

Remarks are presented under the following headings:

Introduction
Orthogonal rotations
Oblique rotations
Promax rotation

#### Introduction

For an introduction to rotation, see Harman (1976) and Gorsuch (1983).

rotatemat applies a linear transformation T to the specified matrix  $matrix\_L$ , which we will call A, so that the result  $c(A(T')^{-1})$  minimizes a criterion function c() over all matrices T in a class of feasible transformations.

Two classes are supported: orthogonal (orthonormal) and oblique. Orthonormal rotations comprise all orthonormal matrices  $\mathbf{T}$ , such that  $\mathbf{T}'\mathbf{T} = \mathbf{T}\mathbf{T}' = \mathbf{I}$ ; here  $\mathbf{A}(\mathbf{T}')^{-1}$  simplifies to  $\mathbf{A}\mathbf{T}$ . Oblique rotations are characterized by diag( $\mathbf{T}'\mathbf{T}$ ) = 1. All supported rotation criteria are invariant with respect to permutations of the columns and change of signs of the columns. rotatemat returns the solution with positive column sums and with columns sorted by the L2 norm; columns are ordered with respect to the L1 norm if the columns have the same L2 norm.

A wide variety of criteria c() is available, representing different ways to measure the "simplicity" of a matrix. Most of these criteria can be applied with both orthogonal and oblique rotations. A discussion of the different criteria and of the rotations with which they may be combined is provided in *Rotation criteria*.

A factor analysis of 24 psychological tests on 145 seventh- and eighth-grade school children with four retained factors is used for illustration. Factors were extracted with maximum likelihood. The loadings are reported by Harman (1976). We enter the factor loadings as a Stata matrix with 24 rows and four columns. For more information, we add full descriptive labels as comments and short labels as row names.

```
. matrix input L = (
>
     601
            019
                   388
                          221 \
                                             Visual perception
     372
           -025
                   252
                          132 \
>
                                             Cubes
                          144 \
                                             Paper form board
>
     413
           -117
                   388
           -100
                   254
>
     487
                          192 \
                                             Flags
     691
           -304
                  -279
                          035 \
                                             General information
>
           -409
                  -200
     690
                         -076 \
                                             Paragraph comprehension
>
>
     677
           -409
                  -292
                          084 \
                                             Sentence completion
                                             Word classification
>
     674
           -189
                  -099
                          122 \
>
     697
           -454
                  -212
                         -080 \
                                             Word meaning
>
     476
            534
                  -486
                          092 \
                                             Addition
>
     558
            332
                  -142
                         -090 \
                                             Code
>
     472
            508
                  -139
                          256 \
                                             Counting dots
     602
            244
                   028
                                             Straight-curved capitals
>
                          295 \
                                             Word recognition
>
     423
            058
                   015
                         -415 \
>
     394
            089
                   097
                         -362 \
                                             Number recognition
     510
            095
                   347
                         -249 \
                                             Figure recognition
>
                                             Object-number
>
     466
            197
                  -004
                         -381 \
                                             Number-figure
>
     515
            312
                   152
                         -147 \
                                             Figure-word
>
     443
            089
                   109
                         -150 \
>
     614
           -118
                   126
                         -038 \
                                             Deduction
                                             Numerical puzzles
>
     589
            227
                   057
                          123 \
>
     608
           -107
                   127
                         -038 \
                                             Problem reasoning
     687
           -044
                   138
                          098 \
                                             Series completion
>
     651
            177
                 -212
                        -017 )
                                             Arithmetic problems
. matrix colnames L = F1 F2 F3 F4
  matrix rownames L = visual
                                    cubes
                                                board
                                    general
                         flags
                                                paragraph
>
>
                         sentence
                                    wordclas
                                               wordmean
>
                         add
                                    code
                                                dots
>
                         capitals
                                    wordrec
                                                numbrec
>
                         figrec
                                    obj-num
                                                num-fig
                         fig-word
>
                                    deduct
                                                numpuzz
                         reason
                                    series
                                                arith
```

. matrix L = L/1000

Thus using rotatemat, we can study various rotations of L without access to the full data or the correlation matrix.

### **Orthogonal rotations**

We can rotate the matrix L according to an extensive list of criteria, including orthogonal rotations.

### Example 1: Orthogonal varimax rotation

The default rotation, orthogonal varimax, is probably the most popular method:

. rotatemat L, format(%6.3f)

Rotation of L[24,4]

Criterion varimax
Rotation class orthogonal
Kaiser normalization off

Rotated factors

	F1	F2	F3	F4
visual	0.247	0.151	0.679	0.128
cubes	0.171	0.060	0.425	0.078
board	0.206	-0.049	0.549	0.097
flags	0.295	0.068	0.504	0.050
general	0.765	0.214	0.117	0.067
paragraph	0.802	0.074	0.122	0.160
sentence	0.826	0.148	0.117	-0.008
wordclas	0.612	0.230	0.290	0.061
wordmean	0.840	0.049	0.112	0.152
add	0.166	0.846	-0.076	0.082
code	0.222	0.533	0.134	0.313
dots	0.048	0.705	0.257	0.025
capitals	0.240	0.500	0.450	0.020
wordrec	0.249	0.124	0.032	0.526
numbrec	0.178	0.109	0.106	0.499
figrec	0.158	0.076	0.401	0.510
obj-num	0.197	0.262	0.060	0.539
num-fig	0.096	0.352	0.311	0.422
fig-word	0.204	0.175	0.232	0.336
deduct	0.443	0.115	0.365	0.255
numpuzz	0.233	0.428	0.389	0.169
reason	0.432	0.120	0.363	0.256
series	0.440	0.228	0.472	0.184
arith	0.409	0.509	0.150	0.228

#### Orthogonal rotation

	F1	F2	F3	F4
F1 F2 F3 F4	-0.632 -0.376	0.438 0.737 -0.458 0.234	0.049 0.760	0.352 0.232 0.268 -0.866

The varimax rotation T of A maximizes the (raw) varimax criterion over all orthogonal T, which for  $p \times f$  matrices is defined as (Harman 1976)

$$c_{\text{varimax}}(\mathbf{A}) = \frac{1}{p} \sum_{i=1}^{f} \left\{ \left( \sum_{i=1}^{p} A_{ij}^{4} \right) - \frac{1}{p} \left( \sum_{i=1}^{p} A_{ij}^{2} \right)^{2} \right\}$$

The criterion  $c_{\text{varimax}}(\mathbf{A})$  can be interpreted as the sum over the columns of the variances of the squares of the loadings  $A_{ij}$ . A column with large variance will typically consist of many small values and a few large values. Achieving such "simple" columnwise distributions is often helpful for interpretation.

#### Technical note

The raw varimax criterion as defined here has been criticized because it weights variables by the size of their loadings, that is, by their communalities. This is often not desirable. A common rotation strategy is to weight all rows equally by rescaling to the same rowwise sum of squared loadings. This is known as the Kaiser normalization. You may request this normalized solution with the normalize option. The default in rotatemat and in rotate (see [MV] rotate) is not to normalize.

Many other criteria for the rotation of matrices have been proposed and studied in the literature. Most of these criteria can be stated in terms of a "simplicity function". For instance, quartimax rotation (Carroll 1953) seeks to achieve interpretation within rows—in a factor analytic setup, this means that variables should have a high loading on a few factors and a low loading on the other factors. The quartimax criterion is defined as (Harman 1976)

$$c_{\text{quartimax}}(\mathbf{A}) = \left(\frac{1}{pf} \sum_{i=1}^{p} \sum_{j=1}^{f} A_{ij}^{4}\right) - \left(\frac{1}{pf} \sum_{i=1}^{p} \sum_{j=1}^{f} A_{ij}^{2}\right)^{2}$$

### Example 2: Orthogonal quartimax rotation

We display the quartimax solution, use blanks to represent loadings with absolute values smaller than 0.3, and suppress the display of the rotation matrix.

. rotatemat L, quartimax format(%6.3f) norotation blanks(0.3) Rotation of L[24,4]

Criterion quartimax
Rotation class orthogonal
Kaiser normalization off
Criterion value -1.032898
Number of iterations 35

Rotated factors (blanks represent abs()<.3)

	F1	F2	F3	F4
visual	0.374		0.630	
cubes			0.393	
board			0.513	
flags	0.379		0.450	
general	0.791			
paragraph	0.827			
sentence	0.838			
wordclas	0.669			
wordmean	0.860			
add		0.829		
code	0.316	0.521		
dots		0.701		
capitals	0.348	0.482	0.393	
wordrec	0.316			0.492
numbrec				0.469
figrec			0.382	0.470
obj-num				0.503
num-fig		0.357		0.383
fig-word				
deduct	0.528			
numpuzz	0.342	0.414	0.340	
reason	0.517			
series	0.543		0.395	
arith	0.490	0.478		
	L			

4

Some of the criteria supported by rotatemat are defined as one-parameter families. The oblimin( $\gamma$ ) criterion and the Crawford and Ferguson cf( $\kappa$ ) criterion families contain the varimax and quartimax criteria as special cases; that is, they can be obtained by certain values of  $\gamma$  and  $\kappa$ , respectively. Intermediate parameter values provide compromises between varimax's aim of column simplification and quartimax's aim of row simplification. Varimax and quartimax are equivalent to oblimin(1) and oblimin(0), respectively. A compromise, oblimin(0.5), is also known as biquartimax.

### Example 3: Orthogonal biquartimax rotation

Because the varimax and quartimax solutions are so close for our matrix L, the biquartimax compromise will also be rather close.

. rotatemat L, oblimin(0.5) format(%6.3f) norotation (output omitted)

#### □ Technical note

You may have noticed a difference between the output of rotatemat in the default case or equivalently when we type

. rotatemat L, varimax

and in other cases. In the default case, no mention is made of the criterion value and the number of iterations. rotatemat uses a fast special algorithm for this most common case, whereas for other rotations it uses a general gradient projection algorithm (GPF) proposed by Jennrich (2001, 2002); see also Bernaards and Jennrich (2005). The general algorithm is used to obtain the varimax rotation if you specify the option vgpf rather than varimax.

The rotations we have illustrated are orthogonal—the lengths of the rows and the angles between the rows are not affected by the rotations. We may verify—we do not show this in the manual to conserve paper—that after an orthogonal rotation of L

```
. matlist L*L'
and
. matlist r(AT)*r(AT)'
return the same 24 by 24 matrix, whereas
. matlist r(T)*r(T)'
```

. matlist r(T)'\*r(T)

both return a  $2 \times 2$  identity matrix. rotatemat returns in r(AT) the rotated matrix and in r(T) the rotation matrix.

### **Oblique rotations**

rotatemat provides a second class of rotations: oblique rotations. These rotations maintain the norms of the rows of the matrix but not their inner products. In geometric terms, interpreting the rows of the matrix to be rotated as vectors, both the orthogonal and the oblique rotations maintain the lengths of the vectors. Under orthogonal transformations, the angles between the vectors are also left unchanged—these transformations comprise true reorientations in space and reflections. Oblique rotations do not conserve angles between vectors. If the vectors are orthogonal before rotations—as will be the case if we are rotating factor or component loading matrices—this will no longer be the case after the rotation. The "freedom" to select angles between the rows allows oblique rotations to generate simpler loading structures than the orthogonal rotations—sometimes much simpler. In a factor analytic setting, the disadvantage is, however, that the rotated factors are correlated.

rotatemat can obtain oblique rotations for most of the criteria that are available for orthogonal rotations; some of the criteria (such as the entropy criterion) are available only for the orthogonal case.

#### 090

#### Example 4: Oblique oblimin rotation

We illustrate with the psychological tests matrix L and apply the oblique oblimin criterion.

. rotatemat L, oblimin oblique format(%6.3f) blanks(0.3)

Rotation of L[24,4]

Criterion oblimin(0)
Rotation class oblique
Kaiser normalization off
Criterion value .1957363
Number of iterations 78

Rotated factors (blanks represent abs()<.3)

	F1	F2	F3	F4
visual		0.686		
cubes		0.430		
board		0.564		
flags		0.507		
general	0.771			
paragraph	0.808			
sentence	0.865			
wordclas	0.560			
wordmean	0.857			
add			0.864	
code			0.460	0.305
dots			0.701	
capitals		0.437	0.442	
wordrec				0.571
numbrec				0.543
figrec		0.314		0.540
obj-num				0.584
num-fig				0.438
fig-word				0.341
deduct	0.325			
numpuzz		0.344	0.347	
reason	0.311			
series		0.417		
arith			0.428	

Oblique rotation

	F1	F2	F3	F4
F1 F2 F3 F4	-0.483 -0.299	0.019 0.587	0.584 0.651 -0.435 0.213	0.213 0.207

The option oblique requested an oblique rotation rather than the default orthogonal. You may verify that r(AT) equals L \* inv(r(T)) within reasonable roundoff with

```
. matlist r(AT) - L * inv(r(T)')
  (output omitted)
```

The correlation between the rotated dimensions is easily obtained.

. mat	list r(T)	' * r(T)			
		F1	F2	F3	F4
	F1	1			
	F2	.4026978	1		
	F3	.294928	.2555824	1	
	F4	.4146879	.3784689	.3183115	1

#### **Promax rotation**

rotatemat also offers promax rotation.

### ➤ Example 5: Oblique promax rotation

We use the matrix L to illustrate promax rotation.

. rotatemat L, promax blanks(0.3) format(%6.3f)

Rotation of L[24,4]

Criterion promax(3) Rotation class oblique Kaiser normalization off

Rotated factors (blanks represent abs()<.3)

	F1	F2	F3	F4
visual		0.775		
cubes		0.487		
board		0.647		
flags		0.572		
general	0.786			
paragraph	0.825			
sentence	0.888			
wordclas	0.543			
wordmean	0.878			
add			0.921	
code			0.466	
dots			0.728	
capitals		0.468	0.441	
wordrec				0.606
numbrec				0.570
figrec		0.364		0.539
obj-num				0.610
num-fig				0.425
fig-word				0.337
deduct		0.323		
numpuzz		0.369	0.336	
reason		0.322		
series		0.462		
arith			0.436	

#### Oblique rotation

	F1	F2	F3	F4
F1 F2 F3 F4	0.841 -0.462 -0.282 -0.012	0.478	-0.386	0.743 0.215 0.159 -0.614

The correlation between the rotated dimensions can be obtained as

. matlist r(T) \* r(T)

	F1	F2	F3	F4
F1	1			
F2	.5491588	1		
F3	.3807942	.4302401	1	
F4	.4877064	.5178414	.4505817	1

4

Stored results

rotatemat stores the following in r():

Scalars

r(f) criterion value

r(iter) number of GPF iterations

r(rc) return code

r(nnconv) number of nonconvergent trials; protect() only

Macros

r(cmd) rotatemat

r(ctitle) descriptive label of rotation method

r(ctitle12) version of r(ctitle) at most 12 characters long

r(criterion) criterion name (e.g., oblimin)

r(class) orthogonal or oblique

r(normalization) kaiser or none r(carg) criterion argument

Matrices

r(T) optimal transformation  $\mathbf{T}$ r(AT) optimal  $\mathbf{AT} = \mathbf{A}(\mathbf{T}')^{-1}$ r(fmin) minimums found; protect() only

### Methods and formulas

rotatemat minimizes a scalar-valued criterion function  $c(\mathbf{AT})$  with respect to the set of orthogonal matrices  $\mathbf{T'T} = \mathbf{I}$ , or  $c(\mathbf{A(T')}^{-1})$  with respect to the normal matrix,  $\operatorname{diag}(\mathbf{T'T}) = \mathbf{1}$ . For orthonormal  $\mathbf{T}$ ,  $\mathbf{T} = (\mathbf{T'})^{-1}$ .

The rotation criteria can be conveniently written in terms of scalar-valued functions; see Bernaards and Jennrich (2005). Define the inner product  $\langle \mathbf{A}, \mathbf{B} \rangle = \operatorname{trace}(\mathbf{A}'\mathbf{B})$ .  $|\mathbf{A}| = \sqrt{\langle \mathbf{A}, \mathbf{A} \rangle}$  is called the Frobenius norm of the matrix  $\mathbf{A}$ . Let  $\mathbf{A}$  be a  $p \times k$  matrix. Denote by  $\mathbf{X}^2$  the direct product  $\mathbf{X} \cdot \mathbf{X}$ . See Harman (1976) for information on many of the rotation criteria and references to the authors originally proposing the criteria. Sometimes we list an alternative reference. Our notation is similar to that of Bernaards and Jennrich (2005).

rotatemat uses the iterative "gradient projection algorithm" (Jennrich 2001, 2002) for the optimization of the criterion over the permissible transformations. Different versions are provided for optimal orthogonal and oblique rotations; see Bernaards and Jennrich (2005).

#### Varimax (orthogonal only)

Varimax is equivalent to oblimin with  $\gamma = 1$  or to the Crawford-Ferguson family with  $\kappa = 1/p$ ; see below.

#### Quartimax (orthogonal only)

$$c(\mathbf{\Lambda}) = \sum_{i} \sum_{r} \lambda_{ir}^{4} = -\frac{1}{4} \left\langle \mathbf{\Lambda}^{2}, \mathbf{\Lambda}^{2} \right\rangle$$

#### Equamax (orthogonal only)

Equamax is equivalent to oblimin with  $\gamma=p/2$  or to the Crawford-Ferguson family with  $\kappa=f/(2p)$ ; see below.

#### Parsimax (orthogonal only)

Parsimax is equivalent to the Crawford-Ferguson family with  $\kappa = (f-1)/(p+f-2)$ ; see below.

#### Entropy (orthogonal only); see Jennrich (2004)

$$c(\mathbf{\Lambda}) = -\frac{1}{2} \left\langle \mathbf{\Lambda}^2, \log \mathbf{\Lambda}^2 \right\rangle$$

Tandem principal 1 (orthogonal only); see Comrey (1967)

$$c(\mathbf{\Lambda}) = -\langle \mathbf{\Lambda}^2, (\mathbf{\Lambda}\mathbf{\Lambda}')^2 \mathbf{\Lambda}^2 \rangle$$

Tandem principal 2 (orthogonal only); see Comrey (1967)

$$c(\mathbf{\Lambda}) = \langle \mathbf{\Lambda}^2, \{ \mathbf{1}\mathbf{1}' - (\mathbf{\Lambda}\mathbf{\Lambda}')^2 \} \mathbf{\Lambda}^2 \rangle$$

#### Promax (oblique only)

Promax does not fit in the maximizing-of-a-simplicity-criterion framework that is at the core of rotatemat. The promax method (Hendrickson and White 1964) was proposed before computing power became widely available. The promax rotation comprises three steps:

- 1. Perform an orthogonal rotation on A; rotatemat uses varimax.
- 2. Raise the elements of the rotated matrix to some power, preserving the signs of the elements. Typically, the power is taken from the range [2,4]. This operation is meant to distinguish more clearly between small and large values.
- 3. The matrix from step 2 is used as the target for an oblique Procrustean rotation from the original matrix A. The method to compute this rotation in promax is different from the method in the procrustes command (see [MV] procrustes). The latter produces the real least-squares oblique rotation; promax uses an approximation.

#### Oblimin; see Jennrich (1979)

$$c(\mathbf{\Lambda}) = \frac{1}{4} \left\langle \mathbf{\Lambda}^2, \{ \mathbf{I} - (\gamma/p) \mathbf{1} \mathbf{1}' \} \mathbf{\Lambda}^2 (\mathbf{1} \mathbf{1}' - \mathbf{I}) \right\rangle$$

Orthomax and oblimin are equivalent when restricted to orthogonal rotations. Special cases of oblimin() include the following:

$\gamma$	Special case
0	quartimin
1/2	biquartimin
p/2	equamax
1	varimax

#### Crawford and Ferguson (1970) family

$$c(\mathbf{\Lambda}) = \frac{1-\kappa}{4} \left\langle \mathbf{\Lambda}^2, \mathbf{\Lambda}^2 (\mathbf{1}\mathbf{1}' - \mathbf{I}) \right\rangle + \frac{\kappa}{4} \left\langle \mathbf{\Lambda}^2, (\mathbf{1}\mathbf{1}' - \mathbf{I})\mathbf{\Lambda}^2 \right\rangle$$

When restricted to orthogonal transformations, cf() and oblimin() are in fact equivalent. Special cases of cf() include the following:

$\kappa$	Special case
0	quartimax
1/p	varimax
f/(2p)	equamax
(f-1)/(p+f-2)	parsimax
1	factor parsimony

### Bentler's invariant pattern simplicity; see Bentler (1977)

$$c(\mathbf{\Lambda}) = \log[\det\{(\mathbf{\Lambda}^2)'\mathbf{\Lambda}^2\}] - \log(\det[\operatorname{diag}\{(\mathbf{\Lambda}^2)'\mathbf{\Lambda}^2\}])$$

#### **Oblimax**

$$c(\mathbf{\Lambda}) = -\log(\langle \mathbf{\Lambda}^2, \mathbf{\Lambda}^2 \rangle) + 2\log(\langle \mathbf{\Lambda}, \mathbf{\Lambda} \rangle)$$

For orthogonal transformations, oblimax is equivalent to quartimax; see above.

#### Quartimin

$$c(\mathbf{\Lambda}) = \sum_{r \neq s} \sum_{i} \lambda_{ir}^{2} \lambda_{is}^{2} = -\frac{1}{4} \left\langle \mathbf{\Lambda}^{2}, \mathbf{\Lambda}^{2} (\mathbf{1}\mathbf{1}' - \mathbf{I}) \right\rangle$$

#### **Target**

$$c(\mathbf{\Lambda}) = \frac{1}{2} |\mathbf{\Lambda} - \mathbf{H}|^2$$

for given target matrix **H**.

#### Partially specified target

$$c(\mathbf{\Lambda}) = |\mathbf{W} \cdot (\mathbf{\Lambda} - \mathbf{H})|^2$$

for given target matrix  $\mathbf{H}$ , nonnegative weighting matrix  $\mathbf{W}$  (usually zero-one valued) and with denoting the direct product.

#### References

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### Also see

[MV] rotate — Orthogonal and oblique rotations after factor and pca

[MV] **procrustes** — Procrustes transformation

#### **Title**

**scoreplot** — Score and loading plots

Description Quick start Menu Syntax

Options Remarks and examples Also see

### Description

scoreplot produces scatterplots of the score variables after factor, factormat, pca, or pcamat, and scatterplots of the discriminant score variables after discrim lda or candisc.

loadingplot produces scatterplots of the loadings (factors or components) after factor, factormat, pca, or pcamat, and the standardized discriminant function loadings after discrim lda or candisc.

#### **Quick start**

Plot score variables

Plot score variables after a command such as pca or factor scoreplot

As above, but add labels found in variable mylabel scoreplot, mlabel(mylabel)

As above, but increase number of factors from 2 to 4 scoreplot, mlabel(mylabel) factors(4)

As above, but use unrotated results and combine plots instead of displaying matrix plot scoreplot, mlabel(mylabel) factors(4) combined norotated

Plot loadings

Plot the loadings after a command such as pca or factor loadingplot

As above, but increase the number of factors from 2 to 4 loadingplot, factors(4)

As above, but use unrotated results and combine plots instead of displaying matrix plot loadingplot, factors(4) combined norotated

#### Menu

#### scoreplot

Statistics > Multivariate analysis > Factor and principal component analysis > Postestimation > Score variables plot

### loadingplot

Statistics > Multivariate analysis > Factor and principal component analysis > Postestimation > Loading plot

### **Syntax**

Y axis, X axis, Titles, Overall twoway\_options

```
Plot score variables
    scoreplot [if] [in] [, scoreplot_options]
 Plot the loadings (factors, components, or discriminant functions)
    loadingplot |, loadingplot_options |
 scoreplot_options
                              Description
Main
                              number of factors/scores to be plotted; default is factors(2)
 factors(#)
 components(#)
                              synonym for factors()
                              use unrotated factors or scores, even if rotated results exist
 norotated
                              graph as a matrix plot, available only when factors(2) is specified;
 matrix
                                default is a scatterplot
 combined
                              graph as a combined plot, available when factors (\# > 2); default
                                is a matrix plot
 half
                              graph lower half only; allowed only with matrix
 graph_matrix_options
                              affect the rendition of the matrix graph
 combine_options
                              affect the rendition of the combined graph
                              options for predict generating score variables
 scoreopt(predict_opts)
 marker_options
                              change look of markers (color, size, etc.)
 marker_label_options
                              change look or position of marker labels
Y axis, X axis, Titles, Overall
 twoway_options
                              any options other than by () documented in [G-3] twoway_options
 loadingplot_options
                              Description
Main
 factors(#)
                              number of factors/scores to be plotted; default is factors(2)
                              synonym for factors()
 components(#)
                              use unrotated factors or scores, even if rotated results exist
 norotated
                              graph as a matrix plot, available only when factors(2) is specified;
 matrix
                                default is a scatterplot
                              graph as a combined plot, available when factors (\# > 2); default
 combined
                                is a matrix plot
 half
                              graph lower half only; allowed only with matrix
 graph_matrix_options
                              affect the rendition of the matrix graph
 combine_options
                              affect the rendition of the combined graph
 maxlength(#)
                              abbreviate variable names to # characters; default is maxlength(12)
 marker_options
                              change look of markers (color, size, etc.)
                              change look or position of marker labels
 marker_label_options
```

any options other than by () documented in [G-3] twoway\_options

### **Options**

Main

factors (#) produces plots for all combinations of score variables up to #. # should not exceed the number of retained factors (components or discriminant functions) and defaults to 2. components() is a synonym. No plot is produced with factors(1).

norotated uses unrotated results, even when rotated results are available. The default is to use rotated results if they are available. norotated is ignored if rotated results are not available.

matrix specifies that plots be produced using graph matrix; see [G-2] graph matrix. This is the default when three or more factors are specified. This option may not be used with combined.

combined specifies that plots be produced using graph combine; see [G-2] graph combine. This option may not be used with matrix.

half specifies that only the lower half of the matrix be graphed. half can be specified only with the matrix option.

graph\_matrix\_options affect the rendition of the matrix plot; see [G-2] graph matrix.

combine\_options affect the rendition of the combined plot; see [G-2] **graph combine**. combine\_options may not be specified unless factors() is greater than 2.

scoreopt(predict\_opts), an option used with scoreplot, specifies options for predict to generate the score variables. For example, after factor, scoreopt(bartlett) specifies that Bartlett scoring be applied.

maxlength(#), an option used with loadingplot, causes the variable names (used as point markers) to be abbreviated to # characters. The abbrev() function performs the abbreviation, and if # is less than 5, it is treated as 5; see [FN] **String functions**.

marker\_options affect the rendition of markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] marker\_options.

marker\_label\_options specify if and how the markers are to be labeled; see [G-3] marker\_label\_options.

Y axis, X axis, Titles, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option).

### Remarks and examples

One of the main results from a principal component analysis, factor analysis, or a linear discriminant analysis is a set of eigenvectors that are called components, factors, or linear discriminant functions. These are stored in what is called a loading matrix. pca, pcamat, factor, and factormat store the loading matrix in e(L). If there were p variables involved in the PCA or factor analysis, and f components or factors were retained, there will be p rows and f columns in the resulting loading matrix. discrim lda and candisc store the standardized canonical discriminant function coefficients or loadings in  $e(L\_std)$ .

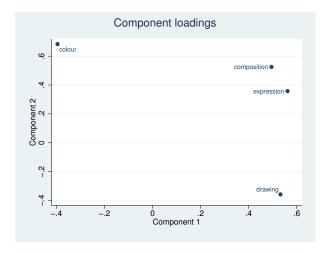
The columns of the loading matrix are in order of importance. For instance, with PCA, the first column of the loading matrix is the component that accounts for the most variance, the second column accounts for the next most variance, and so on.

In a loading plot, the values from one column of the loading matrix are plotted against the values from another column of the loading matrix. Of most interest is the plot of the first and second columns (the first and second components, factors, or discriminant functions), and this is what loadingplot produces by default. The rows of the loading matrix provide the points to be graphed. Variable names are automatically used as the marker labels for these points.

#### Example 1: Loading plot

We use the Renaissance painters' data introduced in example 2 of [MV] **biplot**. There are four attribute variables recorded for 10 painters. We examine the first two principal component loadings for this dataset.

- . use http://www.stata-press.com/data/r14/renpainters (Scores by Roger de Piles for Renaissance Painters)
- . pca composition drawing colour expression
  (output omitted)
- . loadingplot



From the first component, we see that color (or colour, if you prefer) is separated from the other three attributes (variables): composition, expression, and drawing. From the second component, the difference in drawing stands out.

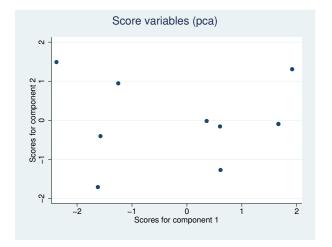
4

Score plots approach the view of the loading matrix from the perspective of the observations. predict after pca and factor produces scores; see [MV] pca postestimation and [MV] factor postestimation. predict after discrim lda and candisc can request discriminant function scores; see [MV] discrim lda postestimation. A score for an observation from a particular column of the loading matrix is obtained as the linear combination of that observation's data by using the coefficients found in the loading. From the raw variables, the linear combinations described in the columns of the loading matrix are applied to generate new component or factor score variables. A score plot graphs one score variable against another. By default, scoreplot graphs the scores generated from the first and second columns of the loading matrix (the first two components or factors).

#### Example 2: Score plot

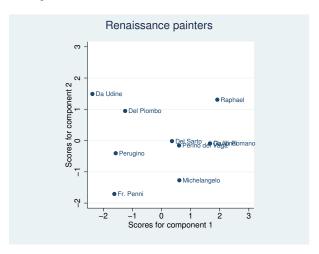
We continue with the PCA of the Renaissance painters.

. scoreplot



Unlike loadingplot, which can use the variable names as labels, scoreplot does not automatically know how to label the points after factor and pca. The graph above is not helpful. The *marker\_label\_option* mlabel() takes care of this.

- . scoreplot, mlabel(painter) aspect(1) xlabel(-2(1)3) ylabel(-2(1)3)
- > title(Renaissance painters)



We added a few other options to improve the graph. We extended the axes to include the value 3 so that there would be room for the marker labels, imposed an aspect ratio of 1, and added a title.

The score plot gives us a feeling for the similarities and differences between the painters. Da Udine is in an opposite corner from Michelangelo. The other two corners have Fr. Penni and Raphael.

You could refer to the loading plot and compare it with this score plot to see that the corner with Da Udine is most associated with the colour variable, whereas the corner with Michelangelo

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is best associated with drawing. Raphael is in the corner where the variables composition and expression are predominant.

If you like to make these kinds of associations between the variables and the observations, you will enjoy using the biplot command. It provides a joint view of the variables and observations; see [MV] biplot.

1

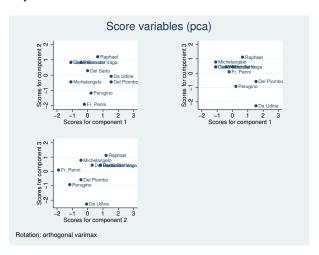
After a rotation, the rotated factor or component loading matrix is stored in e(r\_L). By default, both loadingplot and scoreplot work with the rotated loadings if they are available. The norotated option allows you to obtain the graphs for the unrotated loadings and scores.

You can also request a matrix or combined graph for all combinations of the first several components or factors with the components() option (or the alias factors()).

#### Example 3: Score plots after a rotation

Even though the results from our initial look at the principal components of the Renaissance painters seem clear enough, we continue our demonstration by showing the score plots for the first three components after a rotation. See [MV] rotate for information on rotation in general, and see [MV] pca postestimation for specific guidance and warnings concerning rotation after a PCA.

- . rotate (output omitted)
- . scoreplot, mlabel(painter) components(3) combined aspect(.8)
- > xlabel(-2(1)3) ylabel(-2(1)2)



By default, the rotation information was included as a note in the graph. We specified components (3) to obtain all paired plots between the first three components. The combined option selected the combined view instead of the default matrix view of the graphs. The aspect(), xlabel(), and ylabel() options provide reasonable use of the graphing region while providing the same scale in the horizontal and vertical directions.

1

As the number of factors() or components() increases, the graphing area for each plot gets smaller. Although the default matrix view (option matrix) may be the most natural, the combined view (option combined) displays half as many graphs. However, the combined view uses more space for the labeling of axes than the matrix view. Regardless of the choice, with many requested factors or components, the graphs become too small to be of any use. In loadingplot, the maxlength() option will trim the variable name marker labels that are automatically included. This may help reduce overlap when multiple small graphs are shown. You can go further and remove these marker labels by using the mlabel("") option.

Other examples of loadingplot and scoreplot are found in [MV] pca postestimation, [MV] factor postestimation, [MV] discrim Ida, and [MV] discrim Ida postestimation.

#### Also see

[MV] **candisc** — Canonical linear discriminant analysis

[MV] discrim lda — Linear discriminant analysis

[MV] discrim lda postestimation — Postestimation tools for discrim lda

[MV] **factor** — Factor analysis

[MV] **factor postestimation** — Postestimation tools for factor and factormat

[MV] pca — Principal component analysis

[MV] pca postestimation — Postestimation tools for pca and pcamat

[MV] screeplot — Scree plot

#### **Title**

screeplot — Scree plot

Description Quick start Menu Syntax
Options Remarks and examples Stored results References

Also see

### Description

screeplot produces a scree plot of the eigenvalues of a covariance or correlation matrix.

screeplot automatically obtains the eigenvalues after candisc, discrim lda, factor, factormat, pca, and pcamat. screeplot also works automatically to plot singular values after ca and camat, canonical correlations after canon, and eigenvalues after manova, mca, mds, mdsmat, and mdslong.

screeplot lets you obtain a scree plot in other cases by directly specifying eigvals, a vector containing the eigenvalues.

### **Quick start**

Scree plot of the eigenvalues after a command such as pca or factor screeplot

Add a horizontal line at the mean of the eigenvalues screeplot, mean

Scree plot with confidence intervals after pca screeplot, ci

#### Menu

 ${\it Statistics} > {\it Multivariate}$  analysis  $> {\it Factor}$  and principal component analysis  $> {\it Postestimation} > {\it Scree}$  plot of eigenvalues

### **Syntax**

```
screeplot [eigvals] [, options]
```

scree is a synonym for screeplot.

options	Description
Main	
<pre>neigen(#)</pre>	graph only largest # eigenvalues; default is to plot all eigenvalues
Mean	
<u>me</u> an	graph horizontal line at the mean of the eigenvalues
<pre>meanlopts(cline_options)</pre>	affect rendition of the mean line
CI	
ci[(ci_options)]	<pre>graph confidence intervals (after pca only); ci is a synonym for ci(asymptotic)</pre>
Plot	
cline_options	affect rendition of the lines connecting points
marker_options	change look of markers (color, size, etc.)
Add plots	
addplot(plot)	add other plots to the generated graph
Y axis, X axis, Titles, Legend, Overall	
twoway_options	any options other than by() documented in [G-3] twoway_options

ci_options	Description
<u>asymptotic</u>	compute asymptotic confidence intervals; the default
<u>he</u> teroskedastic	compute heteroskedastic bootstrap confidence intervals
<u>ho</u> moskedastic	compute homoskedastic bootstrap confidence intervals
area_options	affect the rendition of the confidence bands
<u>tab</u> le	produce a table of confidence intervals
<u>l</u> evel(#)	set confidence level; default is level(95)
<u>r</u> eps(#)	number of bootstrap simulations; default is reps (200)
seed(str)	random-number seed used for the bootstrap simulations

## **Options**

neigen(#) specifies the number of eigenvalues to plot. The default is to plot all eigenvalues.

mean displays a horizontal line at the mean of the eigenvalues.

meanlopts(cline\_options) affects the rendition of the mean reference line added using the mean option; see [G-3] cline\_options.

CI

- ci[(ci\_options)] displays confidence intervals for the eigenvalues. The option ci is a synonym for ci(asymptotic). The following methods for estimating confidence intervals are available:
  - ci(asymptotic) specifies the asymptotic distribution of the eigenvalues of a central Wishart distribution, the distribution of the covariance matrix of a sample from a multivariate normal distribution. The asymptotic theory applied to correlation matrices is not fully correct, probably giving confidence intervals that are somewhat too narrow.
  - ci(heteroskedastic) specifies a parametric bootstrap by using the percentile method and assuming that the eigenvalues are from a matrix that is multivariate normal with the same eigenvalues as observed.
  - ci (homoskedastic) specifies a parametric bootstrap by using the percentile method and assuming that the eigenvalues are from a matrix that is multivariate normal with all eigenvalues equal to the mean of the observed eigenvalues. For a PCA of a correlation matrix, this mean is 1.
  - ci (area\_options) affects the rendition of the confidence bands; see [G-3] area\_options.
  - ci(table) produces a table with the confidence intervals.
  - ci(level(#)) specifies the confidence level, as a percentage, for confidence intervals. The default is level(95) or as set by set level; see [U] 20.7 Specifying the width of confidence intervals.
  - ci(reps(#)) specifies the number of simulations to be performed for estimating the confidence intervals. This option is valid only when heteroskedastic or homoskedastic is specified. The default is reps(200).
  - ci(seed(str)) sets the random-number seed used for the parametric bootstrap. Setting the seed makes sure that results are reproducible. See set seed in [R] set seed. This option is valid only when heteroskedastic or homoskedastic is specified.

The confidence intervals are not adjusted for "simultaneous inference".

cline\_options affect the rendition of the lines connecting the plotted points; see [G-3] cline\_options.

marker\_options affect the rendition of markers drawn at the plotted points, including their shape, size, color, and outline; see [G-3] marker\_options.

Add plots

addplot(plot) provides a way to add other plots to the generated graph; see [G-3] addplot\_option.

Y axis, X axis, Titles, Legend, Overall

twoway\_options are any of the options documented in [G-3] twoway\_options, excluding by(). These include options for titling the graph (see [G-3] title\_options) and for saving the graph to disk (see [G-3] saving\_option).

### Remarks and examples

Cattell (1966) introduced scree plots, which are visual tools used to help determine the number of important components or factors in multivariate settings, such as principal component analysis and factor analysis; see [MV] **pca** and [MV] **factor**. The scree plot is examined for a natural break between the large eigenvalues and the remaining small eigenvalues. The word "scree" is used in reference to the appearance of the large eigenvalues as the hill and the small eigenvalues as the debris

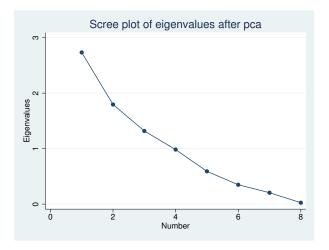
of loose rocks at the bottom of the hill. Examples of scree plots can be found in most books that discuss principal component analysis or factor analysis, including Rabe-Hesketh and Everitt (2007), Hamilton (1992, 249–288), Rencher and Christensen (2012), and Hamilton (2013, chap. 11).

#### Example 1: Scree plots after principal component analysis

Multivariate commands, such as pca and factor (see [MV] pca and [MV] factor), produce eigenvalues and eigenvectors. The screeplot command graphs the eigenvalues, so you can decide how many components or factors to retain.

We demonstrate scree plots after a principal component analysis. Say that we have been hired by the restaurant industry to study expenditures on eating and drinking. We have data on 898 U.S. cities:

- . use http://www.stata-press.com/data/r14/emd
  (1980 City Data)
- . pca ln\_eat hhsize
   (output omitted)
- . screeplot

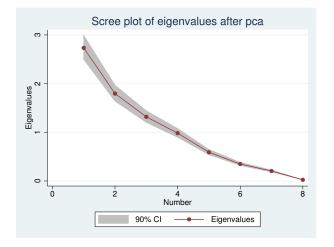


This scree plot does not suggest a natural break between high and low eigenvalues.

We render this same scree plot with the addition of confidence bands by using the ci() option. The asymptotic suboption selects confidence intervals that are based on the assumption of asymptotic normality. Because the asymptotic theory applied to correlation matrices is not fully correct, we also use the level() suboption to adjust the confidence interval. The table suboption displays a table of the eigenvalues and lower and upper confidence interval values.

. scree, ci(asympt level(90) table) (caution is advised in interpreting an asymptotic theory-based confidence interval of eigenvalues of a correlation matrix)

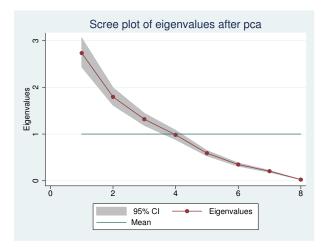
	eigval	low	high
Comp1 Comp2 Comp3 Comp4 Comp5 Comp6	2.733531 1.795623 1.318192 .9829996 .5907632 .3486276 .2052582	2.497578 1.640628 1.204408 .8981487 .5397695 .3185346 .1875407	2.991777 1.965261 1.442725 1.075867 .6465744 .3815635 .2246496
Comp8	.0250056	.0228472	.027368



screeplot warned us about using asymptotic confidence intervals with eigenvalues based on a correlation matrix. screeplot knew that the eigenvalues were based on a correlation matrix instead of a covariance matrix by examining the information available in the e() results from the pca that we ran.

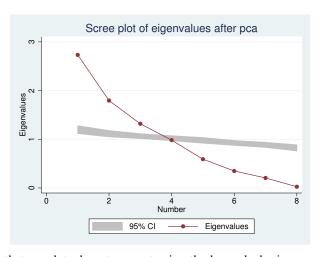
Instead of displaying an asymptotic confidence band, we now display a parametric bootstrap confidence interval. We select the heteroskedastic suboption of ci() that allows for unequal eigenvalues. The reps() and seed() suboptions control the execution of the bootstrap. The mean option provides a horizontal line at the mean of the eigenvalues, here at 1 because we are dealing with a principal component analysis performed on a correlation matrix.

. scree, ci(hetero reps(1000) seed(18228)) mean



Our final scree plot switches to computing the bootstrap confidence intervals on the basis of the assumption that the eigenvalues are equal to the mean of the observed eigenvalues (using the homoskedastic suboption of ci()). We again set the seed by using the seed() suboption.

. scree, ci(homo seed(56227))



The graph indicates that our data do not support using the homoskedastic assumption.

r(eigvals)

#### Stored results

```
screeplot stores the following in r():
```

Scalars
r(level) confidence level for confidence intervals

Macros
r(Ctype) correlation or covariance
r(ci) method for estimating confidence interval
r(rngstate) random-number state used for parametric bootstrap

Matrices
r(ci) confidence intervals

eigenvalues

Scree is an English word with Old Norse origins. In geomorphology, scree denotes an accumulation of loose, coarse, usually angular debris at the foot of steep rock slopes (Luckman 2004). The accumulation must be sufficiently thick to be independent of the underlying slope; thus thin veneers of rock particles do not qualify. Screes are themselves quite steep; angles between  $30^{\circ}$  and  $40^{\circ}$  are common.

Outside geomorphology, and, notably, in some discussions of scree plots, the term is commonly misapplied to imply deposits on much gentler slopes, or those gentler slopes themselves, and by extension parts of curves thought similar to either.

However appropriate in general or in particular, the term *scree plot* is so widely used in multivariate statistics that it is echoed in the name of this Stata command.

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Rabe-Hesketh, S., and B. S. Everitt. 2007. A Handbook of Statistical Analyses Using Stata. 4th ed. Boca Raton, FL: Chapman & Hall/CRC.

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### Also see

```
    [MV] factor — Factor analysis
    [MV] mds — Multidimensional scaling for two-way data
    [MV] pca — Principal component analysis
```

# **Glossary**

agglomerative hierarchical clustering methods. Agglomerative hierarchical clustering methods are bottom-up methods for hierarchical clustering. Each observation begins in a separate group. The closest pair of groups is agglomerated or merged in each iteration until all the data are in one cluster. This process creates a hierarchy of clusters. Contrast to divisive hierarchical clustering methods.

anti-image correlation matrix or anti-image covariance matrix. The image of a variable is defined as that part which is predictable by regressing each variable on all the other variables; hence, the anti-image is the part of the variable that cannot be predicted. The anti-image correlation matrix **A** is a matrix of the negatives of the partial correlations among variables. Partial correlations represent the degree to which the factors explain each other in the results. The diagonal of the anti-image correlation matrix is the Kaiser–Meyer–Olkin measure of sampling adequacy for the individual variables. Variables with small values should be eliminated from the analysis. The anti-image covariance matrix **C** contains the negatives of the partial covariances and has one minus the squared multiple correlations in the principal diagonal. Most of the off-diagonal elements should be small in both anti-image matrices in a good factor model. Both anti-image matrices can be calculated from the inverse of the correlation matrix **R** via

$$\begin{split} \mathbf{A} &= \{ \text{diag}(\mathbf{R}) \}^{-1} \mathbf{R} \{ \text{diag}(\mathbf{R}) \}^{-1} \\ \mathbf{C} &= \{ \text{diag}(\mathbf{R}) \}^{-1/2} \mathbf{R} \{ \text{diag}(\mathbf{R}) \}^{-1/2} \end{split}$$

Also see Kaiser-Meyer-Olkin measure of sampling adequacy.

**average-linkage clustering**. Average-linkage clustering is a hierarchical clustering method that uses the average proximity of observations between groups as the proximity measure between the two groups.

**Bayes's theorem**. Bayes's theorem states that the probability of an event, A, conditional on another event, B, is generally different from the probability of B conditional on A, although the two are related. Bayes's theorem is that

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

where P(A) is the marginal probability of A, and P(A|B) is the conditional probability of A given B, and likewise for P(B) and P(B|A).

**Bentler's invariant pattern simplicity rotation**. Bentler's (1977) rotation maximizes the invariant pattern simplicity. It is an oblique rotation that minimizes the criterion function

$$c(\mathbf{\Lambda}) = -\log[|(\mathbf{\Lambda}^2)'\mathbf{\Lambda}^2|] + \log[|\operatorname{diag}\{(\mathbf{\Lambda}^2)'\mathbf{\Lambda}^2\}|]$$

See Crawford–Ferguson rotation for a definition of  $\Lambda$ . Also see oblique rotation.

between matrix and within matrix. The between and within matrices are SSCP matrices that measure the spread between groups and within groups, respectively. These matrices are used in multivariate analysis of variance and related hypothesis tests: Wilks's lambda, Roy's largest root, Lawley—Hotelling trace, and Pillai's trace.

Here we have k independent random samples of size n. The between matrix  $\mathbf{H}$  is given by

$$\mathbf{H} = n \sum_{i=1}^{k} (\overline{\mathbf{y}}_{i\bullet} - \overline{\mathbf{y}}_{\bullet\bullet}) (\overline{\mathbf{y}}_{i\bullet} - \overline{\mathbf{y}}_{\bullet\bullet})' = \sum_{i=1}^{k} \frac{1}{n} \mathbf{y}_{i\bullet} \mathbf{y}'_{i\bullet} - \frac{1}{kn} \mathbf{y}_{\bullet\bullet} \mathbf{y}'_{\bullet\bullet}$$

The within matrix E is defined as

$$\mathbf{E} = \sum_{i=1}^{k} \sum_{j=1}^{n} (\mathbf{y}_{ij} - \overline{\mathbf{y}}_{i\bullet}) (\mathbf{y}_{ij} - \mathbf{y}_{i\bullet})' = \sum_{i=1}^{k} \sum_{j=1}^{n} \mathbf{y}_{ij} \mathbf{y}'_{ij} - \sum_{i=1}^{k} \frac{1}{n} \mathbf{y}_{i\bullet} \mathbf{y}'_{i\bullet}$$

Also see SSCP matrix.

**biplot**. A biplot is a scatterplot which represents both observations and variables simultaneously. There are many different biplots; variables in biplots are usually represented by arrows and observations are usually represented by points.

biquartimax rotation or biquartimin rotation. Biquartimax rotation and biquartimin rotation are synonyms. They put equal weight on the varimax and quartimax criteria, simplifying the columns and rows of the matrix. This is an oblique rotation equivalent to an oblimin rotation with  $\gamma=0.5$ . Also see varimax rotation, quartimax rotation, and oblimin rotation.

boundary solution or Heywood solution. See Heywood case.

**CA**. See correspondence analysis.

canonical correlation analysis. Canonical correlation analysis attempts to describe the relationships between two sets of variables by finding linear combinations of each so that the correlation between the linear combinations is maximized.

**canonical discriminant analysis**. Canonical linear discriminant analysis is LDA where describing how groups are separated is of primary interest. Also see *linear discriminant analysis*.

**canonical loadings**. The canonical loadings are coefficients of canonical linear discriminant functions. Also see *canonical discriminant analysis* and *loading*.

canonical variate set. The canonical variate set is a linear combination or weighted sum of variables obtained from canonical correlation analysis. Two sets of variables are analyzed in canonical correlation analysis. The first canonical variate of the first variable set is the linear combination in standardized form that has maximal correlation with the first canonical variate from the second variable set. The subsequent canonical variates are uncorrelated to the previous and have maximal correlation under that constraint.

**centered data**. Centered data has zero mean. You can center data x by taking  $x - \overline{x}$ .

**centroid-linkage clustering**. Centroid-linkage clustering is a hierarchical clustering method that computes the proximity between two groups as the proximity between the group means.

**classical scaling**. Classical scaling is a method of performing MDS via an eigen decomposition. This is contrasted to modern MDS, which is achieved via the minimization of a loss function. Also see *multidimensional scaling* and *modern scaling*.

**classification**. Classification is the act of allocating or classifying observations to groups as part of discriminant analysis. In some sources, classification is synonymous with cluster analysis.

**classification function**. Classification functions can be obtained after LDA or QDA. They are functions based on Mahalanobis distance for classifying observations to the groups. See *discriminant function* for an alternative. Also see *linear discriminant analysis* and *quadratic discriminant analysis*.

classification table. A classification table, also known as a confusion matrix, gives the count of observations from each group that are classified into each of the groups as part of a discriminant analysis. The element at (i,j) gives the number of observations that belong to the ith group but were classified into the jth group. High counts are expected on the diagonal of the table where observations are correctly classified, and small values are expected off the diagonal. The columns of the matrix are categories of the predicted classification; the rows represent the actual group membership.

**cluster analysis**. Cluster analysis is a method for determining natural groupings or clusters of observations.

cluster tree. See dendrogram.

clustering. See cluster analysis.

**common factors**. Common factors are found by factor analysis. They linearly reconstruct the original variables. In factor analysis, reconstruction is defined in terms of prediction of the correlation matrix of the original variables.

**communality**. Communality is the proportion of a variable's variance explained by the common factors in factor analysis. It is also "1 – uniqueness". Also see *uniqueness*.

**complete-linkage clustering**. Complete-linkage clustering is a hierarchical clustering method that uses the farthest pair of observations between two groups to determine the proximity of the two groups.

**component scores**. Component scores are calculated after PCA. Component scores are the coordinates of the original variables in the space of principal components.

**Comrey's tandem 1 and 2 rotations**. Comrey (1967) describes two rotations, the first (tandem 1) to judge which "small" factors should be dropped, the second (tandem 2) for "polishing".

Tandem principle 1 minimizes the criterion

$$c(\mathbf{\Lambda}) = \left\langle \mathbf{\Lambda}^2, (\mathbf{\Lambda}\mathbf{\Lambda}')^2 \mathbf{\Lambda}^2 \right\rangle$$

Tandem principle 2 minimizes the criterion

$$c(\mathbf{\Lambda}) = \langle \mathbf{\Lambda}^2, \{ \mathbf{1}\mathbf{1}' - (\mathbf{\Lambda}\mathbf{\Lambda}')^2 \} \mathbf{\Lambda}^2 \rangle$$

See Crawford-Ferguson rotation for a definition of  $\Lambda$ .

**configuration**. The configuration in MDS is a representation in a low-dimensional (usually 2-dimensional) space with distances in the low-dimensional space approximating the dissimilarities or disparities in high-dimensional space. Also see *multidimensional scaling*, *dissimilarity*, and *disparity*.

**configuration plot.** A configuration plot after MDS is a (usually 2-dimensional) plot of labeled points showing the low-dimensional approximation to the dissimilarities or disparities in high-dimensional space. Also see *multidimensional scaling*, *dissimilarity*, and *disparity*.

**confusion matrix**. A confusion matrix is a synonym for a classification table after discriminant analysis. See *classification table*.

contrast or contrasts. In ANOVA, a contrast in k population means is defined as a linear combination

$$\delta = c_1 \mu_1 + c_2 \mu_2 + \dots + c_k \mu_k$$

where the coefficients satisfy

$$\sum_{i=1}^{k} c_i = 0$$

In the multivariate setting (MANOVA), a contrast in k population mean vectors is defined as

$$\boldsymbol{\delta} = c_1 \boldsymbol{\mu}_1 + c_2 \boldsymbol{\mu}_2 + \cdots c_k \boldsymbol{\mu}_k$$

where the coefficients again satisfy

$$\sum_{i=1}^{k} c_i = 0$$

The univariate hypothesis  $\delta=0$  may be tested with contrast (or test) after ANOVA. The multivariate hypothesis  $\delta=0$  may be tested with manovatest after MANOVA.

**correspondence analysis.** Correspondence analysis (CA) gives a geometric representation of the rows and columns of a two-way frequency table. The geometric representation is helpful in understanding the similarities between the categories of variables and associations between variables. CA is calculated by singular value decomposition. Also see *singular value decomposition*.

correspondence analysis projection. A correspondence analysis projection is a line plot of the row and column coordinates after CA. The goal of this graph is to show the ordering of row and column categories on each principal dimension of the analysis. Each principal dimension is represented by a vertical line; markers are plotted on the lines where the row and column categories project onto the dimensions. Also see *correspondence analysis*.

costs. Costs in discriminant analysis are the cost of misclassifying observations.

**covarimin rotation**. Covarimin rotation is an orthogonal rotation equivalent to varimax. Also see *varimax rotation*.

**Crawford–Ferguson rotation**. Crawford–Ferguson (1970) rotation is a general oblique rotation with several interesting special cases.

Special cases of the Crawford-Ferguson rotation include

$\kappa$	Special case
$ \begin{array}{c} 0 \\ 1/p \\ f/(2p) \\ (f-1)/(p+f-2) \\ 1 \end{array} $	quartimax / quartimin varimax / covarimin equamax parsimax factor parsimony
p = number of rows of f = number of column	

Where A is the matrix to be rotated, T is the rotation and  $\Lambda = AT$ . The Crawford-Ferguson rotation is achieved by minimizing the criterion

$$c(\pmb{\Lambda}) = \frac{1-\kappa}{4} \left\langle \pmb{\Lambda}^2, \pmb{\Lambda}^2 (\pmb{1} \pmb{1}' - \mathbf{I}) \right\rangle + \frac{\kappa}{4} \left\langle \pmb{\Lambda}^2, (\pmb{1} \pmb{1}' - \mathbf{I}) \pmb{\Lambda}^2 \right\rangle$$

Also see oblique rotation.

- crossed variables or stacked variables. In CA and MCA crossed categorical variables may be formed from the interactions of two or more existing categorical variables. Variables that contain these interactions are called crossed or stacked variables.
- crossing variables or stacking variables. In CA and MCA, crossing or stacking variables are the existing categorical variables whose interactions make up a crossed or stacked variable.
- curse of dimensionality. The curse of dimensionality is a term coined by Richard Bellman (1961) to describe the problem caused by the exponential increase in size associated with adding extra dimensions to a mathematical space. On the unit interval, 10 evenly spaced points suffice to sample with no more distance than 0.1 between them; however a unit square requires 100 points, and a unit cube requires 1000 points. Many multivariate statistical procedures suffer from the curse of dimensionality. Adding variables to an analysis without adding sufficient observations can lead to imprecision.
- dendrogram or cluster tree. A dendrogram or cluster tree graphically presents information about how observations are grouped together at various levels of (dis)similarity in hierarchical cluster analysis. At the bottom of the dendrogram, each observation is considered its own cluster. Vertical lines extend up for each observation, and at various (dis)similarity values, these lines are connected to the lines from other observations with a horizontal line. The observations continue to combine until, at the top of the dendrogram, all observations are grouped together. Also see hierarchical clustering.
- dilation. A dilation stretches or shrinks distances in Procrustes rotation.
- dimension. A dimension is a parameter or measurement required to define a characteristic of an object or observation. Dimensions are the variables in the dataset. Weight, height, age, blood pressure, and drug dose are examples of dimensions in health data. Number of employees, gross income, net income, tax, and year are examples of dimensions in data about companies.
- discriminant analysis. Discriminant analysis is used to describe the differences between groups and to exploit those differences when allocating (classifying) observations of unknown group membership. Discriminant analysis is also called classification in many references.
- discriminant function. Discriminant functions are formed from the eigenvectors from Fisher's approach to LDA. See linear discriminant analysis. See classification function for an alternative.
- discriminating variables. Discriminating variables in a discriminant analysis are analyzed to determine differences between groups where group membership is known. These differences between groups are then exploited when classifying observations to the groups.
- **disparity**. Disparities are transformed dissimilarities, that is, dissimilarity values transformed by some function. The class of functions to transform dissimilarities to disparities may either be 1) a class of metric, or known functions such as linear functions or power functions that can be parameterized by real scalars or 2) a class of more general (nonmetric) functions, such as any monotonic function. Disparities are used in MDS. Also see dissimilarity, multidimensional scaling, metric scaling, and nonmetric scaling.
- dissimilarity, dissimilarity matrix, and dissimilarity measure. Dissimilarity or a dissimilarity measure is a quantification of the difference between two things, such as observations or variables or groups of observations or a method for quantifying that difference. A dissimilarity matrix is a matrix containing dissimilarity measurements. Euclidean distance is one example of a dissimilarity measure. Contrast to similarity. Also see proximity and Euclidean distance.
- divisive hierarchical clustering methods. Divisive hierarchical clustering methods are top-down methods for hierarchical clustering. All the data begin as a part of one large cluster; with each iteration, a cluster is broken into two to create two new clusters. At the first iteration there are two

clusters, then three, and so on. Divisive methods are very computationally expensive. Contrast to agglomerative hierarchical clustering methods.

**eigenvalue**. An eigenvalue is the scale factor by which an eigenvector is multiplied. For many multivariate techniques, the size of an eigenvalue indicates the importance of the corresponding eigenvector. Also see *eigenvector*.

**eigenvector**. An eigenvector of a linear transformation is a nonzero vector that is either left unaffected or simply multiplied by a scale factor after the transformation.

Here x is an eigenvector of linear transformation A with eigenvalue  $\lambda$ :

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

For many multivariate techniques, eigenvectors form the basis for analysis and interpretation. Also see *loading*.

equamax rotation. Equamax rotation is an orthogonal rotation whose criterion is a weighted sum of the varimax and quartimax criteria. Equamax reflects a concern for simple structure within the rows and columns of the matrix. It is equivalent to oblimin with  $\gamma = p/2$ , or to the Crawford-Ferguson family with  $\kappa = f/2p$ , where p is the number of rows of the matrix to be rotated, and f is the number of columns. Also see orthogonal rotation, varimax rotation, quartimax rotation, oblimin rotation, and Crawford-Ferguson rotation.

**Euclidean distance**. The Euclidean distance between two observations is the distance one would measure with a ruler. The distance between vector  $\mathbf{P} = (P_1, P_2, \dots, P_n)$  and  $\mathbf{Q} = (Q_1, Q_2, \dots, Q_n)$  is given by

$$D(\mathbf{P}, \mathbf{Q}) = \sqrt{(P_1 - Q_1)^2 + (P_2 - Q_2)^2 + \dots + (P_n - Q_n)^2} = \sqrt{\sum_{i=1}^n (P_i - Q_i)^2}$$

**factor**. A factor is an unobserved random variable that is thought to explain variability among observed random variables.

**factor analysis**. Factor analysis is a statistical technique used to explain variability among observed random variables in terms of fewer unobserved random variables called factors. The observed variables are then linear combinations of the factors plus error terms.

If the correlation matrix of the observed variables is  ${\bf R}$ , then  ${\bf R}$  is decomposed by factor analysis as

$$\mathbf{R} = \mathbf{\Lambda} \mathbf{\Phi} \mathbf{\Lambda}' + \mathbf{\Psi}$$

 $\Lambda$  is the loading matrix, and  $\Psi$  contains the specific variances, for example, the variance specific to the variable not explained by the factors. The default unrotated form assumes uncorrelated common factors,  $\Phi = I$ .

factor loading plot. A factor loading plot produces a scatter plot of the factor loadings after factor analysis.

**factor loadings**. Factor loadings are the regression coefficients which multiply the factors to produce the observed variables in the factor analysis.

**factor parsimony**. Factor parsimony is an oblique rotation, which maximizes the column simplicity of the matrix. It is equivalent to a Crawford–Ferguson rotation with  $\kappa=1$ . Also see *oblique rotation* and *Crawford–Ferguson rotation*.

factor scores. Factor scores are computed after factor analysis. Factor scores are the coordinates of the original variables, x, in the space of the factors. The two types of scoring are regression scoring (Thomson 1951) and Bartlett (1937, 1938) scoring.

Using the symbols defined in *factor analysis*, the formula for regression scoring is

$$\hat{\mathbf{f}} = \mathbf{\Lambda}' \mathbf{R}^{-1} \mathbf{x}$$

In the case of oblique rotation the formula becomes

$$\widehat{\mathbf{f}} = \mathbf{\Phi} \mathbf{\Lambda}' \mathbf{R}^{-1} \mathbf{x}$$

The formula for Bartlett scoring is

$$\widehat{\mathbf{f}} = \mathbf{\Gamma}^{-1} \mathbf{\Lambda}' \mathbf{\Psi}^{-1} \mathbf{x}$$

where

$$\Gamma = \mathbf{\Lambda}' \mathbf{\Psi}^{-1} \mathbf{\Lambda}$$

Also see factor analysis.

**Heywood case** or **Heywood solution**. A Heywood case can appear in factor analysis output; this indicates that a boundary solution, called a Heywood solution, was produced. The geometric assumptions underlying the likelihood-ratio test are violated, though the test may be useful if interpreted cautiously.

hierarchical clustering and hierarchical clustering methods. In hierarchical clustering, the data is placed into clusters via iterative steps. Contrast to partition clustering. Also see agglomerative hierarchical clustering methods and divisive hierarchical clustering methods.

**Hotelling's T-squared generalized means test.** Hotelling's T-squared generalized means test is a multivariate test that reduces to a standard t test if only one variable is specified. It tests whether one set of means is zero or if two sets of means are equal.

inertia. In CA, the inertia is related to the definition in applied mathematics of "moment of inertia", which is the integral of the mass times the squared distance to the centroid. Inertia is defined as the total Pearson chi-squared for the two-way table divided by the total number of observations, or the sum of the squared singular values found in the singular value decomposition.

total inertia = 
$$\frac{1}{n}\chi^2 = \sum_k \lambda_k^2$$

In MCA, the inertia is defined analogously. In the case of the indicator or Burt matrix approach, it is given by the formula

total inertia = 
$$\left(\frac{q}{q-1}\right)\sum\phi_t^2 - \frac{(J-q)}{q^2}$$

where q is the number of active variables, J is the number of categories and  $\phi_t$  is the tth (unadjusted) eigenvalue of the eigen decomposition. In JCA the total inertia of the modified Burt matrix is defined as the sum of the inertias of the off-diagonal blocks. Also see correspondence analysis and multiple correspondence analysis.

iterated principal-factor method. The iterated principal-factor method is a method for performing factor analysis in which the communalities  $\hat{h}_i^2$  are estimated iteratively from the loadings in  $\widehat{\Lambda}$  using

$$\widehat{h}_i^2 = \sum_{j=1}^m \widehat{\lambda}_{ij}^2$$

Also see factor analysis and communality.

JCA. An acronym for joint correspondence analysis; see multiple correspondence analysis.

joint correspondence analysis. See multiple correspondence analysis.

**Kaiser–Meyer–Olkin measure of sampling adequacy**. The Kaiser–Meyer–Olkin (KMO) measure of sampling adequacy takes values between 0 and 1, with small values meaning that the variables have too little in common to warrant a factor analysis or PCA. Historically, the following labels have been given to values of KMO (Kaiser 1974):

0.00 to 0.49	unacceptable
0.50 to 0.59	miserable
0.60 to 0.69	mediocre
0.70 to 0.79	middling
0.80 to 0.89	meritorious
0.90 to 1.00	marvelous

**kmeans**. Kmeans is a method for performing partition cluster analysis. The user specifies the number of clusters, k, to create using an iterative process. Each observation is assigned to the group whose mean is closest, and then based on that categorization, new group means are determined. These steps continue until no observations change groups. The algorithm begins with k seed values, which act as the k group means. There are many ways to specify the beginning seed values. Also see *partition clustering*.

**kmedians**. Kmedians is a variation of kmeans. The same process is performed, except that medians instead of means are computed to represent the group centers at each step. Also see *kmeans* and *partition clustering*.

KMO. See Kaiser-Meyer-Olkin measure of sampling adequacy.

KNN. See kth nearest neighbor.

**Kruskal stress**. The Kruskal stress measure (Kruskal 1964; Cox and Cox 2001, 63) used in MDS is given by

Kruskal
$$(\widehat{\mathbf{D}}, \mathbf{E}) = \left\{ \frac{\sum (E_{ij} - \widehat{D}_{ij})^2}{\sum E_{ij}^2} \right\}^{1/2}$$

where  $D_{ij}$  is the dissimilarity between objects i and j,  $1 \le i, j \le n$ , and  $\widehat{D}_{ij}$  is the disparity, that is, the transformed dissimilarity, and  $E_{ij}$  is the Euclidean distance between rows i and j of the matching configuration. Kruskal stress is an example of a loss function in modern MDS. After classical MDS, estat stress gives the Kruskal stress. Also see classical scaling, multidimensional scaling, and stress.

**kth nearest neighbor**. kth-nearest-neighbor (KNN) discriminant analysis is a nonparametric discrimination method based on the k nearest neighbors of each observation. Both continuous and binary data can be handled through the different similarity and dissimilarity measures. KNN analysis can distinguish irregular-shaped groups, including groups with multiple modes. Also see discriminant analysis and nonparametric methods.

**Lawley-Hotelling trace**. The Lawley-Hotelling trace is a test statistic for the hypothesis test  $H_0$ :  $\mu_1 = \mu_2 = \cdots = \mu_k$  based on the eigenvalues  $\lambda_1, \lambda_2, \ldots, \lambda_s$  of  $\mathbf{E^{-1}H}$ . It is defined as

$$U^{(s)} = \operatorname{trace}(\mathbf{E}^{-1}\mathbf{H}) = \sum_{i=1}^{s} \lambda_i$$

where **H** is the between matrix and **E** is the within matrix, see between matrix.

LDA. See linear discriminant analysis.

**leave one out**. In discriminant analysis, classification of an observation while leaving it out of the estimation sample is done to check the robustness of the analysis; thus the phrase "leave one out" (LOO). Also see *discriminant analysis*.

**linear discriminant analysis.** Linear discriminant analysis (LDA) is a parametric form of discriminant analysis. In Fisher's (1936) approach to LDA, linear combinations of the discriminating variables provide maximal separation between the groups. The Mahalanobis (1936) formulation of LDA assumes that the observations come from multivariate normal distributions with equal covariance matrices. Also see *discriminant analysis* and *parametric methods*.

linkage. In cluster analysis, the linkage refers to the measure of proximity between groups or clusters.

**loading**. A loading is a coefficient or weight in a linear transformation. Loadings play an important role in many multivariate techniques, including factor analysis, PCA, MANOVA, LDA, and canonical correlations. In some settings, the loadings are of primary interest and are examined for interpretability. For many multivariate techniques, loadings are based on an eigenanalysis of a correlation or covariance matrix. Also see *eigenvector*.

loading plot. A loading plot is a scatter plot of the loadings after LDA, factor analysis or PCA.

**logistic discriminant analysis.** Logistic discriminant analysis is a form of discriminant analysis based on the assumption that the likelihood ratios of the groups have an exponential form. Multinomial logistic regression provides the basis for logistic discriminant analysis. Because multinomial logistic regression can handle binary and continuous regressors, logistic discriminant analysis is also appropriate for binary and continuous discriminating variables. Also see *discriminant analysis*.

LOO. See leave one out.

**loss**. Modern MDS is performed by minimizing a loss function, also called a loss criterion. The loss quantifies the difference between the disparities and the Euclidean distances.

Loss functions include Kruskal's stress and its square, both normalized with either disparities or distances, the strain criterion which is equivalent to classical metric scaling when the disparities equal the dissimilarities, and the Sammon (1969) mapping criterion which is the sum of the scaled, squared differences between the distances and the disparities, normalized by the sum of the disparities.

Also see multidimensional scaling, Kruskal stress, classical scaling, and disparity.

**Mahalanobis distance**. The Mahalanobis distance measure is a scale-invariant way of measuring distance. It takes into account the correlations of the dataset.

**Mahalanobis transformation**. The Mahalanobis transformation takes a Cholesky factorization of the inverse of the covariance matrix  $S^{-1}$  in the formula for Mahalanobis distance and uses it to transform the data. If we have the Cholesky factorization  $S^{-1} = \mathbf{L}'\mathbf{L}$ , then the Mahalanobis transformation of  $\mathbf{x}$  is  $\mathbf{z} = \mathbf{L}\mathbf{x}$ , and  $\mathbf{z}'\mathbf{z} = D_M^2(\mathbf{x})$ .

MANCOVA. MANCOVA is multivariate analysis of covariance. See multivariate analysis of variance.

MANOVA. multivariate analysis of variance.

mass. In CA and MCA, the mass is the marginal probability. The sum of the mass over the active row or column categories equals 1.

**matching coefficient.** The matching similarity coefficient is used to compare two binary variables. If a is the number of observations that both have value 1, and d is the number of observations that both have value 0, and b, c are the number of (1,0) and (0,1) observations, respectively, then the matching coefficient is given by

$$\frac{a+d}{a+b+c+d}$$

Also see similarity measure.

**matching configuration**. In MDS, the matching configuration is the low dimensional configuration whose distances approximate the high-dimensional dissimilarities or disparities. Also see *multidimensional scaling*, *dissimilarity*, and *disparity*.

matching configuration plot. After MDS, this is a scatter plot of the matching configuration.

**maximum likelihood factor method**. The maximum likelihood factor method is a method for performing factor analysis that assumes multivariate normal observations. It maximizes the determinant of the partial correlation matrix; thus, this solution is also meaningful as a descriptive method for nonnormal data. Also see *factor analysis*.

MCA. See multiple correspondence analysis.

MDS. See multidimensional scaling.

MDS configuration plot. See configuration plot.

**measure**. A measure is a quantity representing the proximity between objects or method for determining the proximity between objects. Also see *proximity*.

**median-linkage clustering**. Median-linkage clustering is a hierarchical clustering method that uses the distance between the medians of two groups to determine the similarity or dissimilarity of the two groups. Also see *cluster analysis* and *agglomerative hierarchical clustering methods*.

**metric scaling.** Metric scaling is a type of MDS, in which the dissimilarities are transformed to disparities via a class of known functions. This is contrasted to *nonmetric scaling*. Also see *multidimensional scaling*.

**minimum entropy rotation**. The minimum entropy rotation is an orthogonal rotation achieved by minimizing the deviation from uniformity (entropy). The minimum entropy criterion (Jennrich 2004) is

$$c(\mathbf{\Lambda}) = -\frac{1}{2} \left\langle \mathbf{\Lambda}^2, \log \mathbf{\Lambda}^2 \right\rangle$$

See Crawford–Ferguson rotation for a definition of  $\Lambda$ . Also see orthogonal rotation.

**misclassification rate**. The misclassification rate calculated after discriminant analysis is, in its simplest form, the fraction of observations incorrectly classified. See *discriminant analysis*.

**modern scaling**. Modern scaling is a form of MDS that is achieved via the minimization of a loss function that compares the disparities (transformed dissimilarities) in the higher-dimensional space and the distances in the lower-dimensional space. Contrast to *classical scaling*. Also see *dissimilarity*, *disparity*, *multidimensional scaling*, and *loss*.

multidimensional scaling. Multidimensional scaling (MDS) is a dimension-reduction and visualization technique. Dissimilarities (for instance, Euclidean distances) between observations in a high-dimensional space are represented in a lower-dimensional space which is typically two dimensions

so that the Euclidean distance in the lower-dimensional space approximates in some sense the dissimilarities in the higher-dimensional space. Often the higher-dimensional dissimilarities are first transformed to disparities, and the disparities are then approximated by the distances in the lower-dimensional space. Also see *dissimilarity*, *disparity*, *classical scaling*, *loss*, *modern scaling*, *metric scaling*, and *nonmetric scaling*.

multiple correspondence analysis. Multiple correspondence analysis (MCA) and joint correspondence analysis (JCA) are methods for analyzing observations on categorical variables. MCA and JCA analyze a multiway table and are usually viewed as an extension of CA. Also see *correspondence* analysis.

multivariate analysis of covariance. See multivariate analysis of variance.

multivariate analysis of variance. Multivariate analysis of variance (MANOVA) is used to test hypotheses about means. Four multivariate statistics are commonly computed in MANOVA: Wilks's lambda, Pillai's trace, Lawley–Hotelling trace, and Roy's largest root. Also see Wilks's lambda, Pillai's trace, Lawley–Hotelling trace, and Roy's largest root.

multivariate regression. Multivariate regression is a method of estimating a linear (matrix) model

$$Y = XB + \Xi$$

Multivariate regression is estimated by least-squares regression, and it can be used to test hypotheses, much like MANOVA.

nearest neighbor. See kth nearest neighbor.

nonmetric scaling. Nonmetric scaling is a type of modern MDS in which the dissimilarities may be transformed to disparities via any monotonic function as opposed to a class of known functions. Contrast to metric scaling. Also see multidimensional scaling, dissimilarity, disparity, and modern scaling.

**nonparametric methods**. Nonparametric statistical methods, such as KNN discriminant analysis, do not assume the population fits any parameterized distribution.

**normalization**. Normalization presents information in a standard form for interpretation. In CA the row and column coordinates can be normalized in different ways depending on how one wishes to interpret the data. Normalization is also used in rotation, MDS, and MCA.

**oblimax rotation**. Oblimax rotation is a method for oblique rotation which maximizes the number of high and low loadings. When restricted to orthogonal rotation, oblimax is equivalent to quartimax rotation. Oblimax minimizes the oblimax criterion

$$c(\mathbf{\Lambda}) = -\log(\langle \mathbf{\Lambda}^2, \mathbf{\Lambda}^2 \rangle) + 2\log(\langle \mathbf{\Lambda}, \mathbf{\Lambda} \rangle)$$

See Crawford–Ferguson rotation for a definition of  $\Lambda$ . Also see oblique rotation, orthogonal rotation, and quartimax rotation.

**oblimin rotation**. Oblimin rotation is a general method for oblique rotation, achieved by minimizing the oblimin criterion

$$c(\mathbf{\Lambda}) = \frac{1}{4} \langle \mathbf{\Lambda}^2, \{ \mathbf{I} - (\gamma/p) \mathbf{1} \mathbf{1}' \} \mathbf{\Lambda}^2 (\mathbf{1} \mathbf{1}' - \mathbf{I}) \rangle$$

Oblimin has several interesting special cases:

$\gamma$	Special case			
0	quartimax / quartimin			
1/2	biquartimax / biquartimin			
1	varimax / covarimin			
p/2	equamax			
$p = \text{number of rows of } \mathbf{A}.$				

See Crawford-Ferguson rotation for a definition of  $\Lambda$  and  $\Lambda$ . Also see oblique rotation.

**oblique rotation** or **oblique transformation**. An oblique rotation maintains the norms of the rows of the matrix but not their inner products. In geometric terms, this maintains the lengths of vectors, but not the angles between them. In contrast, in orthogonal rotation, both are preserved.

**ordination**. Ordination is the ordering of a set of data points with respect to one or more axes. MDS is a form of ordination.

**orthogonal rotation** or **orthogonal transformation**. Orthogonal rotation maintains both the norms of the rows of the matrix and also inner products of the rows of the matrix. In geometric terms, this maintains both the lengths of vectors and the angles between them. In contrast, oblique rotation maintains only the norms, that is, the lengths of vectors.

**parametric methods**. Parametric statistical methods, such as LDA and QDA, assume the population fits a parameterized distribution. For example, for LDA we assume the groups are multivariate normal with equal covariance matrices.

**parsimax rotation**. Parsimax rotation is an orthogonal rotation that balances complexity between the rows and the columns. It is equivalent to the Crawford–Ferguson family with  $\kappa = (f-1)/(p+f-2)$ , where p is the number of rows of the original matrix, and f is the number of columns. See *orthogonal rotation* and *Crawford–Ferguson rotation*.

partially specified target rotation. Partially specified target rotation minimizes the criterion

$$c(\mathbf{\Lambda}) = \|\mathbf{W} \otimes (\mathbf{\Lambda} - \mathbf{H})\|^2$$

for a given target matrix  $\mathbf{H}$  and a nonnegative weighting matrix  $\mathbf{W}$  (usually zero-one valued). See *Crawford-Ferguson rotation* for a definition of  $\boldsymbol{\Lambda}$ .

partition clustering and partition cluster-analysis methods. Partition clustering methods break the observations into a distinct number of nonoverlapping groups. This is accomplished in one step, unlike hierarchical cluster-analysis methods, in which an iterative procedure is used. Consequently, this method is quicker and will allow larger datasets than the hierarchical clustering methods. Contrast to hierarchical clustering. Also see kmeans and kmedians.

PCA. See principal component analysis.

**Pillai's trace**. Pillai's trace is a test statistic for the hypothesis test  $H_0: \mu_1 = \mu_2 = \cdots = \mu_k$  based on the eigenvalues  $\lambda_1, \ldots, \lambda_s$  of  $\mathbf{E}^{-1}\mathbf{H}$ . It is defined as

$$V^{(s)} = \operatorname{trace}[(\mathbf{E} + \mathbf{H})^{-1}\mathbf{H}] = \sum_{i=1}^{s} \frac{\lambda_i}{1 + \lambda_i}$$

where **H** is the between matrix and **E** is the within matrix. See between matrix.

- **posterior probabilities**. After discriminant analysis, the posterior probabilities are the probabilities of a given observation being assigned to each of the groups based on the prior probabilities, the training data, and the particular discriminant model. Contrast to *prior probabilities*.
- **principal component analysis**. Principal component analysis (PCA) is a statistical technique used for data reduction. The leading eigenvectors from the eigen decomposition of the correlation or the covariance matrix of the variables describe a series of uncorrelated linear combinations of the variables that contain most of the variance. In addition to data reduction, the eigenvectors from a PCA are often inspected to learn more about the underlying structure of the data.
- **principal factor method**. The principal factor method is a method for factor analysis in which the factor loadings, sometimes called factor patterns, are computed using the squared multiple correlations as estimates of the communality. Also see *factor analysis* and *communality*.
- **prior probabilities** Prior probabilities in discriminant analysis are the probabilities of an observation belonging to a group before the discriminant analysis is performed. Prior probabilities are often based on the prevalence of the groups in the population as a whole. Contrast to *posterior probabilities*.
- **Procrustes rotation**. A Procrustes rotation is an orthogonal or oblique transformation, that is, a restricted Procrustes transformation without translation or dilation (uniform scaling).
- **Procrustes transformation**. The goal of Procrustes transformation is to transform the source matrix **X** to be as close as possible to the target **Y**. The permitted transformations are any combination of dilation (uniform scaling), rotation and reflection (that is, orthogonal or oblique transformations), and translation. Closeness is measured by residual sum of squares. In some cases, unrestricted Procrustes transformation is desired; this allows the data to be transformed not just by orthogonal or oblique rotations, but by all conformable regular matrices **A**. Unrestricted Procrustes transformation is equivalent to a multivariate regression.

The name comes from Procrustes of Greek mythology; Procrustes invited guests to try his iron bed. If the guest was too tall for the bed, Procrustes would amputate the guest's feet, and if the guest was too short, he would stretch the guest out on a rack.

Also see orthogonal rotation, oblique rotation, dilation, and multivariate regression.

- promax power rotation. Promax power rotation is an oblique rotation. It does not fit in the minimizing-a-criterion framework that is at the core of most other rotations. The promax method (Hendrickson and White 1964) was proposed before computing power became widely available. The promax rotation consists of three steps:
  - 1. Perform an orthogonal rotation.
  - 2. Raise the elements of the rotated matrix to some power, preserving the sign of the elements. Typically the power is in the range  $2 \le power \le 4$ . This operation is meant to distinguish clearly between small and large values.
  - 3. The matrix from step two is used as the target for an oblique Procrustean rotation from the original matrix.
- **proximity, proximity matrix**, and **proximity measure**. Proximity or a proximity measure means the nearness or farness of two things, such as observations or variables or groups of observations or a method for quantifying the nearness or farness between two things. A proximity is measured by a similarity or dissimilarity. A proximity matrix is a matrix of proximities. Also see *similarity* and *dissimilarity*.
- QDA. See quadratic discriminant analysis.
- quadratic discriminant analysis. Quadratic discriminant analysis (QDA) is a parametric form of discriminant analysis and is a generalization of LDA. Like LDA, QDA assumes that the observations

come from a multivariate normal distribution, but unlike LDA, the groups are not assumed to have equal covariance matrices. Also see *discriminant analysis*, *linear discriminant analysis*, and *parametric methods*.

**quartimax rotation**. Quartimax rotation maximizes the variance of the squared loadings within the rows of the matrix. It is an orthogonal rotation that is equivalent to minimizing the criterion

$$c(\mathbf{\Lambda}) = \sum_{i} \sum_{r} \lambda_{ir}^4 = -\frac{1}{4} \left\langle \mathbf{\Lambda}^2, \mathbf{\Lambda}^2 \right\rangle$$

See Crawford–Ferguson rotation for a definition of  $\Lambda$ .

**quartimin rotation**. Quartimin rotation is an oblique rotation that is equivalent to quartimax rotation when quartimin is restricted to orthogonal rotations. Quartimin is equivalent to oblimin rotation with  $\gamma = 0$ . Also see *quartimax rotation*, oblique rotation, orthogonal rotation, and oblimin rotation.

**reflection**. A reflection is an orientation reversing orthogonal transformation, that is, a transformation that involves negating coordinates in one or more dimensions. A reflection is a Procrustes transformation.

**repeated measures**. Repeated measures data have repeated measurements for the subjects over some dimension, such as time—for example test scores at the start, midway, and end of the class. The repeated observations are typically not independent. Repeated-measures ANOVA is one approach for analyzing repeated measures data, and MANOVA is another. Also see *sphericity*.

**rotation**. A rotation is an orientation preserving orthogonal transformation. A rotation is a Procrustes transformation.

**Roy's largest root**. Roy's largest root test is a test statistic for the hypothesis test  $H_0: \mu_1 = \cdots = \mu_k$  based on the largest eigenvalue of  $\mathbf{E}^{-1}\mathbf{H}$ . It is defined as

$$\theta = \frac{\lambda_1}{1 + \lambda_1}$$

Here **H** is the between matrix, and **E** is the within matrix. See between matrix.

**Sammon mapping criterion**. The Sammon (1969) mapping criterion is a loss criterion used with MDS; it is the sum of the scaled, squared differences between the distances and the disparities, normalized by the sum of the disparities. Also see *multidimensional scaling*, *modern scaling*, and *loss*.

score. A score for an observation after factor analysis, PCA, or LDA is derived from a column of the loading matrix and is obtained as the linear combination of that observation's data by using the coefficients found in the loading.

score plot. A score plot produces scatterplots of the score variables after factor analysis, PCA, or LDA.

scree plot. A scree plot is a plot of eigenvalues or singular values ordered from greatest to least after an eigen decomposition or singular value decomposition. Scree plots help determine the number of factors or components in an eigen analysis. Scree is the accumulation of loose stones or rocky debris lying on a slope or at the base of a hill or cliff; this plot is called a scree plot because it looks like a scree slope. The goal is to determine the point where the mountain gives way to the fallen rock.

**Shepard diagram**. A Shepard diagram after MDS is a 2-dimensional plot of high-dimensional dissimilarities or disparities versus the resulting low-dimensional distances. Also see *multidimensional scaling*.

similarity, similarity matrix, and similarity measure. A similarity or a similarity measure is a quantification of how alike two things are, such as observations or variables or groups of observations, or a method for quantifying that alikeness. A similarity matrix is a matrix containing similarity measurements. The matching coefficient is one example of a similarity measure. Contrast to dissimilarity. Also see proximity and matching coefficient.

single-linkage clustering. Single-linkage clustering is a hierarchical clustering method that computes the proximity between two groups as the proximity between the closest pair of observations between the two groups.

singular value decomposition. A singular value decomposition (SVD) is a factorization of a rectangular matrix. It says that if M is an  $m \times n$  matrix, there exists a factorization of the form

$$\mathbf{M} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^*$$

where U is an  $m \times m$  unitary matrix,  $\Sigma$  is an  $m \times n$  matrix with nonnegative numbers on the diagonal and zeros off the diagonal, and  $V^*$  is the conjugate transpose of V, an  $n \times n$  unitary matrix. If M is a real matrix, then so is V, and  $V^* = V'$ .

sphericity. Sphericity is the state or condition of being a sphere. In repeated measures ANOVA, sphericity concerns the equality of variance in the difference between successive levels of the repeated measure. The multivariate alternative to ANOVA, called MANOVA, does not require the assumption of sphericity. Also see repeated measures.

SSCP matrix. SSCP is an acronym for the sums of squares and cross products. Also see between matrix.

stacked variables. See crossed variables.

stacking variables. See crossing variables.

standardized data. Standardized data has a mean of zero and a standard deviation of one. You can standardize data x by taking  $(x - \overline{x})/\sigma$ , where  $\sigma$  is the standard deviation of the data.

stopping rules. Stopping rules for hierarchical cluster analysis are used to determine the number of clusters. A stopping-rule value (also called an index) is computed for each cluster solution, that is, at each level of the hierarchy in hierarchical cluster analysis. Also see hierarchical clustering.

stress. See Kruskal stress and loss.

structure. Structure, as in factor structure, is the correlations between the variables and the common factors after factor analysis. Structure matrices are available after factor analysis and LDA. Also see factor analysis and linear discriminant analysis.

supplementary rows or columns or supplementary variables. Supplementary rows or columns can be included in CA, and supplementary variables can be included in MCA. They do not affect the CA or MCA solution, but they are included in plots and tables with statistics of the corresponding row or column points. Also see correspondence analysis and multiple correspondence analysis.

**SVD**. See singular value decomposition.

target rotation. Target rotation minimizes the criterion

$$c(\mathbf{\Lambda}) = \frac{1}{2} \|\mathbf{\Lambda} - \mathbf{H}\|^2$$

for a given target matrix **H**.

See Crawford–Ferguson rotation for a definition of  $\Lambda$ .

- **taxonomy**. Taxonomy is the study of the general principles of scientific classification. It also denotes classification, especially the classification of plants and animals according to their natural relationships. Cluster analysis is a tool used in creating a taxonomy and is synonymous with numerical taxonomy. Also see *cluster analysis*.
- **tetrachoric correlation**. A tetrachoric correlation estimates the correlation coefficients of binary variables by assuming a latent bivariate normal distribution for each pair of variables, with a threshold model for manifest variables.
- **ties**. After discriminant analysis, ties in classification occur when two or more posterior probabilities are equal for an observation. They are most common with KNN discriminant analysis.
- total inertia or total principal inertia. The total (principal) inertia in CA and MCA is the sum of the principal inertias. In CA, total inertia is the Pearson  $\chi^2/n$ . In CA, the principal inertias are the singular values; in MCA the principal inertias are the eigenvalues. Also see *correspondence* analysis and multiple correspondence analysis.
- **uniqueness.** In factor analysis, the uniqueness is the percentage of a variable's variance that is not explained by the common factors. It is also "1 communality". Also see *communality*.
- **unrestricted transformation**. An unrestricted transformation is a Procrustes transformation that allows the data to be transformed, not just by orthogonal and oblique rotations, but by all conformable regular matrices. This is equivalent to a multivariate regression. Also see *Procrustes transformation* and *multivariate regression*.
- varimax rotation. Varimax rotation maximizes the variance of the squared loadings within the columns of the matrix. It is an orthogonal rotation equivalent to oblimin with  $\gamma=1$  or to the Crawford–Ferguson family with  $\kappa=1/p$ , where p is the number of rows of the matrix to be rotated. Also see orthogonal rotation, oblimin rotation, and Crawford–Ferguson rotation.
- **Ward's linkage clustering.** Ward's-linkage clustering is a hierarchical clustering method that joins the two groups resulting in the minimum increase in the error sum of squares.
- weighted-average linkage clustering. Weighted-average linkage clustering is a hierarchical clustering method that uses the weighted average similarity or dissimilarity of the two groups as the measure between the two groups.
- Wilks's lambda. Wilks's lambda is a test statistic for the hypothesis test  $H_0: \mu_1 = \mu_2 = \cdots = \mu_k$  based on the eigenvalues  $\lambda_1, \ldots, \lambda_s$  of  $\mathbf{E}^{-1}\mathbf{H}$ . It is defined as

$$\Lambda = \frac{|\mathbf{E}|}{|\mathbf{E} + \mathbf{H}|} = \prod_{i=1}^{s} \frac{1}{1 + \lambda_i}$$

where **H** is the between matrix and **E** is the within matrix. See between matrix.

**Wishart distribution**. The Wishart distribution is a family of probability distributions for nonnegative-definite matrix-valued random variables ("random matrices"). These distributions are of great importance in the estimation of covariance matrices in multivariate statistics.

within matrix. See between matrix.

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## Subject and author index

See the combined subject index and the combined author index in the Glossary and Index.