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cluster linkage — Hierarchical cluster analysis

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

Same 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

Same 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

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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 *linkage* [*varlist*] [*if*] [*in*] [, *cluster_options*]

Cluster analysis of a dissimilarity matrix

clustermat *linkage matname* [*if*] [*in*] [, *clustermat_options*]

linkage	Description
<u>single</u>linkage	single-linkage cluster analysis
<u>average</u>linkage	average-linkage cluster analysis
completelinkage	complete-linkage cluster analysis
<u>wav</u>eragelinkage	weighted-average linkage cluster analysis
<u>med</u>ianlinkage	median-linkage cluster analysis
<u>cen</u>troidlinkage	centroid-linkage cluster analysis
<u>wards</u>linkage	Ward's linkage cluster analysis

cluster_options	Description
Main	
<u>measure</u>(*measure*)	similarity or dissimilarity measure
<u>name</u>(*clname*)	name of resulting cluster analysis
Advanced	
<u>generate</u>(*stub*)	prefix for generated variables; default prefix is *clname*

clustermat_options	Description
Main	
<u>shape</u>(*shape*)	shape (storage method) of *matname*
add	add cluster information to data currently in memory
clear	replace data in memory with cluster information
<u>labelvar</u>(*varname*)	place dissimilarity matrix row names in *varname*
<u>name</u>(*clname*)	name of resulting cluster analysis
Advanced	
force	perform clustering after fixing *matname* problems
<u>generate</u>(*stub*)	prefix for generated variables; default prefix is *clname*

shape	*matname* is stored as a
full	square symmetric matrix; the default
lower	vector of rowwise lower triangle (with diagonal)
llower	vector of rowwise strict lower triangle (no diagonal)
upper	vector of rowwise upper triangle (with diagonal)
uupper	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 Euclidean). 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.

$$D_{11} \ D_{21} \ D_{22} \ D_{31} \ D_{32} \ D_{33} \ \ldots \ D_{n1} \ D_{n2} \ \ldots \ D_{nn}$$

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.

$$D_{21} \ D_{31} \ D_{32} \ D_{41} \ D_{42} \ D_{43} \ \ldots \ D_{n1} \ D_{n2} \ \ldots \ D_{n,n-1}$$

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.

$$D_{11} \ D_{12} \ \ldots \ D_{1n} \ D_{22} \ D_{23} \ \ldots \ D_{2n} \ D_{33} \ D_{34} \ \ldots \ D_{3n} \ \ldots \ D_{nn}$$

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.

$$D_{12} \ D_{13} \ \ldots \ D_{1n} \ D_{23} \ D_{24} \ \ldots \ D_{2n} \ D_{34} \ D_{35} \ \ldots \ D_{3n} \ \ldots \ D_{n-1,n}$$

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.
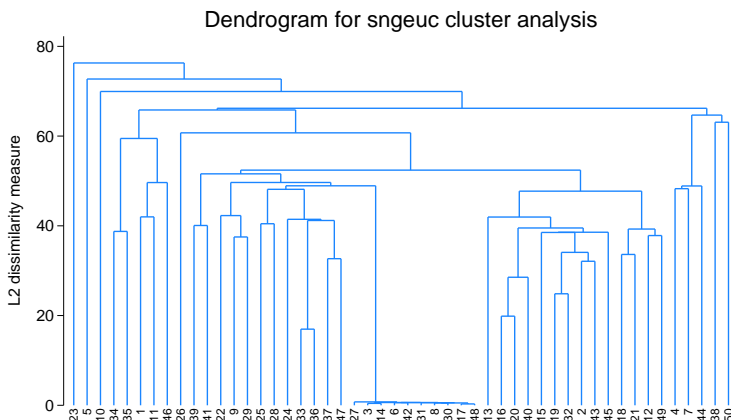
Although all 50 plants are supposed to be of the same type, you decide to perform a cluster analysis to see if there are subgroups or anomalies among them. You arbitrarily decide to use single-linkage clustering with the default Euclidean distance.

```
. use https://www.stata-press.com/data/r19/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**.

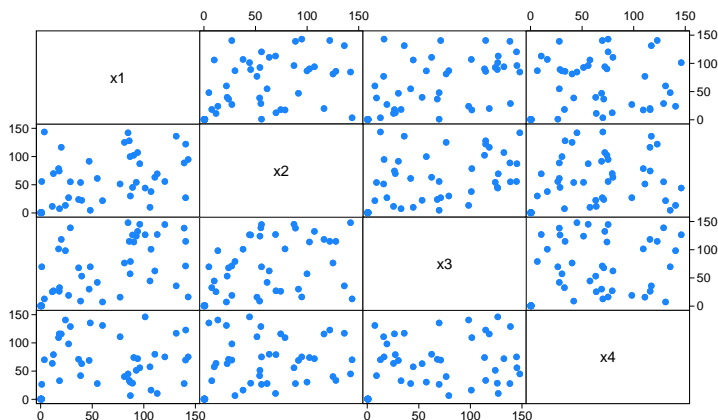What you really want to see is the dendrogram for this cluster analysis; see [MV] **cluster dendrogram**.

```
. cluster dendrogram sngeuc, xlabel(, angle(90) labsize(*.75))
```

Dendrogram for sngeuc cluster analysis

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.
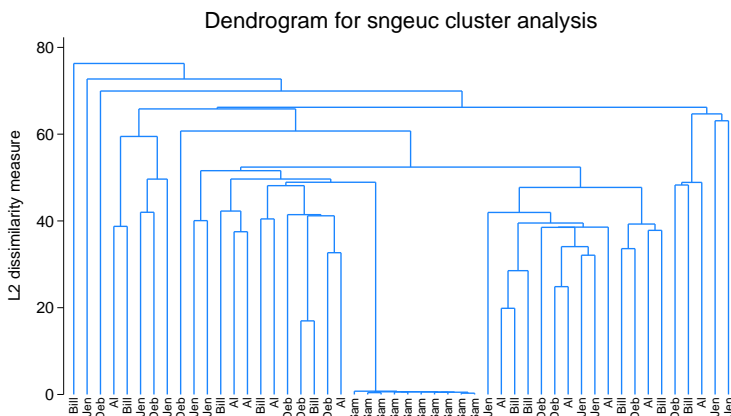
```
. graph matrix x1 x2 x3 x4
```


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))
```

Dendrogram for sngeuc cluster analysis

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.

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▷ 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.
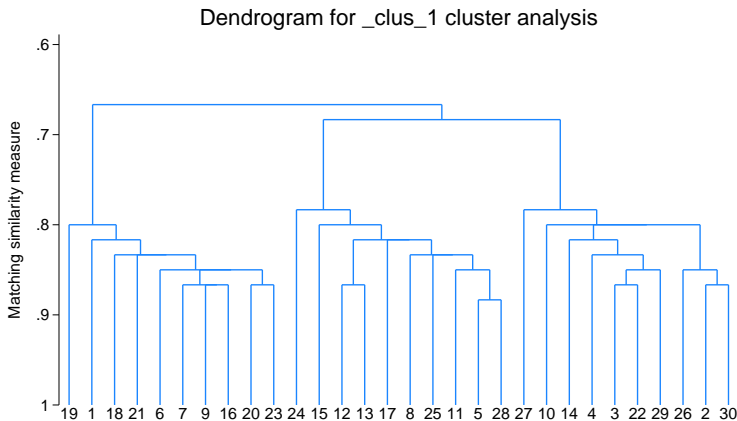
Among the analyses you try is the following cluster analysis. You decide to use single-linkage clustering with the simple matching binary coefficient because it is easy to understand. Just for fun, though it makes no difference to you, you specify the generate() option to force the generated variables to have zstub as a prefix. You let Stata pick a name for your cluster analysis by not specifying the name() option.

```
. use https://www.stata-press.com/data/r19/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
```


Dendrogram for _clus_1 cluster analysis

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, nototals
```

	truegrp		
	1	2	3
grp3			
1		10	
2			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, nototals
```

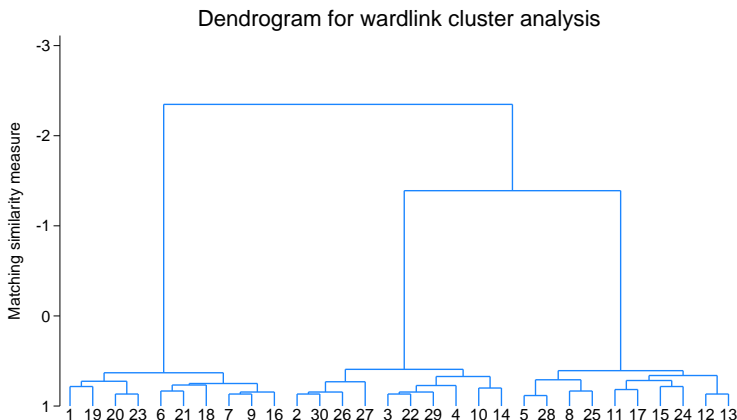|	truegrp		
	1	2	3
medgrp3			
1		10	
2	10		
3			10

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
```

Dendrogram for wardlink cluster analysis

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, nototals
```

	truegrp		
	1	2	3
wardgrp3			
1		10	
2	10		
3			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.
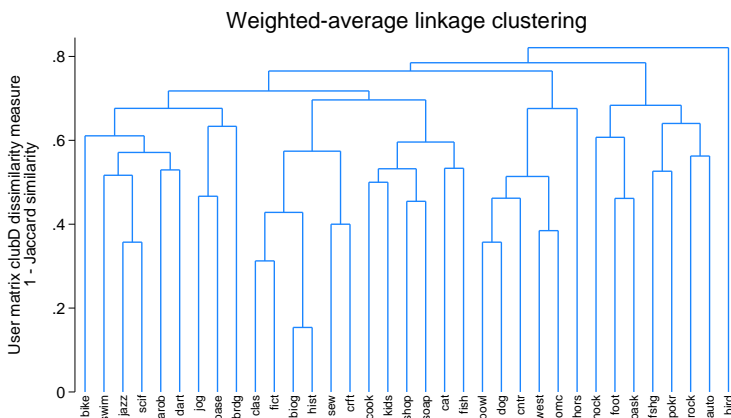
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▷ Example 3

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 https://www.stata-press.com/data/r19/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 *measure*s, 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 US 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** — Introduction to cluster-analysis commands

[MV] **cluster dendrogram** — Dendrograms for hierarchical cluster analysis

[MV] **cluster generate** — Generate grouping variables from a cluster analysis

[MV] **cluster notes** — Cluster analysis notes

[MV] **cluster stop** — Cluster-analysis stopping rules

[MV] **cluster utility** — List, rename, use, and drop cluster analyses

[MV] **clustermat** — Introduction to clustermat commands