## 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 membership, probabilities of group membership, etc.

\*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	
<u>c</u> lassification	group membership classification; the default when one variable is specified and group() is not specified
pr	probability of group membership; the default when group() is specified or when multiple variables are specified
<u>mah</u> alanobis	Mahalanobis squared distance between observations and groups
<u>clsc</u> ore	group classification function score
* <u>looc</u> lass	leave-one-out group membership classification; may be used only when one new variable is specified
*loopr	leave-one-out probability of group membership
* <u>loom</u> ahal	leave-one-out Mahalanobis squared distance between observations and groups
options	Description
Main	
<pre>group(group)</pre>	the group for which the statistic is to be calculated
Options	
<u>pri</u> ors( <i>priors</i> ) <u>tie</u> s( <i>ties</i> )	group prior probabilities; defaults to e(grouppriors) 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. Leaveone-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 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(first) 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

 $\label{eq:statistics} Statistics > Postestimation$ 

## Syntax for estat

Group correlation matrices and p-values

estat <u>cor</u>relations [, *correlations\_options*]

Group covariance matrices

estat covariance [, covariance\_options]

Mahalanobis and generalized squared distances between the group means

<pre>estat grdistances [ , grdistances_options ]</pre>				
correlations_options Description				
Main				
р	display two-sided <i>p</i> -values			
<u>for</u> mat(% <i>fmt</i> )	numeric display format; default is %9.0g			
nohalf	display full matrix even if symmetric			
covariance_options	Description			
Main				
<u>for</u> mat(% <i>fmt</i> )	numeric display format; default is %9.0g			
nohalf display full matrix even if symmetric				

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	
<pre>priors(priors)</pre>	group prior probabilities; defaults to e(grouppriors)

collect is allowed with all estat commands; see [U] 11.1.10 Prefix commands.

#### Options for estat

Options for estat are presented under the following headings:

Options for estat correlations 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 and Navarro Alberto (2017).

We perform a quadratic discriminant analysis on this dataset and demonstrate the use of estat and predict.

```
. use https://www.stata-press.com/data/r19/skulls
(Egyptian skulls)
. discrim qda x1 x2 x3 x4, group(predynastic)
Quadratic discriminant analysis
Resubstitution classification summary
```

Кеу			
Number Percent			
True	Classif	ied	
predynastic	Early	Late	Total
Early	9 90.00	1 10.00	10 100.00
Late	3 30.00	7 70.00	10 100.00
Total	12 60.00	8 40.00	20 100.00
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	е			
Group covariance	natrices			
predynastic: Ea	rly			
	x1	x2	x3	x4
x1	40.32222			
x2	7.188889	15.34444		
x3	13.18889	-7.322222	36.9	
x4	16.1	8.077778	-2.144444	11.43333
predynastic: La	te			
	x1	x2	х3	x4
x1	43.12222			
x2	-4.966667	38.98889		
x3	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

	- ± y			
Кеу				
Correlation Two-sided p	-value			
	x	1 x2	x3	x4
x1	1.0000	0		
x2	0.2890 0.4180	1 1.00000 0		
х3	0.3419 0.3335	2 -0.30772 3 0.38707	1.00000	
x4	0.7498 0.0125	4 0.60986 1 0.06119	-0.10440 0.77409	1.00000

```
predynastic: Late
```

Кеу				
Correlation Two-sided p	-value			
	x1	x2	x3	x4
x1	1.00000			
x2	-0.12113 0.73889	1.00000		
х3	0.44598 0.19640	0.33026 0.35133	1.00000	
x4	0.26274 0.46331	0.67577 0.03196	0.45327 0.18830	1.00000

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.

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
                               xЗ
                x1
                                     x4
21. . 127 129 95 51
22. end
. predict grp
(option classification assumed; group classification)
. predict pr1 pr2, pr
. label values grp epoch
. list x* grp pr1 pr2 in 21
              x2
                   xЗ
        x1
                         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		Classification		Probabi	lities			
Obs	x1	x2	xЗ	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 leave-one-out (LOO) classifications, probabilities, classification tables, and error-rate estimates.

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### 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 https://www.stata-press.com/data/r19/rootstock, clear (Table 6.2. Rootstock data, Rencher and Christensen (2012))

```
Table 0.2. Rootstock data, Rencher and Christensen (201
```

```
. 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.

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## Stored results

estat correlations stores the following in r():

Matrices	
r(Rho_#)	group # correlation matrix
r(P_#)	two-sided $p\text{-values}$ for group $\#\operatorname{correlations}$

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, eds. 1985. Data: A Collection of Problems from Many Fields for the Student and Research Worker. New York: Springer. https://doi.org/10.1007/978-1-4612-5098-2.
- Everitt, B. S., and G. Dunn. 2001. Applied Multivariate Data Analysis. 2nd ed. London: Arnold.
- Manly, B. F. J., and J. A. Navarro Alberto. 2017. Multivariate Statistical Methods: A Primer. 4th ed. Boca Raton, FL: CRC Press.

Rencher, A. C., and W. F. Christensen. 2012. Methods of Multivariate Analysis. 3rd ed. Hoboken, NJ: Wiley. https://doi.org/10.1002/9781118391686.

## Also see

- [MV] discrim qda Quadratic discriminant analysis
- [MV] discrim Discriminant analysis
- [MV] discrim estat Postestimation tools for discrim
- [U] 20 Estimation and postestimation commands

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