SAS/STAT® 13.2 User's Guide
The CLUSTER Procedure

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Chapter 33
The CLUSTER Procedure

Contents

Overview: CLUSTER Procedure

The CLUSTER procedure hierarchically clusters the observations in a SAS data set by using one of 11 methods. The data can be coordinates or distances. If the data are coordinates, PROC CLUSTER computes (possibly squared) Euclidean distances. If you want non-Euclidean distances, use the DISTANCE procedure (see Chapter 36) to compute an appropriate distance data set that can then be used as input to PROC CLUSTER.

The clustering methods are: average linkage, the centroid method, complete linkage, density linkage (including Wong's hybrid and *k*th-nearest-neighbor methods), maximum likelihood for mixtures of spherical multivariate normal distributions with equal variances but possibly unequal mixing proportions, the flexible-beta method, McQuitty's similarity analysis, the median method, single linkage, two-stage density linkage, and Ward's minimum-variance method. Each method is described in the section "Clustering Methods" on page 2026.

All methods are based on the usual agglomerative hierarchical clustering procedure. Each observation begins in a cluster by itself. The two closest clusters are merged to form a new cluster that replaces the two old clusters. Merging of the two closest clusters is repeated until only one cluster is left. The various clustering methods differ in how the distance between two clusters is computed.

The CLUSTER procedure is not practical for very large data sets because the CPU time is roughly proportional to the square or cube of the number of observations. The FASTCLUS procedure (see Chapter 38) requires time proportional to the number of observations and thus can be used with much larger data sets than PROC CLUSTER. If you want to cluster a very large data set hierarchically, use PROC FASTCLUS for a preliminary cluster analysis to produce a large number of clusters. Then use PROC CLUSTER to cluster the preliminary clusters hierarchically. This method is illustrated in Example 33.3.

PROC CLUSTER displays a history of the clustering process, showing statistics useful for estimating the number of clusters in the population from which the data are sampled. It creates a dendrogram when ODS Graphics is enabled. PROC CLUSTER also creates an output data set that can be used by the TREE procedure to output the cluster membership at any desired level. For example, to obtain the six-cluster solution, you could first use PROC CLUSTER with the OUTTREE= option, and then use this output data set as the input data set to the TREE procedure. With PROC TREE, specify the NCLUSTERS=6 and the OUT= options to obtain the six-cluster solution. For an example, see Example 105.1 in Chapter 105, "The TREE Procedure."

For coordinate data, Euclidean distances are computed from differences between coordinate values. The use of differences has several important consequences:

- For differences to be valid, the variables must have an interval or stronger scale of measurement. Ordinal or ranked data are generally not appropriate for cluster analysis.
- For Euclidean distances to be comparable, equal differences should have equal practical importance. You might need to transform the variables linearly or nonlinearly to satisfy this condition. For example, if one variable is measured in dollars and one in euros, you might need to convert to the same currency. Or, if ratios are more meaningful than differences, take logarithms.

- Variables with large variances tend to have more effect on the resulting clusters than variables with small variances. If you consider all variables to be equally important, you can use the STD option in PROC CLUSTER to standardize the variables to mean 0 and standard deviation 1. However, standardization is not always appropriate. See Milligan and Cooper (1987) for a Monte Carlo study on various methods of variable standardization. You should remove outliers before using PROC CLUSTER with the STD option unless you specify the TRIM= option. The STDIZE procedure (see Chapter 94) provides additional methods for standardizing variables and imputing missing values.

The ACECLUS procedure (see Chapter 24) is useful for linear transformations of the variables if any of the following conditions hold:

- You have no idea how the variables should be scaled.
- You want to detect natural clusters regardless of whether some variables have more influence than others.
- You want to use a clustering method designed for finding compact clusters, but you want to be able to detect elongated clusters.

Agglomerative hierarchical clustering is discussed in all standard references on cluster analysis, such as Anderberg (1973); Sneath and Sokal (1973); Hartigan (1975); Everitt (1980); Spath (1980). An especially good introduction is given by Massart and Kaufman (1983). Anyone considering doing a hierarchical cluster analysis should study the Monte Carlo results of Milligan (1980); Milligan and Cooper (1985); Cooper and Milligan (1988).

Other essential, though more advanced, references on hierarchical clustering include Hartigan (1977, pp. 60–68; 1981), Wong (1982); Wong and Schaack (1982); Wong and Lane (1983). For a discussion of the confusing terminology in hierarchical cluster analysis, see Blashfield and Aldenderfer (1978).

Getting Started: CLUSTER Procedure

This example shows how you can use the CLUSTER procedure to compute hierarchical clusters of observations in a SAS data set.

Suppose you want to determine whether national figures for birth rates, death rates, and infant death rates can be used to categorize countries. Previous studies indicate that the clusters computed from this type of data can be elongated and elliptical. Thus, you need to perform a linear transformation on the raw data before the cluster analysis.

The following data[1] from Rouncefield (1995) are birth rates, death rates, and infant death rates for 97 countries. The DATA step creates the SAS data set Poverty:

```
data Poverty;
   input Birth Death InfantDeath Country $20. @@;
   datalines;
24.7  5.7  30.8 Albania               12.5 11.9  14.4 Bulgaria
13.4 11.7  11.3 Czechoslovakia        12   12.4   7.6 Former E. Germany
11.6 13.4  14.8 Hungary               14.3 10.2    16 Poland
13.6 10.7  26.9 Romania                 14    9  20.2 Yugoslavia

   ... more lines ...

41.7 10.3    66 Zimbabwe
;
```

The data set Poverty contains the character variable Country and the numeric variables Birth, Death, and InfantDeath, which represent the birth rate per thousand, death rate per thousand, and infant death rate per thousand. The `$20.` in the INPUT statement specifies that the variable Country is a character variable with a length of 20. The double trailing at sign (@@) in the INPUT statement holds the input line for further iterations of the DATA step, specifying that observations are input from each line until all values are read.

Because the variables in the data set do not have equal variance, you must perform some form of scaling or transformation. One method is to standardize the variables to mean zero and variance one. However, when you suspect that the data contain elliptical clusters, you can use the ACECLUS procedure to transform the data such that the resulting within-cluster covariance matrix is spherical. The procedure obtains approximate estimates of the pooled within-cluster covariance matrix and then computes canonical variables to be used in subsequent analyses.

The following statements perform the ACECLUS transformation by using the SAS data set Poverty. The OUT= option creates an output SAS data set called Ace that contains the canonical variable scores:

```
proc aceclus data=Poverty out=Ace p=.03 noprint;
   var Birth Death InfantDeath;
run;
```

The P= option specifies that approximately 3% of the pairs are included in the estimation of the within-cluster covariance matrix. The NOPRINT option suppresses the display of the output. The VAR statement specifies that the variables Birth, Death, and InfantDeath are used in computing the canonical variables.

The following statements invoke the CLUSTER procedure, using the SAS data set Ace created in the previous PROC ACECLUS run:

```
ods graphics on;

proc cluster data=Ace method=ward ccc pseudo print=15 out=tree
   plots=den(height=rsq);
   var can1-can3;
   id country;
run;

ods graphics off;
```

[1] These data have been compiled from the *United Nations Demographic Yearbook 1990* (United Nations publications, Sales No. E/F.91.XII.1, copyright 1991, United Nations, New York) and are reproduced with the permission of the United Nations.

The ODS GRAPHICS ON statement enables ODS Graphics. Ward's minimum-variance clustering method is specified by the METHOD= option. The CCC option displays the cubic clustering criterion, and the PSEUDO option displays pseudo F and t^2 statistics. The PRINT=15 option displays only the last 15 generations of the cluster history. By default, when ODS Graphics is enabled, a dendrogram displaying the semipartial R square is displayed on the X axis. The option PLOTS=DEN(HEIGHT=RSQ) requests a dendrogram with R square displayed instead.

The VAR statement specifies that the canonical variables computed in the ACECLUS procedure are used in the cluster analysis. The ID statement selects the variable Country as the Y axis variable in the dendrogram and also specifies that Country should be added to the Tree output data set.

PROC CLUSTER first displays the table of eigenvalues of the covariance matrix (Figure 33.1). These eigenvalues are used in the computation of the cubic clustering criterion. The first two columns list each eigenvalue and the difference between the eigenvalue and its successor. The last two columns display the individual and cumulative proportion of variation associated with each eigenvalue.

Figure 33.1 Table of Eigenvalues of the Covariance Matrix

The CLUSTER Procedure
Ward's Minimum Variance Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	64.5500051	54.7313223	0.8091	0.8091
2	9.8186828	4.4038309	0.1231	0.9321
3	5.4148519		0.0679	1.0000

Root-Mean-Square Total-Sample Standard Deviation	5.156987

Root-Mean-Square Distance Between Observations	12.63199

Figure 33.2 displays the last 15 generations of the cluster history. First listed are the number of clusters and the names of the clusters joined. The observations are identified either by the ID value or by CLn, where n is the number of the cluster. Next, PROC CLUSTER displays the number of observations in the new cluster and the semipartial R square. The latter value represents the decrease in the proportion of variance accounted for by joining the two clusters.

Figure 33.2 Cluster History

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Tie
15	Oman	CL37	5	0.0039	.957	.933	6.03	132	12.1	
14	CL31	CL22	13	0.0040	.953	.928	5.81	131	9.7	
13	CL41	CL17	32	0.0041	.949	.922	5.70	131	13.1	
12	CL19	CL21	10	0.0045	.945	.916	5.65	132	6.4	
11	CL39	CL15	9	0.0052	.940	.909	5.60	134	6.3	
10	CL76	CL27	6	0.0075	.932	.900	5.25	133	18.1	
9	CL23	CL11	15	0.0130	.919	.890	4.20	125	12.4	
8	CL10	Afghanistan	7	0.0134	.906	.879	3.55	122	7.3	
7	CL9	CL25	17	0.0217	.884	.864	2.26	114	11.6	
6	CL8	CL20	14	0.0239	.860	.846	1.42	112	10.5	
5	CL14	CL13	45	0.0307	.829	.822	0.65	112	59.2	
4	CL16	CL7	28	0.0323	.797	.788	0.57	122	14.8	
3	CL12	CL6	24	0.0323	.765	.732	1.84	153	11.6	
2	CL3	CL4	52	0.1782	.587	.613	-.82	135	48.9	
1	CL5	CL2	97	0.5866	.000	.000	0.00	.	135	

Next listed is the squared multiple correlation, R square, which is the proportion of variance accounted for by the clusters. Figure 33.2 shows that, when the data are grouped into three clusters, the proportion of variance accounted for by the clusters (R square) is just under 77%. The approximate expected value of R square is given in the ERSq column. This expectation is approximated under the null hypothesis that the data have a uniform distribution instead of forming distinct clusters.

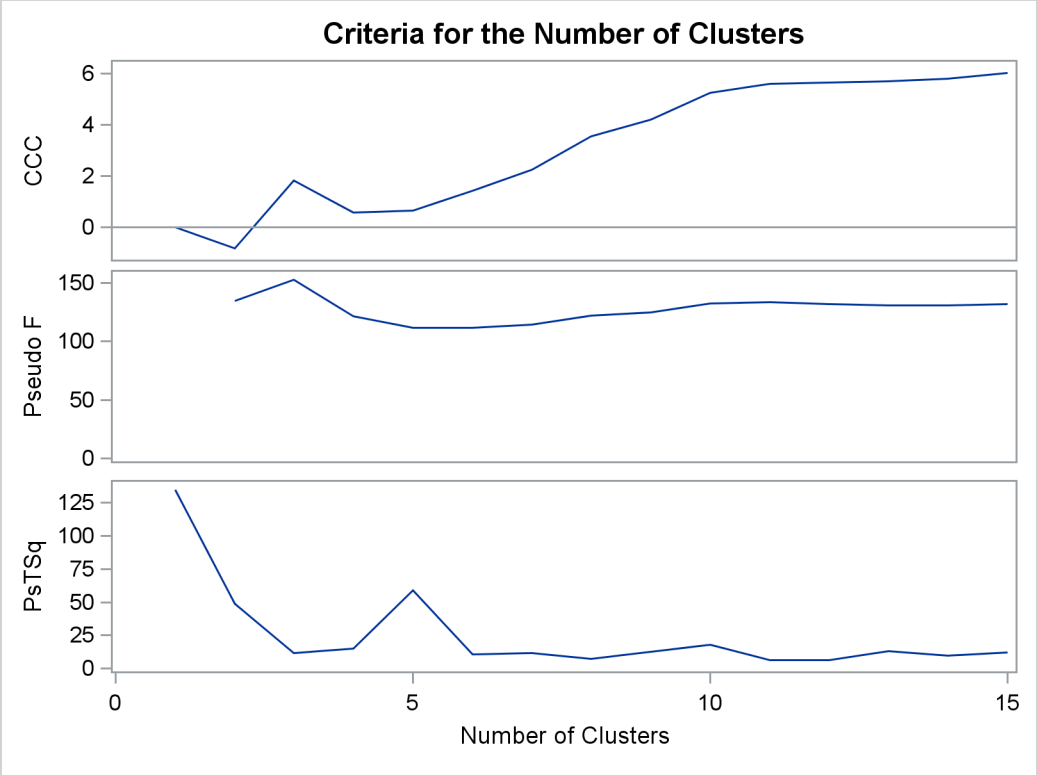
The next three columns display the values of the cubic clustering criterion (CCC), pseudo F (PSF), and t^2 (PST2) statistics. These statistics are useful for estimating the number of clusters in the data.

The final column in Figure 33.2 lists ties for minimum distance; a blank value indicates the absence of a tie. A tie means that the clusters are indeterminate and that changing the order of the observations might change the clusters. See Example 33.4 for ways to investigate the effects of ties.

Figure 33.3 plots the three statistics for estimating the number of clusters. Peaks in the plot of the cubic clustering criterion with values greater than 2 or 3 indicate good clusters; peaks with values between 0 and 2 indicate possible clusters. Large negative values of the CCC can indicate outliers. In Figure 33.3, there is a local peak of the CCC when the number of clusters is three. The CCC drops at four clusters and then steadily increases, leveling off at eleven clusters.

Another method of judging the number of clusters in a data set is to look at the pseudo F statistic (PSF). Relatively large values indicate good numbers of clusters. In Figure 33.3, the pseudo F statistic suggests three clusters or eleven clusters.

Figure 33.3 Plot of Statistics for Estimating the Number of Clusters

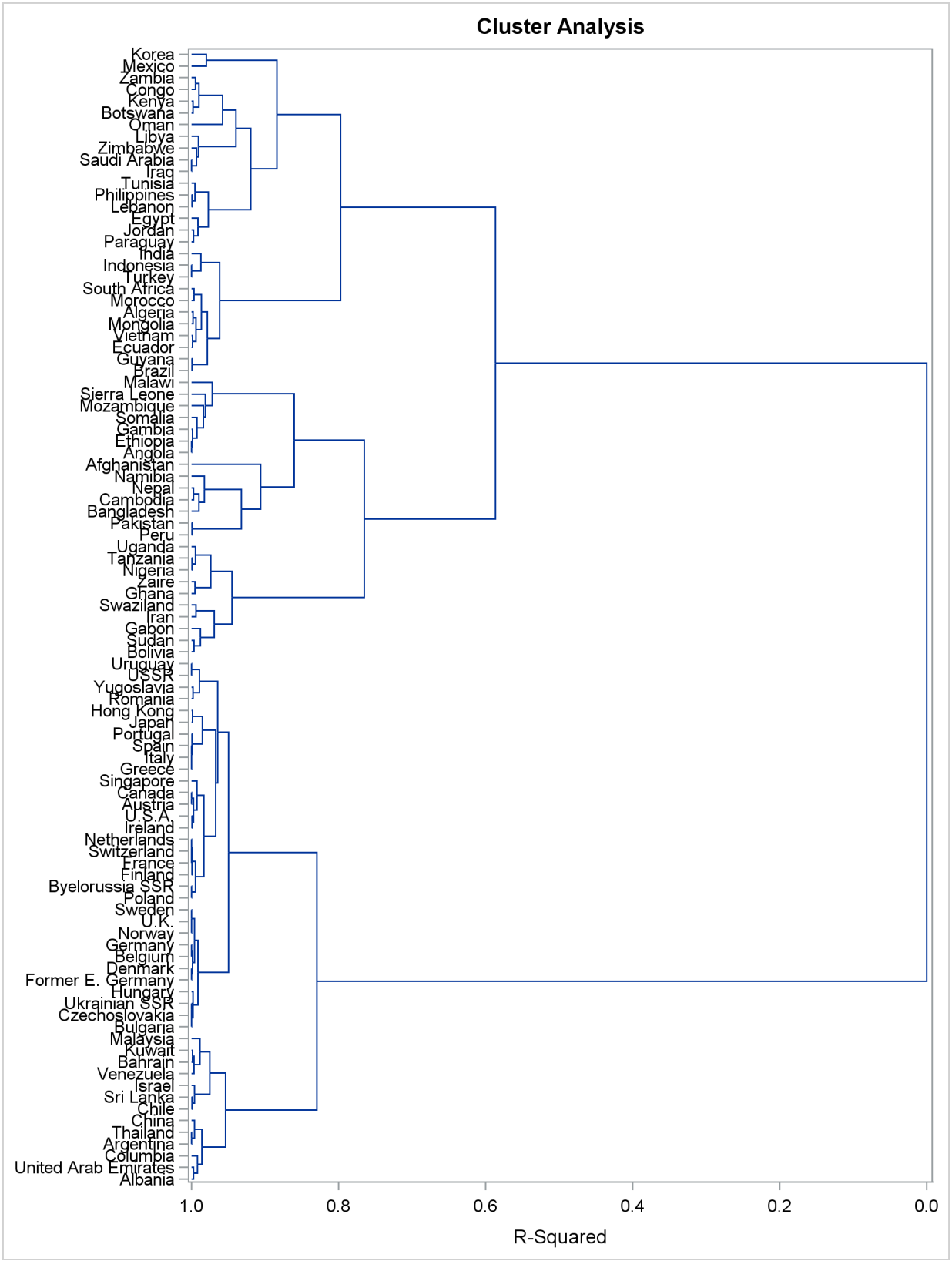


To interpret the values of the pseudo t^2 statistic, look down the column or look at the plot from right to left until you find the first value that is markedly larger than the previous value, then move back up the column or to the right in the plot by one step in the cluster history. In Figure 33.3, you can see possibly good clustering levels at eleven clusters, six clusters, three clusters, and two clusters.

Considered together, these statistics suggest that the data can be clustered into eleven clusters or three clusters. The following statements examine the results of clustering the data into three clusters.

Figure 33.4 displays the dendrogram. The figure provides a graphical view of the information in Figure 33.2. As the number of branches grows to the left from the root, the R square approaches 1; the first three clusters (branches of the tree) account for over half of the variation (about 77%, from Figure 33.4). In other words, only three clusters are necessary to explain over three-fourths of the variation.

Figure 33.4 Dendrogram of Clusters versus R-Square Values



You can use PROC TREE and the output data set from PROC CLUSTER to create a new data set that contains information about cluster membership as follows:

```
proc tree data=Tree out=New nclusters=3 noprint;
   height _rsq_;
   copy can1 can2;
   id country;
run;
```

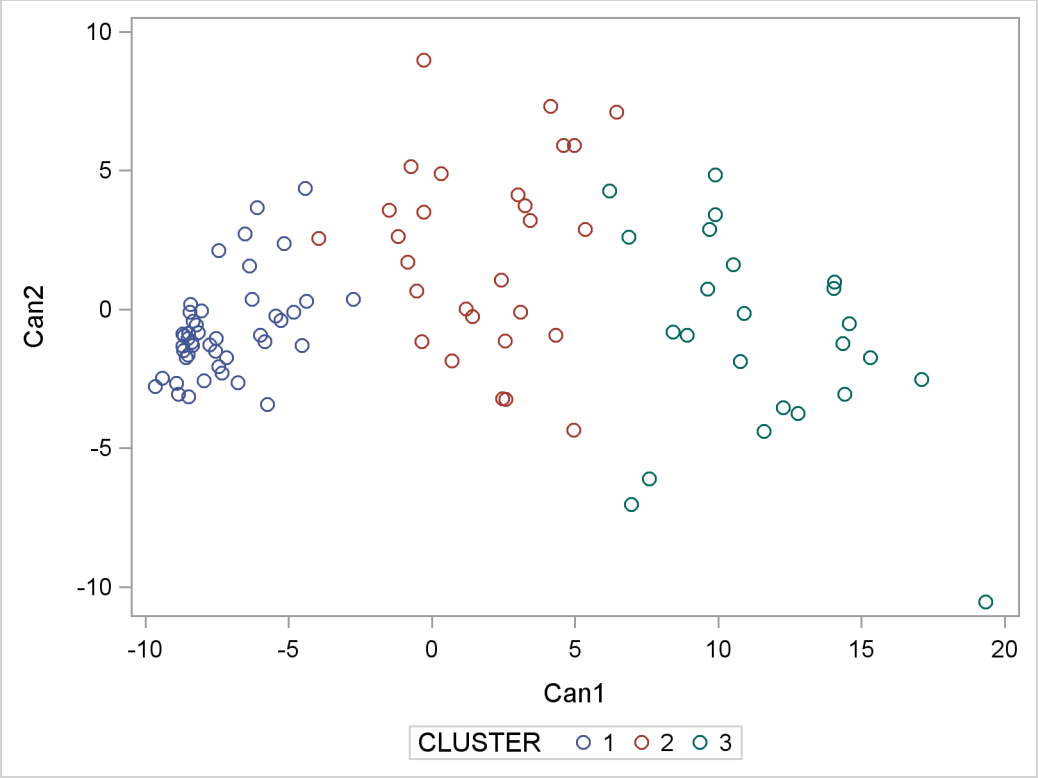
The SAS data set Tree is input. The OUT= option creates an output SAS data set named New that contains information about cluster membership. The NCLUSTERS= option specifies the number of clusters desired in the data set New. The results can be displayed in a scatter plot.

The following statements use the SGPLOT procedure to display the results that are in the SAS data set New:

```
proc sgplot data=New;
   scatter y=can2 x=can1 / group=cluster;
run;
```

The SCATTER statement requests a plot of the two canonical variables, using the value of the variable cluster, which is produced by PROC TREE as the identification variable. The results are displayed in Figure 33.5.

Figure 33.5 Plot of Canonical Variables and Cluster for Three Clusters



The statistics in Figure 33.2 and Figure 33.3, the dendrogram in Figure 33.4, and the plot of the canonical variables in Figure 33.5 assist in the estimation of the number of clusters in the data. There seems to be reasonable separation in the clusters. However, you must use this information, along with experience and knowledge of the field, to help in deciding the correct number of clusters.

Syntax: CLUSTER Procedure

The following statements are available in the CLUSTER procedure:

PROC CLUSTER METHOD=*name* < *options* > **;**
BY *variables* **;**
COPY *variables* **;**
FREQ *variable* **;**
ID *variable* **;**
RMSSTD *variable* **;**
VAR *variables* **;**

Only the PROC CLUSTER statement is required, except that the FREQ statement is required when the RMSSTD statement is used; otherwise the FREQ statement is optional. Usually only the VAR statement and possibly the ID and COPY statements are needed in addition to the PROC CLUSTER statement. The rest of this section provides detailed syntax information for each of the preceding statements, beginning with the PROC CLUSTER statement. The remaining statements are covered in alphabetical order.

PROC CLUSTER Statement

PROC CLUSTER METHOD=*name* < *options* > **;**

The PROC CLUSTER statement invokes the CLUSTER procedure. It also specifies a clustering method, and optionally specifies details for clustering methods, data sets, data processing, and displayed output.

Table 33.1 summarizes the *options* available in the PROC CLUSTER statement.

Table 33.1 PROC CLUSTER Statement Options

Option	Description
Specify input and output data sets	
DATA=	Specifies input data set
OUTTREE=	Creates output data set
Specify clustering methods	
BETA=	Specifies beta value for flexible beta method
HYBRID	Specifies Wong's hybrid clustering method
METHOD=	Specifies clustering method
MODE=	Specifies the minimum number of members for modal clusters
PENALTY=	Specifies the penalty coefficient for maximum likelihood
Control data processing prior to clustering	
NOEIGEN	Suppresses computation of eigenvalues
NONORM	Suppresses normalizing of distances
NOSQUARE	Suppresses squaring of distances
STANDARD	Standardizes variables
TRIM=	Omits points with low probability densities
Control density estimation	
K=	Specifies number of neighbors for *k*th-nearest-neighbor density estimation

Table 33.1 *continued*

Option	Description
R=	Specifies radius of sphere of support for uniform-kernel density estimation
Ties	
NOTIE	Suppresses checking for ties
Control display of the cluster history	
CCC	Displays cubic clustering criterion
NOID	Suppresses display of ID values
PRINT=	Specifies number of generations to display
PSEUDO	Displays pseudo F and t^2 statistics
RMSSTD	Displays root mean square standard deviation
RSQUARE	Displays R square and semipartial R square
Control other aspects of output	
NOPRINT	Suppresses display of all output
PLOTS=	Specifies ODS graphics details
SIMPLE	Displays simple summary statistics

METHOD=*name*

The METHOD= specification determines the clustering method used by the procedure. Any one of the following 11 methods can be specified for *name*:

AVERAGE | AVE requests average linkage (group average, unweighted pair-group method using arithmetic averages, UPGMA). Distance data are squared unless you specify the NOSQUARE option.

CENTROID | CEN requests the centroid method (unweighted pair-group method using centroids, UPGMC, centroid sorting, weighted-group method). Distance data are squared unless you specify the NOSQUARE option.

COMPLETE | COM requests complete linkage (furthest neighbor, maximum method, diameter method, rank order typal analysis). To reduce distortion of clusters by outliers, the TRIM= option is recommended.

DENSITY | DEN requests density linkage, which is a class of clustering methods using nonparametric probability density estimation. You must also specify either the K=, R=, or HYBRID option to indicate the type of density estimation to be used. See also the MODE= and DIM= options in this section.

EML requests maximum-likelihood hierarchical clustering for mixtures of spherical multivariate normal distributions with equal variances but possibly unequal mixing proportions. Use METHOD=EML only with coordinate data. See the PENALTY= option for details. The NONORM option does not affect the reported likelihood values but does affect other unrelated criteria. The EML method is much slower than the other methods in the CLUSTER procedure.

FLEXIBLE | FLE requests the Lance-Williams flexible-beta method. See the BETA= option in this section.

MCQUITTY | MCQ requests McQuitty's similarity analysis (weighted average linkage, weighted pair-group method using arithmetic averages, WPGMA).

MEDIAN | MED requests Gower's median method (weighted pair-group method using centroids, WPGMC). Distance data are squared unless you specify the NOSQUARE option.

SINGLE | SIN requests single linkage (nearest neighbor, minimum method, connectedness method, elementary linkage analysis, or dendritic method). To reduce chaining, you can use the TRIM= option with METHOD=SINGLE.

TWOSTAGE | TWO requests two-stage density linkage. You must also specify the K=, R=, or HYBRID option to indicate the type of density estimation to be used. See also the MODE= and DIM= options in this section.

WARD | WAR requests Ward's minimum-variance method (error sum of squares, trace W). Distance data are squared unless you specify the NOSQUARE option. To reduce distortion by outliers, the TRIM= option is recommended. See the NONORM option.

The following list provides details about the other *options*.

BETA=*n*

specifies the beta parameter for METHOD=FLEXIBLE. The value of *n* should be less than 1, usually between 0 and –1. By default, BETA=–0.25. Milligan (1987) suggests a somewhat smaller value, perhaps –0.5, for data with many outliers.

CCC

displays the cubic clustering criterion and approximate expected R square under the uniform null hypothesis (Sarle 1983). The statistics associated with the RSQUARE option, R square and semipartial R square, are also displayed. The CCC option applies only to coordinate data. The CCC option is not appropriate with METHOD=SINGLE because of the method's tendency to chop off tails of distributions. Computation of the CCC requires the eigenvalues of the covariance matrix. If the number of variables is large, computing the eigenvalues requires much computer time and memory.

DATA=*SAS-data-set*

names the input data set that contains observations to be clustered. By default, the procedure uses the most recently created SAS data set. If the data set is TYPE=DISTANCE, the data are interpreted as a distance matrix; the number of variables must equal the number of observations in the data set or in each BY group. The distances are assumed to be Euclidean, but the procedure accepts other types of distances or dissimilarities. If the data set is not TYPE=DISTANCE, the data are interpreted as coordinates in a Euclidean space, and Euclidean distances are computed. For more about TYPE=DISTANCE data sets, see Chapter A, "Special SAS Data Sets."

Data set types (such as TYPE=DISTANCE) do not persist when you copy or modify a data set. You must specify the TYPE= data set option for the new data set, as in the following example:

```
data dist2(type=distance);
   set dist;
run;
```

If you do not specify the TYPE=DISTANCE data set option, the new data set is the default TYPE=DATA. If you use the new data set in a procedure that accepts both TYPE=DATA or TYPE=DISTANCE data sets (such as PROC CLUSTER or PROC MODECLUS), the results will be incorrect.

You cannot use a TYPE=CORR data set as input to PROC CLUSTER, since the procedure uses dissimilarity measures. Instead, you can use a DATA step or the IML procedure to extract the correlation matrix from a TYPE=CORR data set and transform the values to dissimilarities such as 1 – r or $1 - r^2$, where r is the correlation.

All methods produce the same results when used with coordinate data as when used with Euclidean distances computed from the coordinates. However, the DIM= option must be used with distance data if you specify METHOD=TWOSTAGE or METHOD=DENSITY or if you specify the TRIM= option.

Certain methods that are most naturally defined in terms of coordinates require *squared* Euclidean distances to be used in the combinatorial distance formulas (Lance and Williams 1967). For this reason, distance data are automatically squared when used with METHOD=AVERAGE, METHOD=CENTROID, METHOD=MEDIAN, or METHOD=WARD. If you want the combinatorial formulas to be applied to the (unsquared) distances with these methods, use the NOSQUARE option.

DIM=*n*

specifies the dimensionality used when computing density estimates with the TRIM= option, METHOD=DENSITY, or METHOD=TWOSTAGE. The values of n must be greater than or equal to 1. The default is the number of variables if the data are coordinates; the default is 1 if the data are distances.

HYBRID

requests the Wong (1982) hybrid clustering method in which density estimates are computed from a preliminary cluster analysis using the k-means method. The DATA= data set must contain means, frequencies, and root mean square standard deviations of the preliminary clusters (see the FREQ and RMSSTD statements). To use HYBRID, you must use either a FREQ statement or a DATA= data set that contains a _FREQ_ variable, and you must also use either an RMSSTD statement or a DATA= data set that contains an _RMSSTD_ variable.

The MEAN= data set produced by the FASTCLUS procedure is suitable for input to the CLUSTER procedure for hybrid clustering. Since this data set contains _FREQ_ and _RMSSTD_ variables, you can use it as input and then omit the FREQ and RMSSTD statements.

You must specify either METHOD=DENSITY or METHOD=TWOSTAGE with the HYBRID option. You cannot use this option in combination with the TRIM=, K=, or R= option.

K=*n*

specifies the number of neighbors to use for kth-nearest-neighbor density estimation (Silverman 1986, pp. 19–21 and 96–99). The number of neighbors (n) must be at least two but less than the number of observations. See the MODE= option, which follows.

Density estimation is used with the TRIM=, METHOD=DENSITY, and METHOD=TWOSTAGE options.

MODE=*n*

specifies that, when two clusters are joined, each must have at least *n* members in order for either cluster to be designated a modal cluster. If you specify MODE=1, each cluster must also have a maximum density greater than the fusion density in order for either cluster to be designated a modal cluster.

Use the MODE= option only with METHOD=DENSITY or METHOD=TWOSTAGE. With METHOD=TWOSTAGE, the MODE= option affects the number of modal clusters formed. With METHOD=DENSITY, the MODE= option does not affect the clustering process but does determine the number of modal clusters reported on the output and identified by the _MODE_ variable in the output data set.

If you specify the K= option, the default value of MODE= is the same as the value of K= because the use of *k*th-nearest-neighbor density estimation limits the resolution that can be obtained for clusters with fewer than *k* members. If you do not specify the K= option, the default is MODE=2.

If you specify MODE=0, the default value is used instead of 0.

If you specify a FREQ statement or if a _FREQ_ variable appears in the input data set, the MODE= value is compared with the number of actual observations in the clusters being joined, not with the sum of the frequencies in the clusters.

NOEIGEN

suppresses computation of the eigenvalues of the covariance matrix and substitutes the variances of the variables for the eigenvalues when computing the cubic clustering criterion. The NOEIGEN option saves time if the number of variables is large, but it should be used only if the variables are nearly uncorrelated. If you specify the NOEIGEN option and the variables are highly correlated, the cubic clustering criterion might be very liberal. The NOEIGEN option applies only to coordinate data.

NOID

suppresses the display of ID values for the clusters joined at each generation of the cluster history.

NONORM

prevents the distances from being normalized to unit mean or unit root mean square with most methods. With METHOD=WARD, the NONORM option prevents the between-cluster sum of squares from being normalized by the total sum of squares to yield a squared semipartial correlation. The NONORM option does not affect the reported likelihood values with METHOD=EML, but it does affect other unrelated criteria, such as the _DIST_ variable.

NOPRINT

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 20, "Using the Output Delivery System."

NOSQUARE

prevents input distances from being squared with METHOD=AVERAGE, METHOD=CENTROID, METHOD=MEDIAN, or METHOD=WARD.

If you specify the NOSQUARE option with distance data, the data are assumed to be squared Euclidean distances for computing R-square and related statistics defined in a Euclidean coordinate system.

If you specify the NOSQUARE option with coordinate data with METHOD=CENTROID, METHOD=MEDIAN, or METHOD=WARD, then the combinatorial formula is applied to unsquared

Euclidean distances. The resulting cluster distances do not have their usual Euclidean interpretation and are therefore labeled "False" in the output.

NOTIE
prevents PROC CLUSTER from checking for ties for minimum distance between clusters at each generation of the cluster history. If your data are measured with such precision that ties are unlikely, then you can specify the NOTIE option to reduce slightly the time and space required by the procedure. See the section "Ties" on page 2037 for more information.

OUTTREE=*SAS-data-set*
creates an output data set that can be used by the TREE procedure to draw a tree diagram. If you want to create a SAS data set in a permanent library, you must specify a two-level name. For more information about permanent libraries and SAS data sets, see *SAS Language Reference: Concepts*. If you omit the OUTTREE= option, the data set is named by using the DATA*n* convention and is not permanently saved. If you do not want to create an output data set, use OUTTREE=_NULL_.

PENALTY=*p*
specifies the penalty coefficient used with METHOD=EML. See the section "Clustering Methods" on page 2026 for more information. Values for *p* must be greater than zero. By default, PENALTY=2.

PLOTS <(*global-plot-options***)> <=** *plot-request* **>**

PLOTS <(*global-plot-options***)> <=** (*plot-request* **<...** *plot-request* **>)>**
controls the plots produced through ODS Graphics.

ODS Graphics must be enabled before plots can be requested. For example:

```
ods graphics on;

proc cluster method=ward plots=all;
run;

ods graphics off;
```

For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 606 in Chapter 21, "Statistical Graphics Using ODS."

By default, PROC CLUSTER produces a dendrogram. PROC CLUSTER can also produce plots of the cubic clustering criterion, the pseudo F statistic, and the pseudo t^2 statistic from the cluster history table. These statistics are useful for estimating the number of clusters. Each statistic is plotted against the number of clusters. You can request that PROC CLUSTER create these graphs by specifying the CCC or PSEUDO options, or by specifying the statistics in a *plot-request* in the PLOT option. PROC CLUSTER might be unable to compute the statistics in some cases; for details, see the CCC and PSEUDO options. If a statistic cannot be computed, it cannot be plotted. PROC CLUSTER plots all of these statistics that are computed unless you tell it specifically what to plot using PLOTS=.

PROC CLUSTER has a CCC and PSEUDO option as well as CCC and PSEUDO *plot-requests*. All four options are illustrated in the following step:

```
ods graphics on;

proc cluster ccc pseudo plots=(ccc pseudo);
run;

ods graphics off;
```

The maximum number of clusters shown in all the plots is the minimum of the following quantities:

- the number of observations
- the value of the PRINT= option, if that option is specified
- the maximum number of clusters for which CCC is computed, if the CCC is plotted

The *global-plot-options* apply to all plots generated by the CLUSTER procedure. The *global-plot-options* are as follows:

MAXCLUS=*n*
: right-truncates the CCC, PSF, and PST2 plots at the *n* value. This prevents these plots from losing resolution when a large number of clusters are plotted. The default is MAXCLUS=200.

MAXPOINTS=*n*

MAXPTS=*n*
: suppresses the dendrogram when the number of clusters exceeds the *n* value. This prevents an unreadable plot from being produced. The default is MAXPOINTS=200.

UNPACKPANEL

UNPACK
: breaks a plot that is otherwise paneled into separate plots for each statistic.

ONLY
: suppresses the default plots. Only plots specifically requested are displayed.

The following *plot-requests* can be specified:

ALL
: generates all possible plots. The CCC and PSEUDO options must be specified to obtain the CCC, PSF and PST2 plots in addition to the dendrogram.

CCC
: implicitly specifies the CCC option and, if possible, plots the cubic clustering criterion against the number of clusters.

DENDROGRAM < (*dendrogram-options* **) >**
: requests a dendrogram and specifies *dendrogram-options*. A dendrogram is created by default unless the ONLY *global-plot-option* is requested.

  Unlike most graphs, the size of the dendrogram can vary as a function of the number of objects that appear in the dendrogram. You can specify the following *dendrogram-options* to control the size and appearance of the dendrogram:

COMPUTEHEIGHT=*a b*

CH=*a b*

specifies the constants for computing the height of the dendrogram. For n points being clustered, intercept a, and slope b, the height is based in part on $a + bn$. For a horizontal dendrogram, the default (given in pixels) is COMPUTEHEIGHT=100 12, the default height in pixels is max(100 + 12n, 480), the default height in inches is max(1.04167 + 0.125n, 5), and the default height in centimeters is max(2.64583 + 0.3175n, 12.7). For a vertical dendrogram, the default height is 480 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.

COMPUTEWIDTH=*a b*

CW=*a b*

specifies the constants for computing the width of the dendrogram. For n points being clustered, intercept a, and slope b, the width is based in part on $a + bn$. For a vertical dendrogram, the default (given in pixels) is COMPUTEWIDTH=100 12, the default width in pixels is max(100 + 12n, 640), the default width in inches is max(1.04167 + 0.125n, 6.66667), and the default width in centimeters is max(2.64583 + 0.3175n, 16.933). For a horizontal dendrogram, the default width is 640 pixels. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this option. Inches equals pixels divided by 96, and centimeters equals inches times 2.54.

HEIGHT=HEIGHT | MODE | NCL | RSQ

H=H | M | N | R

specifies the method for drawing the height of the dendrogram. HEIGHT=HEIGHT is the default.

HEIGHT=HEIGHT specifies the distance or similarity between the last clusters joined, as defined in the section "Clustering Methods" on page 2026.

HEIGHT=MODE pertains to the modal clusters. With METHOD=DENSITY, the mode indicates the number of modal clusters contained by the current cluster. With METHOD=TWOSTAGE, the mode gives the maximum density in each modal cluster and the fusion density, d^*, for clusters containing two or more modal clusters; for clusters that contain no modal clusters, that value of the _MODE_ variable is missing.

HEIGHT=NCL specifies that the number of clusters is used.

HEIGHT=RSQ specifies that the squared multiple correlation is used.

HORIZONTAL | VERTICAL

specifies either a horizontal dendrogram with the objects on the vertical axis (HORIZONTAL) or a vertical dendrogram with the objects on the horizontal axis (VERTICAL). The default is HORIZONTAL.

SETHEIGHT=*height*

SH=*height*

specifies the height of the dendrogram. By default, the height is based on the COMPUTE-HEIGHT= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

SETWIDTH=*width*

SW=*width*

specifies the width of the dendrogram. By default, the width is based on the COMPUTEWIDTH= option. The default unit is pixels, and you can use the UNIT= *dendrogram-option* to change the unit to inches or centimeters for this *dendrogram-option*.

UNIT=PX | IN | CM

specifies the unit (pixels, inches, or centimeters) for the SETHEIGHT=, SETWIDTH=, COMPUTEHEIGHT=, and COMPUTEWIDTH= *dendrogram-options*.

NONE

suppresses all plots.

PSEUDO

implicitly specifies the PSEUDO option and, if possible, plots the pseudo F statistic and the pseudo t^2 statistic against the number of clusters.

PSF

implicitly specifies the PSEUDO option and, if possible, plots the pseudo F statistic against the number of clusters.

PST2

implicitly specifies the PSEUDO option and, if possible, plots the pseudo t^2 statistic against the number of clusters.

You can specify one or more of the *plot-requests* in the same PLOT option. For example, all of the following are valid:

```
proc cluster plots=(ccc pst2);
proc cluster plots=(psf);
proc cluster plots=psf;
```

The first statement plots both the cubic clustering criterion and the pseudo t^2 statistic, while the second and third statements plot the pseudo F statistic only. When you specify only one plot request, you can omit the parentheses around the plot request. When you specify more than one *plot-request*, you must specify parentheses. Otherwise the second and subsequent *plot-requests* are *options*. Since CCC and PSEUDO are both *options* as well as *plot-requests*, the following three statements are valid, but they are not equivalent:

```
proc cluster plots(only)=ccc pseudo;
proc cluster plots(only)=pseudo ccc;
proc cluster plots(only)=(ccc pseudo);
```

The first two examples have one *plot-request* and one procedure *option*. The third example has two *plot-requests*.

The names of the graphs that PROC CLUSTER generates are listed in Table 33.5, along with the required statements and options.

PRINT=*n* | **P=***n*
specifies the number of generations of the cluster history to display. The PRINT= option displays the latest *n* generations; for example, PRINT=5 displays the cluster history from one cluster through five clusters. The value of PRINT= must be a nonnegative integer. The default is to display all generations. Specify PRINT=0 to suppress the cluster history.

PSEUDO
displays pseudo F and t^2 statistics. This option is effective only when the data are coordinates or when METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD is specified. See the section "Miscellaneous Formulas" on page 2033 for more information. The PSEUDO option is not appropriate with METHOD=SINGLE because of the method's tendency to chop off tails of distributions.

R=*n*
specifies the radius of the sphere of support for uniform-kernel density estimation (Silverman 1986, pp. 11–13 and 75–94).

The value of R= must be greater than zero.

Density estimation is used with the TRIM=, METHOD=DENSITY, and METHOD=TWOSTAGE options.

RMSSTD
displays the root mean square standard deviation of each cluster. This option is effective only when the data are coordinates or when METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD is specified.

See the section "Miscellaneous Formulas" on page 2033 for more information.

RSQUARE | **RSQ**
displays the R square and semipartial R square. This option is effective only when the data are coordinates or when METHOD=AVERAGE or METHOD=CENTROID is specified. The R square and semipartial R square statistics are always displayed with METHOD=WARD. See the section "Miscellaneous Formulas" on page 2033 for more information..

SIMPLE | **S**
displays means, standard deviations, skewness, kurtosis, and a coefficient of bimodality. The SIMPLE option applies only to coordinate data. See the section "Miscellaneous Formulas" on page 2033 for more information.

STANDARD | **STD**
standardizes the variables to mean 0 and standard deviation 1. The STANDARD option applies only to coordinate data.

TRIM=*p*
omits points with low estimated probability densities from the analysis. Valid values for the TRIM= option are $0 \leq p < 100$. If $p < 1$, then p is the proportion of observations omitted. If $p \geq 1$, then p is interpreted as a percentage. A specification of TRIM=10, which trims 10% of the points, is a reasonable value for many data sets. Densities are estimated by the kth-nearest-neighbor or uniform-kernel method. Trimmed points are indicated by a negative value of the _FREQ_ variable in the OUTTREE= data set.

You must use either the K= or R= option when you use TRIM=. You cannot use the HYBRID option in combination with TRIM=, so you might want to use the DIM= option instead. If you specify the

STANDARD option in combination with TRIM=, the variables are standardized both before and after trimming.

The TRIM= option is useful for removing outliers and reducing chaining. Trimming is highly recommended with METHOD=WARD or METHOD=COMPLETE because clusters from these methods can be severely distorted by outliers. Trimming is also valuable with METHOD=SINGLE since single linkage is the method most susceptible to chaining. Most other methods also benefit from trimming. However, trimming is unnecessary with METHOD=TWOSTAGE or METHOD=DENSITY when *k*th-nearest-neighbor density estimation is used.

Use of the TRIM= option can spuriously inflate the cubic clustering criterion and the pseudo F and t^2 statistics. Trimming only outliers improves the accuracy of the statistics, but trimming saddle regions between clusters yields excessively large values.

BY Statement

BY *variables* **;**

You can specify a BY statement with PROC CLUSTER to obtain separate analyses of observations in groups that are defined by the BY variables. When a BY statement appears, the procedure expects the input data set to be sorted in order of the BY variables. If you specify more than one BY statement, only the last one specified is used.

If your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data by using the SORT procedure with a similar BY statement.
- Specify the NOTSORTED or DESCENDING option in the BY statement for the CLUSTER procedure. The NOTSORTED option does not mean that the data are unsorted but rather that the data are arranged in groups (according to values of the BY variables) and that these groups are not necessarily in alphabetical or increasing numeric order.
- Create an index on the BY variables by using the DATASETS procedure (in Base SAS software).

For more information about BY-group processing, see the discussion in *SAS Language Reference: Concepts*. For more information about the DATASETS procedure, see the discussion in the *Base SAS Procedures Guide*.

COPY Statement

COPY *variables* **;**

The variables in the COPY statement are copied from the input data set to the OUTTREE= data set. Observations in the OUTTREE= data set that represent clusters of more than one observation from the input data set have missing values for the COPY variables.

FREQ Statement

FREQ *variable* **;**

If one variable in the input data set represents the frequency of occurrence for other values in the observation, specify the variable's name in a FREQ statement. PROC CLUSTER then treats the data set as if each observation appeared n times, where n is the value of the FREQ variable for the observation. Noninteger values of the FREQ variable are truncated to the largest integer less than the FREQ value.

If you omit the FREQ statement but the DATA= data set contains a variable called _FREQ_, then frequencies are obtained from the _FREQ_ variable. If neither a FREQ statement nor an _FREQ_ variable is present, each observation is assumed to have a frequency of one.

If each observation in the DATA= data set represents a cluster (for example, clusters formed by PROC FASTCLUS), the variable specified in the FREQ statement should give the number of original observations in each cluster.

If you specify the RMSSTD statement, a FREQ statement is required. A FREQ statement or _FREQ_ variable is required when you specify the HYBRID option.

With most clustering methods, the same clusters are obtained from a data set with a FREQ variable as from a similar data set without a FREQ variable, if each observation is repeated as many times as the value of the FREQ variable in the first data set. The FLEXIBLE method can yield different results due to the nature of the combinatorial formula. The DENSITY and TWOSTAGE methods are also exceptions because two identical observations can be absorbed one at a time by a cluster with a higher density. If you are using a FREQ statement with either the DENSITY or TWOSTAGE method, see the MODE=option for details.

ID Statement

ID *variable* **;**

The values of the ID variable identify observations in the displayed cluster history and in the OUTTREE= data set. If the ID statement is omitted, each observation is denoted by OBn, where n is the observation number.

RMSSTD Statement

RMSSTD *variable* **;**

If the coordinates in the DATA= data set represent cluster means (for example, formed by the FASTCLUS procedure), you can obtain accurate statistics in the cluster histories for METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD if the data set contains both of the following:

- a variable giving the number of original observations in each cluster (see the discussion of the FREQ statement earlier in this chapter)
- a variable giving the root mean squared standard deviation of each cluster

Specify the name of the variable containing root mean squared standard deviations in the RMSSTD statement. If you specify the RMSSTD statement, you must also specify a FREQ statement.

If you omit the RMSSTD statement but the DATA= data set contains a variable called _RMSSTD_, then the root mean squared standard deviations are obtained from the _RMSSTD_ variable.

An RMSSTD statement or _RMSSTD_ variable is required when you specify the HYBRID option.

A data set created by PROC FASTCLUS, using the MEAN= option, contains _FREQ_ and _RMSSTD_ variables, so you do not have to use FREQ and RMSSTD statements when using such a data set as input to the CLUSTER procedure.

VAR Statement

VAR *variables* **;**

The VAR statement lists numeric variables to be used in the cluster analysis. If you omit the VAR statement, all numeric variables not listed in other statements are used.

Details: CLUSTER Procedure

Clustering Methods

The following notation is used, with lowercase symbols generally pertaining to observations and uppercase symbols pertaining to clusters:

n	number of observations
v	number of variables if data are coordinates
G	number of clusters at any given level of the hierarchy
x_i or $\mathbf{x}_i$	ith observation (row vector if coordinate data)
C_K	Kth cluster, subset of $\{1, 2, \ldots, n\}$
N_K	number of observations in C_K
$\bar{\mathbf{x}}$	sample mean vector
$\bar{\mathbf{x}}_K$	mean vector for cluster C_K
$\|\mathbf{x}\|$	Euclidean length of the vector $\mathbf{x}$—that is, the square root of the sum of the squares of the elements of $\mathbf{x}$
T	$\sum_{i=1}^{n} \|\mathbf{x}_i - \bar{\mathbf{x}}\|^2$
W_K	$\sum_{i \in C_k} \|\mathbf{x}_i - \bar{\mathbf{x}}_K\|^2$
P_G	$\sum W_J$, where summation is over the G clusters at the Gth level of the hierarchy
B_{KL}	$W_M - W_K - W_L$ if $C_M = C_K \cup C_L$
$d(\mathbf{x}, \mathbf{y})$	any distance or dissimilarity measure between observations or vectors $\mathbf{x}$ and $\mathbf{y}$
D_{KL}	any distance or dissimilarity measure between clusters C_K and C_L

The distance between two clusters can be defined either directly or combinatorially (Lance and Williams 1967)—that is, by an equation for updating a distance matrix when two clusters are joined. In all of the following combinatorial formulas, it is assumed that clusters C_K and C_L are merged to form C_M, and the formula gives the distance between the new cluster C_M and any other cluster C_J.

For an introduction to most of the methods used in the CLUSTER procedure, see Massart and Kaufman (1983).

Average Linkage

The following method is obtained by specifying METHOD=AVERAGE. The distance between two clusters is defined by

$$D_{KL} = \frac{1}{N_K N_L} \sum_{i \in C_K} \sum_{j \in C_L} d(x_i, x_j)$$

If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then

$$D_{KL} = \|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2 + \frac{W_K}{N_K} + \frac{W_L}{N_L}$$

The combinatorial formula is

$$D_{JM} = \frac{N_K D_{JK} + N_L D_{JL}}{N_M}$$

In average linkage the distance between two clusters is the average distance between pairs of observations, one in each cluster. Average linkage tends to join clusters with small variances, and it is slightly biased toward producing clusters with the same variance.

Average linkage was originated by Sokal and Michener (1958).

Centroid Method

The following method is obtained by specifying METHOD=CENTROID. The distance between two clusters is defined by

$$D_{KL} = \|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2$$

If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{N_K D_{JK} + N_L D_{JL}}{N_M} - \frac{N_K N_L D_{KL}}{N_M^2}$$

In the centroid method, the distance between two clusters is defined as the (squared) Euclidean distance between their centroids or means. The centroid method is more robust to outliers than most other hierarchical methods but in other respects might not perform as well as Ward's method or average linkage (Milligan 1980).

The centroid method was originated by Sokal and Michener (1958).

Complete Linkage

The following method is obtained by specifying METHOD=COMPLETE. The distance between two clusters is defined by

$$D_{KL} = \max_{i \in C_K} \max_{j \in C_L} d(x_i, x_j)$$

The combinatorial formula is

$$D_{JM} = \max(D_{JK}, D_{JL})$$

In complete linkage, the distance between two clusters is the maximum distance between an observation in one cluster and an observation in the other cluster. Complete linkage is strongly biased toward producing clusters with roughly equal diameters, and it can be severely distorted by moderate outliers (Milligan 1980).

Complete linkage was originated by Sørensen (1948).

Density Linkage

The phrase *density linkage* is used here to refer to a class of clustering methods that use nonparametric probability density estimates (for example, Hartigan 1975, pp. 205–212; Wong 1982; Wong and Lane 1983). Density linkage consists of two steps:

1. A new dissimilarity measure, d^*, based on density estimates and adjacencies is computed. If x_i and x_j are adjacent (the definition of *adjacency* depends on the method of density estimation), then $d^*(x_i, x_j)$ is the reciprocal of an estimate of the density midway between x_i and x_j; otherwise, $d^*(x_i, x_j)$ is infinite.
2. A single linkage cluster analysis is performed using d^*.

The CLUSTER procedure supports three types of density linkage: the *k*th-nearest-neighbor method, the uniform-kernel method, and Wong's hybrid method. These are obtained by using METHOD=DENSITY and the K=, R=, and HYBRID options, respectively.

kth-Nearest-Neighbor Method

The *k*th-nearest-neighbor method (Wong and Lane 1983) uses *k*th-nearest-neighbor density estimates. Let $r_k(x)$ be the distance from point x to the *k*th-nearest observation, where k is the value specified for the K= option. Consider a closed sphere centered at x with radius $r_k(x)$. The estimated density at x, $f(x)$, is the proportion of observations within the sphere divided by the volume of the sphere. The new dissimilarity measure is computed as

$$d^*(x_i, x_j) = \begin{cases} \frac{1}{2}\left(\frac{1}{f(x_i)} + \frac{1}{f(x_j)}\right) & \text{if } d(x_i, x_j) \le \max(r_k(x_i), r_k(x_j)) \\ \infty & \text{otherwise} \end{cases}$$

Wong and Lane (1983) show that *k*th-nearest-neighbor density linkage is strongly set consistent for high-density (density-contour) clusters if k is chosen such that $k/n \to 0$ and $k/\ln(n) \to \infty$ as $n \to \infty$. Wong and Schaack (1982) discuss methods for estimating the number of population clusters by using *k*th-nearest-neighbor clustering.

Uniform-Kernel Method

The uniform-kernel method uses uniform-kernel density estimates. Let r be the value specified for the R= option. Consider a closed sphere centered at point x with radius r. The estimated density at x, $f(x)$, is the proportion of observations within the sphere divided by the volume of the sphere. The new dissimilarity measure is computed as

$$d^*(x_i, x_j) = \begin{cases} \frac{1}{2}\left(\frac{1}{f(x_i)} + \frac{1}{f(x_j)}\right) & \text{if } d(x_i, x_j) \le r \\ \infty & \text{otherwise} \end{cases}$$

Wong's Hybrid Method

The Wong (1982) hybrid clustering method uses density estimates based on a preliminary cluster analysis by the k-means method. The preliminary clustering can be done by the FASTCLUS procedure, by using the MEAN= option to create a data set containing cluster means, frequencies, and root mean squared standard deviations. This data set is used as input to the CLUSTER procedure, and the HYBRID option is specified with METHOD=DENSITY to request the hybrid analysis. The hybrid method is appropriate for very large data sets but should not be used with small data sets—say, than those with fewer than 100 observations in the original data. The term *preliminary cluster* refers to an observation in the DATA= data set.

For preliminary cluster C_K, N_K and W_K are obtained from the input data set, as are the cluster means or the distances between the cluster means. Preliminary clusters C_K and C_L are considered adjacent if the midpoint between $\bar{x}_K$ and $\bar{\mathbf{x}}_L$ is closer to either $\bar{\mathbf{x}}_K$ or $\bar{\mathbf{x}}_L$ than to any other preliminary cluster mean or, equivalently, if $d^2(\bar{\mathbf{x}}_K, \bar{\mathbf{x}}_L) < d^2(\bar{\mathbf{x}}_K, \bar{\mathbf{x}}_M) + d^2(\bar{\mathbf{x}}_L, \bar{\mathbf{x}}_M)$ for all other preliminary clusters C_M, $M \neq K$ or L. The new dissimilarity measure is computed as

$$d^*(\bar{\mathbf{x}}_K, \bar{\mathbf{x}}_L) = \begin{cases} \frac{\left(W_K + W_L + \frac{1}{4}(N_K + N_L)d^2(\bar{\mathbf{x}}_K, \bar{\mathbf{x}}_L)\right)^{\frac{v}{2}}}{(N_K + N_L)^{1+\frac{v}{2}}} & \text{if } C_K \text{ and } C_L \text{ are adjacent} \\ \infty & \text{otherwise} \end{cases}$$

Using the K= and R= Options

The values of the K= and R= options are called *smoothing parameters*. Small values of K= or R= produce jagged density estimates and, as a consequence, many modes. Large values of K= or R= produce smoother density estimates and fewer modes. In the hybrid method, the smoothing parameter is the number of clusters in the preliminary cluster analysis. The number of modes in the final analysis tends to increase as the number of clusters in the preliminary analysis increases. Wong (1982) suggests using $n^{0.3}$ preliminary clusters, where n is the number of observations in the original data set. There is no rule of thumb for selecting K= values. For all types of density linkage, you should repeat the analysis with several different values of the smoothing parameter (Wong and Schaack 1982).

There is no simple answer to the question of which smoothing parameter to use (Silverman 1986, pp. 43–61, 84–88, and 98–99). It is usually necessary to try several different smoothing parameters. A reasonable first guess for the R= option in many coordinate data sets is given by

$$\left[\frac{2^{v+2}(v+2)\Gamma(\frac{v}{2}+1)}{nv^2}\right]^{\frac{1}{v+4}} \sqrt{\sum_{l=1}^{v} s_l^2}$$

where s_l^2 is the standard deviation of the lth variable. The estimate for R= can be computed in a DATA step by using the GAMMA function for Γ. This formula is derived under the assumption that the data are

sampled from a multivariate normal distribution and tends, therefore, to be too large (oversmooth) if the true distribution is multimodal. Robust estimates of the standard deviations can be preferable if there are outliers. If the data are distances, the factor $\sum s_l^2$ can be replaced by an average (mean, trimmed mean, median, root mean square, and so on) distance divided by $\sqrt{2}$. To prevent outliers from appearing as separate clusters, you can also specify K=2, or more generally K=m, $m \geq 2$, which in most cases forces clusters to have at least m members.

If the variables all have unit variance (for example, if the STANDARD option is used), Table 33.2 can be used to obtain an initial guess for the R= option.

Since infinite d^* values occur in density linkage, the final number of clusters can exceed one when there are wide gaps between the clusters or when the smoothing parameter results in little smoothing.

Density linkage applies no constraints to the shapes of the clusters and, unlike most other hierarchical clustering methods, is capable of recovering clusters with elongated or irregular shapes. Since density linkage uses less prior knowledge about the shape of the clusters than do methods restricted to compact clusters, density linkage is less effective at recovering compact clusters from small samples than are methods that always recover compact clusters, regardless of the data.

Table 33.2 Reasonable First Guess for the R= Option for Standardized Data

Number of Observations	Number of Variables									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
20	1.01	1.36	1.77	2.23	2.73	3.25	3.81	4.38	4.98	5.60
35	0.91	1.24	1.64	2.08	2.56	3.08	3.62	4.18	4.77	5.38
50	0.84	1.17	1.56	1.99	2.46	2.97	3.50	4.06	4.64	5.24
75	0.78	1.09	1.47	1.89	2.35	2.85	3.38	3.93	4.50	5.09
100	0.73	1.04	1.41	1.82	2.28	2.77	3.29	3.83	4.40	4.99
150	0.68	0.97	1.33	1.73	2.18	2.66	3.17	3.71	4.27	4.85
200	0.64	0.93	1.28	1.67	2.11	2.58	3.09	3.62	4.17	4.75
350	0.57	0.85	1.18	1.56	1.98	2.44	2.93	3.45	4.00	4.56
500	0.53	0.80	1.12	1.49	1.91	2.36	2.84	3.35	3.89	4.45
750	0.49	0.74	1.06	1.42	1.82	2.26	2.74	3.24	3.77	4.32
1000	0.46	0.71	1.01	1.37	1.77	2.20	2.67	3.16	3.69	4.23
1500	0.43	0.66	0.96	1.30	1.69	2.11	2.57	3.06	3.57	4.11
2000	0.40	0.63	0.92	1.25	1.63	2.05	2.50	2.99	3.49	4.03

EML

The following method is obtained by specifying METHOD=EML. The distance between two clusters is given by

$$D_{KL} = nv \ln\left(1 + \frac{B_{KL}}{P_G}\right) - 2\left(N_M \ln(N_M) - N_K \ln(N_K) - N_L \ln(N_L)\right)$$

The EML method joins clusters to maximize the likelihood at each level of the hierarchy under the following assumptions:

- multivariate normal mixture
- equal spherical covariance matrices
- unequal sampling probabilities

The EML method is similar to Ward's minimum-variance method but removes the bias toward equal-sized clusters. Practical experience has indicated that EML is somewhat biased toward unequal-sized clusters. You can specify the PENALTY= option to adjust the degree of bias. If you specify PENALTY=*p*, the formula is modified to

$$D_{KL} = nv \ln\left(1 + \frac{B_{KL}}{P_G}\right) - p\left(N_M \ln(N_M) - N_K \ln(N_K) - N_L \ln(N_L)\right)$$

The EML method was derived by W. S. Sarle of SAS Institute from the maximum likelihood formula obtained by Symons (1981, p. 37, Equation 8) for disjoint clustering. There are currently no other published references on the EML method.

Flexible-Beta Method

The following method is obtained by specifying METHOD=FLEXIBLE. The combinatorial formula is

$$D_{JM} = (D_{JK} + D_{JL})\frac{1-b}{2} + D_{KL}b$$

where b is the value of the BETA= option, or –0.25 by default.

The flexible-beta method was developed by Lance and Williams (1967); see also Milligan (1987).

McQuitty's Similarity Analysis

The following method is obtained by specifying METHOD=MCQUITTY. The combinatorial formula is

$$D_{JM} = \frac{D_{JK} + D_{JL}}{2}$$

The method was independently developed by Sokal and Michener (1958) and McQuitty (1966).

Median Method

The following method is obtained by specifying METHOD=MEDIAN. If $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{D_{JK} + D_{JL}}{2} - \frac{D_{KL}}{4}$$

The median method was developed by Gower (1967).

Single Linkage

The following method is obtained by specifying METHOD=SINGLE. The distance between two clusters is defined by

$$D_{KL} = \min_{i \in C_K} \min_{j \in C_L} d(x_i, x_j)$$

The combinatorial formula is

$$D_{JM} = \min(D_{JK}, D_{JL})$$

In single linkage, the distance between two clusters is the minimum distance between an observation in one cluster and an observation in the other cluster. Single linkage has many desirable theoretical properties (Jardine and Sibson 1971; Fisher and Van Ness 1971; Hartigan 1981) but has fared poorly in Monte Carlo studies (for example, Milligan 1980). By imposing no constraints on the shape of clusters, single linkage sacrifices performance in the recovery of compact clusters in return for the ability to detect elongated and irregular clusters. You must also recognize that single linkage tends to chop off the tails of distributions before separating the main clusters (Hartigan 1981). The notorious chaining tendency of single linkage can be alleviated by specifying the TRIM= option (Wishart 1969, pp. 296–298).

Density linkage and two-stage density linkage retain most of the virtues of single linkage while performing better with compact clusters and possessing better asymptotic properties (Wong and Lane 1983).

Single linkage was originated by Florek et al. (1951b, a) and later reinvented by McQuitty (1957) and Sneath (1957).

Two-Stage Density Linkage

If you specify METHOD=DENSITY, the modal clusters often merge before all the points in the tails have clustered. The option METHOD=TWOSTAGE is a modification of density linkage that ensures that all points are assigned to modal clusters before the modal clusters are permitted to join. The CLUSTER procedure supports the same three varieties of two-stage density linkage as of ordinary density linkage: *k*th-nearest neighbor, uniform kernel, and hybrid.

In the first stage, disjoint modal clusters are formed. The algorithm is the same as the single linkage algorithm ordinarily used with density linkage, with one exception: two clusters are joined only if at least one of the two clusters has fewer members than the number specified by the MODE= option. At the end of the first stage, each point belongs to one modal cluster.

In the second stage, the modal clusters are hierarchically joined by single linkage. The final number of clusters can exceed one when there are wide gaps between the clusters or when the smoothing parameter is small.

Each stage forms a tree that can be plotted by the TREE procedure. By default, the TREE procedure plots the tree from the first stage. To obtain the tree for the second stage, use the option HEIGHT=MODE in the PROC TREE statement. You can also produce a single tree diagram containing both stages, with the number of clusters as the height axis, by using the option HEIGHT=N in the PROC TREE statement. To produce an output data set from PROC TREE containing the modal clusters, use _HEIGHT_ for the HEIGHT variable (the default) and specify LEVEL=0.

Two-stage density linkage was developed by W. S. Sarle of SAS Institute. There are currently no other published references on two-stage density linkage.

Ward's Minimum-Variance Method

The following method is obtained by specifying METHOD=WARD. The distance between two clusters is defined by

$$D_{KL} = B_{KL} = \frac{\|\bar{\mathbf{x}}_K - \bar{\mathbf{x}}_L\|^2}{\frac{1}{N_K} + \frac{1}{N_L}}$$

If $d(\mathbf{x}, \mathbf{y}) = \frac{1}{2}\|\mathbf{x} - \mathbf{y}\|^2$, then the combinatorial formula is

$$D_{JM} = \frac{(N_J + N_K)D_{JK} + (N_J + N_L)D_{JL} - N_J D_{KL}}{N_J + N_M}$$

In Ward's minimum-variance method, the distance between two clusters is the ANOVA sum of squares between the two clusters added up over all the variables. At each generation, the within-cluster sum of squares is minimized over all partitions obtainable by merging two clusters from the previous generation. The sums of squares are easier to interpret when they are divided by the total sum of squares to give proportions of variance (squared semipartial correlations).

Ward's method joins clusters to maximize the likelihood at each level of the hierarchy under the following assumptions:

- multivariate normal mixture
- equal spherical covariance matrices
- equal sampling probabilities

Ward's method tends to join clusters with a small number of observations, and it is strongly biased toward producing clusters with roughly the same number of observations. It is also very sensitive to outliers (Milligan 1980).

Ward (1963) describes a class of hierarchical clustering methods including the minimum variance method.

Miscellaneous Formulas

The root mean squared standard deviation of a cluster C_K is

$$\text{RMSSTD} = \sqrt{\frac{W_K}{v(N_K - 1)}}$$

The R-square statistic for a given level of the hierarchy is

$$R^2 = 1 - \frac{P_G}{T}$$

The squared semipartial correlation for joining clusters C_K and C_L is

$$\text{semipartial } R^2 = \frac{B_{KL}}{T}$$

The bimodality coefficient is

$$b = \frac{m_3^2 + 1}{m_4 + \frac{3(n-1)^2}{(n-2)(n-3)}}$$

where m_3 is skewness and m_4 is kurtosis. Values of b greater than 0.555 (the value for a uniform population) can indicate bimodal or multimodal marginal distributions. The maximum of 1.0 (obtained for the Bernoulli distribution) is obtained for a population with only two distinct values. Very heavy-tailed distributions have small values of b regardless of the number of modes.

Formulas for the cubic-clustering criterion and approximate expected R square are given in Sarle (1983).

The pseudo F statistic for a given level is

$$\text{pseudo } F = \frac{\frac{T-P_G}{G-1}}{\frac{P_G}{n-G}}$$

The pseudo t^2 statistic for joining C_K and C_L is

$$\text{pseudo } t^2 = \frac{B_{KL}}{\frac{W_K+W_L}{N_K+N_L-2}}$$

The pseudo F and t^2 statistics can be useful indicators of the number of clusters, but they are *not* distributed as F and t^2 random variables. If the data are independently sampled from a multivariate normal distribution with a scalar covariance matrix and if the clustering method allocates observations to clusters randomly (which no clustering method actually does), then the pseudo F statistic is distributed as an F random variable with $v(G-1)$ and $v(n-G)$ degrees of freedom. Under the same assumptions, the pseudo t^2 statistic is distributed as an F random variable with v and $v(N_K + N_L - 2)$ degrees of freedom. The pseudo t^2 statistic differs computationally from Hotelling's T^2 in that the latter uses a general symmetric covariance matrix instead of a scalar covariance matrix. The pseudo F statistic was suggested by Caliński and Harabasz (1974). The pseudo t^2 statistic is related to the $J_e(2)/J_e(1)$ statistic of Duda and Hart (1973) by

$$\frac{J_e(2)}{J_e(1)} = \frac{W_K + W_L}{W_M} = \frac{1}{1 + \frac{t^2}{N_K+N_L-2}}$$

See Milligan and Cooper (1985) and Cooper and Milligan (1988) regarding the performance of these statistics in estimating the number of population clusters. Conservative tests for the number of clusters using the pseudo F and t^2 statistics can be obtained by the Bonferroni approach (Hawkins, Muller, and ten Krooden 1982, pp. 337–340).

Ultrametrics

A dissimilarity measure $d(x, y)$ is called an *ultrametric* if it satisfies the following conditions:

- $d(x, x) = 0$ for all x
- $d(x, y) \geq 0$ for all x, y
- $d(x, y) = d(y, x)$ for all x, y
- $d(x, y) \leq \max(d(x, z), d(y, z))$ for all x, y, and z

Any hierarchical clustering method induces a dissimilarity measure on the observations—say, $h(x_i, x_j)$. Let C_M be the cluster with the fewest members that contains both x_i and x_j. Assume C_M was formed by joining C_K and C_L. Then define $h(x_i, x_j) = D_{KL}$.

If the fusion of C_K and C_L reduces the number of clusters from g to $g - 1$, then define $D_{(g)} = D_{KL}$. Johnson (1967) shows that if

$$0 \leq D_{(n)} \leq D_{(n-1)} \leq \cdots \leq D_{(2)}$$

then $h(\cdot, \cdot)$ is an ultrametric. A method that always satisfies this condition is said to be a *monotonic* or *ultrametric clustering method*. All methods implemented in PROC CLUSTER except CENTROID, EML, and MEDIAN are ultrametric (Milligan 1979; Batagelj 1981).

Algorithms

Anderberg (1973) describes three algorithms for implementing agglomerative hierarchical clustering: stored data, stored distance, and sorted distance. The algorithms used by PROC CLUSTER for each method are indicated in Table 33.3. For METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, either the stored data or the stored distance algorithm can be used. For these methods, if the data are distances or if you specify the NOSQUARE option, the stored distance algorithm is used; otherwise, the stored data algorithm is used.

Table 33.3 Three Algorithms for Implementing Agglomerative Hierarchical Clustering

	Algorithm		
Clustering Method	**Stored Data**	**Stored Distance**	**Sorted Distance**
AVERAGE	x	x	
CENTROID	x	x	
COMPLETE		x	
DENSITY			x
EML	x		
FLEXIBLE		x	
MCQUITTY		x	
MEDIAN		x	
SINGLE		x	
TWOSTAGE			x
WARD	x	x	

Note: All of the hierarchical methods accept coordinate data. Methods that require stored or sorted distances automatically calculate distances from the coordinates.

Computational Resources

The CLUSTER procedure stores the data (including the COPY and ID variables) in memory or, if necessary, on disk. If eigenvalues are computed, the covariance matrix is stored in memory. If the stored distance or sorted distance algorithm is used, the distances are stored in memory or, if necessary, on disk.

With coordinate data, the increase in CPU time is roughly proportional to the number of variables. The VAR statement should list the variables in order of decreasing variance for greatest efficiency.

For both coordinate and distance data, the dominant factor determining CPU time is the number of observations. For density methods with coordinate data, the asymptotic time requirements are somewhere between $n \ln(n)$ and n^2, depending on how the smoothing parameter increases. For other methods except EML, time is roughly proportional to n^2. For the EML method, time is roughly proportional to n^3.

PROC CLUSTER runs much faster if the data can be stored in memory and, when the stored distance algorithm is used, if the distance matrix can be stored in memory as well. To estimate the bytes of memory needed for the data, use the following formula and round up to the nearest multiple of d.

$n(vd$	+	$8d + i$	
	+	i	if density estimation or the sorted distance algorithm is used
	+	$3d$	if stored data algorithm is used
	+	$3d$	if density estimation is used
	+	max(8, length of ID variable)	if ID variable is used
	+	length of ID variable	if ID variable is used
	+	sum of lengths of COPY variables)	if COPY variables is used

where

- n is the number of observations
- v is the number of variables
- d is the size of a C variable of type *double*. For most computers, $d = 8$.
- i is the size of a C variable of type *int*. For most computers, $i = 4$.

The number of bytes needed for the distance matrix is $dn(n + 1)/2$.

Missing Values

If the data are coordinates, observations with missing values are excluded from the analysis. If the data are distances, missing values are not permitted in the lower triangle of the distance matrix. The upper triangle is ignored. For more about TYPE=DISTANCE data sets, see Chapter A, "Special SAS Data Sets."

Ties

At each level of the clustering algorithm, PROC CLUSTER must identify the pair of clusters with the minimum distance. Sometimes, usually when the data are discrete, there can be two or more pairs with the same minimum distance. In such cases the tie must be broken in some arbitrary way. If there are ties, then the results of the cluster analysis depend on the order of the observations in the data set. The presence of ties is reported in the SAS log and in the column of the cluster history labeled "Tie" unless the NOTIE option is specified.

PROC CLUSTER breaks ties as follows. Each cluster is identified by the smallest observation number among its members. For each pair of clusters, there is a smaller identification number and a larger identification number. If two or more pairs of clusters are tied for minimum distance between clusters, the pair that has the minimum larger identification number is merged. If there is a tie for minimum larger identification number, the pair that has the minimum smaller identification number is merged.

A tie means that the level in the cluster history at which the tie occurred and possibly some of the subsequent levels are not uniquely determined. Ties that occur early in the cluster history usually have little effect on the later stages. Ties that occur in the middle part of the cluster history are cause for further investigation. Ties that occur late in the cluster history indicate important indeterminacies.

The importance of ties can be assessed by repeating the cluster analysis for several different random permutations of the observations. The discrepancies at a given level can be examined by crosstabulating the clusters obtained at that level for all of the permutations. See Example 33.4 for details.

Size, Shape, and Correlation

In some biological applications, the organisms that are being clustered can be at different stages of growth. Unless it is the growth process itself that is being studied, differences in size among such organisms are not of interest. Therefore, distances among organisms should be computed in such a way as to control for differences in size while retaining information about differences in shape.

If coordinate data are measured on an interval scale, you can control for size by subtracting a measure of the overall size of each observation from each data item. For example, if no other direct measure of size is available, you could subtract the mean of each row of the data matrix, producing a row-centered coordinate matrix. An easy way to subtract the mean of each row is to use PROC STANDARD on the transposed coordinate matrix:

```
proc transpose data= coordinate-datatype;
run;

proc standard m=0;
run;

proc transpose out=row-centered-coordinate-data;
run;
```

Another way to remove size effects from interval-scale coordinate data is to do a principal component analysis and discard the first component (Blackith and Reyment 1971).

If the data are measured on a ratio scale, you can control for size by dividing each observation by a measure of overall size; in this case, the geometric mean is a more natural measure of size than the arithmetic mean. However, it is often more meaningful to analyze the logarithms of ratio-scaled data, in which case you can subtract the arithmetic mean after taking logarithms. You must also consider the dimensions of measurement. For example, if you have measures of both length and weight, you might need to cube the measures of length or take the cube root of the weights. Various other complications can also arise in real applications, such as different growth rates for different parts of the body (Sneath and Sokal 1973).

Issues of size and shape are pertinent to many areas besides biology (for example, Hamer and Cunningham 1981). Suppose you have data consisting of subjective ratings made by several different raters. Some raters tend to give higher overall ratings than other raters. Some raters also tend to spread out their ratings over more of the scale than other raters. If it is impossible for you to adjust directly for rater differences, then distances should be computed in such a way as to control for differences both in size and variability. For example, if the data are considered to be measured on an interval scale, you can subtract the mean of each observation and divide by the standard deviation, producing a row-standardized coordinate matrix. With some clustering methods, analyzing squared Euclidean distances from a row-standardized coordinate matrix is equivalent to analyzing the matrix of correlations among rows, since squared Euclidean distance is an affine transformation of the correlation (Hartigan 1975, p. 64).

If you do an analysis of row-centered or row-standardized data, you need to consider whether the columns (variables) should be standardized before centering or standardizing the rows, after centering or standardizing the rows, or both before and after. If you standardize the columns after standardizing the rows, then strictly speaking you are not analyzing shape because the profiles are distorted by standardizing the columns; however, this type of double standardization might be necessary in practice to get reasonable results. It is not clear whether iterating the standardization of rows and columns can be of any benefit.

The choice of distance or correlation measure should depend on the meaning of the data and the purpose of the analysis. Simulation studies that compare distance and correlation measures are useless unless the data are generated to mimic data from your field of application. Conclusions drawn from artificial data cannot be generalized, because it is possible to generate data such that distances that include size effects work better or such that correlations work better.

You can standardize the rows of a data set by using a DATA step or by using the TRANSPOSE and STANDARD procedures. You can also use PROC TRANSPOSE and then have PROC CORR create a TYPE=CORR data set containing a correlation matrix. If you want to analyze a TYPE=CORR data set with PROC CLUSTER, you must use a DATA step to perform the following steps:

1. Set the data set TYPE= to DISTANCE.
2. Convert the correlations to dissimilarities by computing $1-r$, $\sqrt{1-r}$, $1-r^2$, or some other decreasing function.
3. Delete observations for which the variable _TYPE_ does not have the value 'CORR'.

Output Data Set

The OUTTREE= data set contains one observation for each observation in the input data set, plus one observation for each cluster of two or more observations (that is, one observation for each node of the cluster

tree). The total number of output observations is usually $2n - 1$, where n is the number of input observations. The density methods can produce fewer output observations when the number of clusters cannot be reduced to one.

The label of the OUTTREE= data set identifies the type of cluster analysis performed and is automatically displayed when the TREE procedure is invoked.

The variables in the OUTTREE= data set are as follows:

- the BY variables, if you use a BY statement
- the ID variable, if you use an ID statement
- the COPY variables, if you use a COPY statement
- _NAME_, a character variable giving the name of the node. If the node is a cluster, the name is CL*n*, where *n* is the number of the cluster. If the node is an observation, the name is OB*n*, where *n* is the observation number. If the node is an observation and the ID statement is used, the name is the formatted value of the ID variable.
- _PARENT_, a character variable giving the value of _NAME_ of the parent of the node
- _NCL_, the number of clusters
- _FREQ_, the number of observations in the current cluster
- _HEIGHT_, the distance or similarity between the last clusters joined, as defined in the section "Clustering Methods" on page 2026. The variable _HEIGHT_ is used by the TREE procedure as the default height axis. The label of the _HEIGHT_ variable identifies the between-cluster distance measure. For METHOD=TWOSTAGE, the _HEIGHT_ variable contains the densities at which clusters joined in the first stage; for clusters formed in the second stage, _HEIGHT_ is a very small negative number.

If the input data set contains coordinates, the following variables appear in the output data set:

- the variables containing the coordinates used in the cluster analysis. For output observations that correspond to input observations, the values of the coordinates are the same in both data sets except for some slight numeric error possibly introduced by standardizing and unstandardizing if the STANDARD option is used. For output observations that correspond to clusters of more than one input observation, the values of the coordinates are the cluster means.
- _ERSQ_, the approximate expected value of R square under the uniform null hypothesis
- _RATIO_, equal to (1 – _ERSQ_) / (1 – _RSQ_)
- _LOGR_, natural logarithm of _RATIO_
- _CCC_, the cubic clustering criterion

The variables _ERSQ_, _RATIO_, _LOGR_, and _CCC_ have missing values when the number of clusters is greater than one-fifth the number of observations.

If the input data set contains coordinates and METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then the following variables appear in the output data set:

- _DIST_, the Euclidean distance between the means of the last clusters joined
- _AVLINK_, the average distance between the last clusters joined

If the input data set contains coordinates or METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then the following variables appear in the output data set:

- _RMSSTD_, the root mean squared standard deviation of the current cluster
- _SPRSQ_, the semipartial squared multiple correlation or the decrease in the proportion of variance accounted for due to joining two clusters to form the current cluster
- _RSQ_, the squared multiple correlation
- _PSF_, the pseudo F statistic
- _PST2_, the pseudo t^2 statistic

If METHOD=EML, then the following variable appears in the output data set:

- _LNLR_, the log-likelihood ratio

If METHOD=TWOSTAGE or METHOD=DENSITY, the following variable appears in the output data set:

- _MODE_, pertaining to the modal clusters. With METHOD=DENSITY, the _MODE_ variable indicates the number of modal clusters contained by the current cluster. With METHOD=TWOSTAGE, the _MODE_ variable gives the maximum density in each modal cluster and the fusion density, d^*, for clusters containing two or more modal clusters; for clusters containing no modal clusters, _MODE_ is missing.

If nonparametric density estimates are requested (when METHOD=DENSITY or METHOD=TWOSTAGE and the HYBRID option is not used; or when any of the TRIM=, K= or R= options are used), the output data set contains the following:

- _DENS_, the maximum density in the current cluster

Displayed Output

If you specify the SIMPLE option and the data are coordinates, PROC CLUSTER produces simple descriptive statistics for each variable:

- the Mean
- the standard deviation, Std Dev
- the Skewness
- the Kurtosis
- a coefficient of Bimodality

If the data are coordinates and you do not specify the NOEIGEN option, PROC CLUSTER displays the following:

- the Eigenvalues of the Correlation or Covariance Matrix
- the Difference between successive eigenvalues
- the Proportion of variance explained by each eigenvalue
- the Cumulative proportion of variance explained

If the data are coordinates, PROC CLUSTER displays the Root Mean Squared Total-Sample Standard Deviation of the variables

If the distances are normalized, PROC CLUSTER displays one of the following, depending on whether squared or unsquared distances are used:

- the Root Mean Squared Distance Between Observations
- the Mean Distance Between Observations

For the generations in the clustering process specified by the PRINT= option, PROC CLUSTER displays the following:

- the Number of Clusters or NCL
- the names of the Clusters Joined. The observations are identified by the formatted value of the ID variable, if any; otherwise, the observations are identified by OB*n*, where *n* is the observation number. The CLUSTER procedure displays the entire value of the ID variable in the cluster history instead of truncating at 16 characters. Long ID values might be split onto several lines. Clusters of two or more observations are identified as CL*n*, where *n* is the number of clusters existing after the cluster in question is formed.
- the number of observations in the new cluster, Frequency of New Cluster or FREQ

If you specify the RMSSTD option and the data are coordinates, or if you specify METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then PROC CLUSTER displays the root mean squared standard deviation of the new cluster, RMS Std of New Cluster or RMS Std.

PROC CLUSTER displays the following items if you specify METHOD=WARD. It also displays them if you specify the RSQUARE option and either the data are coordinates or you specify METHOD=AVERAGE or METHOD=CENTROID.

- the decrease in the proportion of variance accounted for resulting from joining the two clusters, Semipartial R-Square or SPRSQ. This equals the between-cluster sum of squares divided by the corrected total sum of squares.
- the squared multiple correlation, R-Square or RSQ. R square is the proportion of variance accounted for by the clusters.

If you specify the CCC option and the data are coordinates, PROC CLUSTER displays the following:

- Approximate Expected R-Square or ERSQ, the approximate expected value of R square under the uniform null hypothesis
- the Cubic Clustering Criterion or CCC. The cubic clustering criterion and approximate expected R square are given missing values when the number of clusters is greater than one-fifth the number of observations.

If you specify the PSEUDO option and the data are coordinates, or if you specify METHOD=AVERAGE, METHOD=CENTROID, or METHOD=WARD, then PROC CLUSTER displays the following:

- Pseudo F or PSF, the pseudo F statistic measuring the separation among all the clusters at the current level
- Pseudo t^2 or PST2, the pseudo t^2 statistic measuring the separation between the two clusters most recently joined

If you specify the NOSQUARE option and METHOD=AVERAGE, PROC CLUSTER displays the (Normalized) Average Distance or (Norm) Aver Dist, the average distance between pairs of objects in the two clusters joined with one object from each cluster.

If you do not specify the NOSQUARE option and METHOD=AVERAGE, PROC CLUSTER displays the (Normalized) RMS Distance or (Norm) RMS Dist, the root mean squared distance between pairs of objects in the two clusters joined with one object from each cluster.

If METHOD=CENTROID, PROC CLUSTER displays the (Normalized) Centroid Distance or (Norm) Cent Dist, the distance between the two cluster centroids.

If METHOD=COMPLETE, PROC CLUSTER displays the (Normalized) Maximum Distance or (Norm) Max Dist, the maximum distance between the two clusters.

If METHOD=DENSITY or METHOD=TWOSTAGE, PROC CLUSTER displays the following:

- Normalized Fusion Density or Normalized Fusion Dens, the value of d^* as defined in the section "Clustering Methods" on page 2026
- the Normalized Maximum Density in Each Cluster joined, including the Lesser or Min, and the Greater or Max, of the two maximum density values

If METHOD=EML, PROC CLUSTER displays the following:

- Log Likelihood Ratio or LNLR
- Log Likelihood or LNLIKE

If METHOD=FLEXIBLE, PROC CLUSTER displays the (Normalized) Flexible Distance or (Norm) Flex Dist, the distance between the two clusters based on the Lance-Williams flexible formula.

If METHOD=MEDIAN, PROC CLUSTER displays the (Normalized) Median Distance or (Norm) Med Dist, the distance between the two clusters based on the median method.

If METHOD=MCQUITTY, PROC CLUSTER displays the (Normalized) McQuitty's Similarity or (Norm) MCQ, the distance between the two clusters based on McQuitty's similarity method.

If METHOD=SINGLE, PROC CLUSTER displays the (Normalized) Minimum Distance or (Norm) Min Dist, the minimum distance between the two clusters.

If you specify the NONORM option and METHOD=WARD, PROC CLUSTER displays the Between-Cluster Sum of Squares or BSS, the ANOVA sum of squares between the two clusters joined.

If you specify neither the NOTIE option nor METHOD=TWOSTAGE or METHOD=DENSITY, PROC CLUSTER displays Tie, where a T in the column indicates a tie for minimum distance and a blank indicates the absence of a tie.

After the cluster history, if METHOD=TWOSTAGE or METHOD=DENSITY, PROC CLUSTER displays the number of modal clusters.

ODS Table Names

PROC CLUSTER assigns a name to each table it creates. You can use these names to reference the table when using the Output Delivery System (ODS) to select tables and create output data sets. These names are listed in Table 33.4. For more information about ODS, see Chapter 20, "Using the Output Delivery System."

Table 33.4 ODS Tables Produced by PROC CLUSTER

ODS Table Name	Description	Statement	Option
ClusterHistory	Observation or clusters joined, frequencies and other cluster statistics	PROC	default
SimpleStatistics	Simple statistics, before or after trimming	PROC	SIMPLE
EigenvalueTable	Eigenvalues of the CORR or COV matrix	PROC	default

Table 33.4 (continued)

ODS Table Name	Description	Statement	Option
RMSStd	Root mean square total sample standard deviation	PROC	default
AvDist	Root mean square distance between observations	PROC	default

ODS Graphics

Statistical procedures use ODS Graphics to create graphs as part of their output. ODS Graphics is described in detail in Chapter 21, "Statistical Graphics Using ODS."

Before you create graphs, ODS Graphics must be enabled (for example, by specifying the ODS GRAPHICS ON statement). For more information about enabling and disabling ODS Graphics, see the section "Enabling and Disabling ODS Graphics" on page 606 in Chapter 21, "Statistical Graphics Using ODS."

The overall appearance of graphs is controlled by ODS styles. Styles and other aspects of using ODS Graphics are discussed in the section "A Primer on ODS Statistical Graphics" on page 605 in Chapter 21, "Statistical Graphics Using ODS."

PROC CLUSTER can produce plots of the cubic clustering criterion, pseudo F, and pseudo t^2 statistics, and a dendrogram. To plot a statistic, you must ask for it to be computed via one or more of the CCC, PSEUDO, or PLOT options.

You can reference every graph produced through ODS Graphics with a name. The names of the graphs that PROC CLUSTER generates are listed in Table 33.5, along with the required statements and options.

Table 33.5 Graphs Produced by PROC CLUSTER

ODS Graph Name	Plot Description	Statement & Option
CubicClusCritPlot	Cubic clustering criterion for the number of clusters	PROC CLUSTER PLOTS=CCC
PseudoFPlot	Pseudo F criterion for the number of clusters	PROC CLUSTER PLOTS=PSF
PseudoTSqPlot	Pseudo t^2 criterion for the number of clusters	PROC CLUSTER PLOTS=PST2
CccAndPsTSqPlot	Cubic clustering criterion and pseudo t^2	PROC CLUSTER PLOTS=(CCC PST2)
CccAndPsfPlot	Cubic clustering criterion and pseudo F	PROC CLUSTER PLOTS=(CCC PSF)
CccPsfAndPsTSqPlot	Cubic clustering criterion, pseudo F, and pseudo t^2	PROC CLUSTER PLOTS=ALL
Dendrogram	Dendrogram (tree diagram)	PROC CLUSTER PLOTS=DENDROGRAM

Examples: CLUSTER Procedure

Example 33.1: Cluster Analysis of Flying Mileages between 10 American Cities

This example clusters 10 American cities based on the flying mileages between them. Six clustering methods are shown with corresponding dendrograms. The EML method cannot be used because it requires coordinate data. The other omitted methods produce the same clusters, although not the same distances between clusters, as one of the illustrated methods: complete linkage and the flexible-beta method yield the same clusters as Ward's method, McQuitty's similarity analysis produces the same clusters as average linkage, and the median method corresponds to the centroid method.

All of the methods suggest a division of the cities into two clusters along the east-west dimension. There is disagreement, however, about which cluster Denver should belong to. Some of the methods indicate a possible third cluster that contains Denver and Houston.

The following step displays the city mileage SAS data set, which is available in the Sashelp library and is designated as a TYPE=DISTANCE data set when it is used by PROC CLUSTER:

```
proc print noobs data=sashelp.mileages;
run;
```

Output 33.1.1 City Mileage Data Set

Atlanta	Chicago	Denver	Houston	LosAngeles	Miami	NewYork	SanFrancisco	Seattle	WashingtonDC	City
0	.	.	.	.	.	.	.	.	.	Atlanta
587	0	.	.	.	.	.	.	.	.	Chicago
1212	920	0	.	.	.	.	.	.	.	Denver
701	940	879	0	.	.	.	.	.	.	Houston
1936	1745	831	1374	0	.	.	.	.	.	Los Angeles
604	1188	1726	968	2339	0	.	.	.	.	Miami
748	713	1631	1420	2451	1092	0	.	.	.	New York
2139	1858	949	1645	347	2594	2571	0	.	.	San Francisco
2182	1737	1021	1891	959	2734	2408	678	0	.	Seattle
543	597	1494	1220	2300	923	205	2442	2329	0	Washington D.C.

A partial listing from the following statements include Output 33.1.2 and Output 33.1.3:

```
title 'Cluster Analysis of Flying Mileages Between 10 American Cities';
ods graphics on;

title2 'Using METHOD=AVERAGE';
proc cluster data=sashelp.mileages(type=distance) method=average pseudo;
   id City;
run;
```

Output 33.1.2 Cluster History Using METHOD=AVERAGE

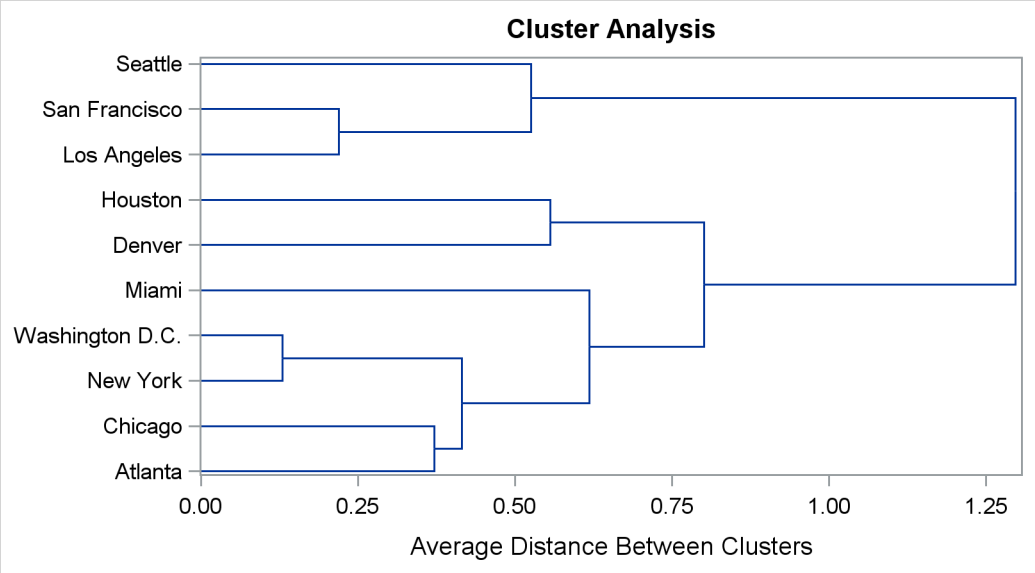
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=AVERAGE

The CLUSTER Procedure
Average Linkage Cluster Analysis

Cluster History

Number of Clusters	Clusters Joined		Freq	Pseudo F Statistic	Pseudo t-Squared	Norm RMS Distance	Tie
9	New York	Washington D.C.	2	66.7	.	0.1297	
8	Los Angeles	San Francisco	2	39.2	.	0.2196	
7	Atlanta	Chicago	2	21.7	.	0.3715	
6	CL7	CL9	4	14.5	3.4	0.4149	
5	CL8	Seattle	3	12.4	7.3	0.5255	
4	Denver	Houston	2	13.9	.	0.5562	
3	CL6	Miami	5	15.5	3.8	0.6185	
2	CL3	CL4	7	16.0	5.3	0.8005	
1	CL2	CL5	10	.	16.0	1.2967	

Output 33.1.3 Dendrogram Using METHOD=AVERAGE



A partial listing from the following statements include Output 33.1.4 and Output 33.1.5:

```
title2 'Using METHOD=CENTROID';
proc cluster data=sashelp.mileages(type=distance) method=centroid pseudo;
   id City;
run;
```

Output 33.1.4 Cluster History Using METHOD=CENTROID

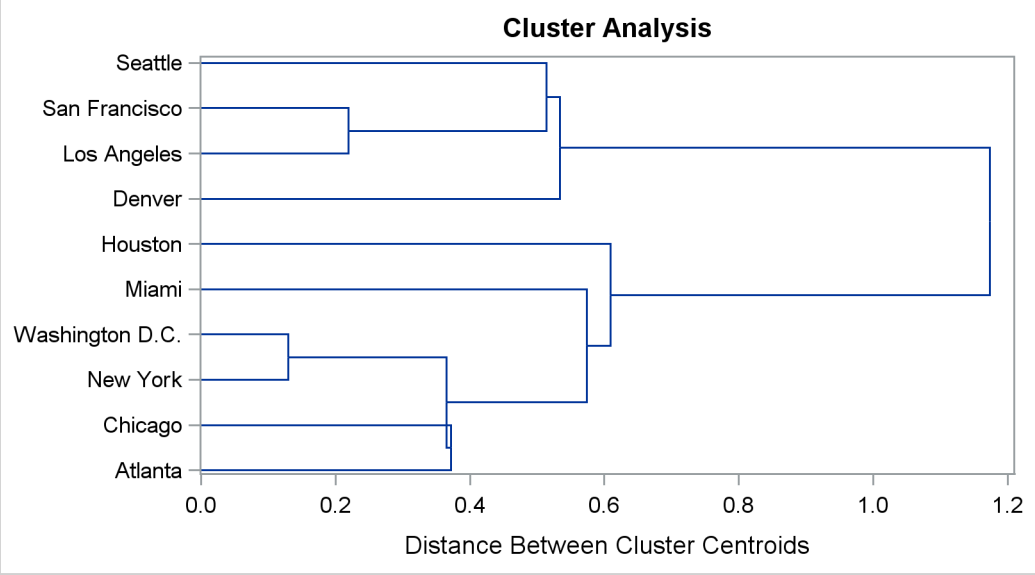
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=CENTROID

The CLUSTER Procedure
Centroid Hierarchical Cluster Analysis

Cluster History

Number of Clusters	Clusters Joined		Freq	Pseudo F Statistic	Pseudo t-Squared	Norm Centroid Distance	Tie
9	New York	Washington D.C.	2	66.7	.	0.1297	
8	Los Angeles	San Francisco	2	39.2	.	0.2196	
7	Atlanta	Chicago	2	21.7	.	0.3715	
6	CL7	CL9	4	14.5	3.4	0.3652	
5	CL8	Seattle	3	12.4	7.3	0.5139	
4	Denver	CL5	4	12.4	2.1	0.5337	
3	CL6	Miami	5	14.2	3.8	0.5743	
2	CL3	Houston	6	22.1	2.6	0.6091	
1	CL2	CL4	10	.	22.1	1.173	

Output 33.1.5 Dendrogram Using METHOD=CENTROID



A partial listing from the following statements include Output 33.1.6 and Output 33.1.7:

```
title2 'Using METHOD=DENSITY K=3';
proc cluster data=sashelp.mileages(type=distance) method=density k=3;
   id City;
run;
```

Output 33.1.6 Cluster History Using METHOD=DENSITY K=3

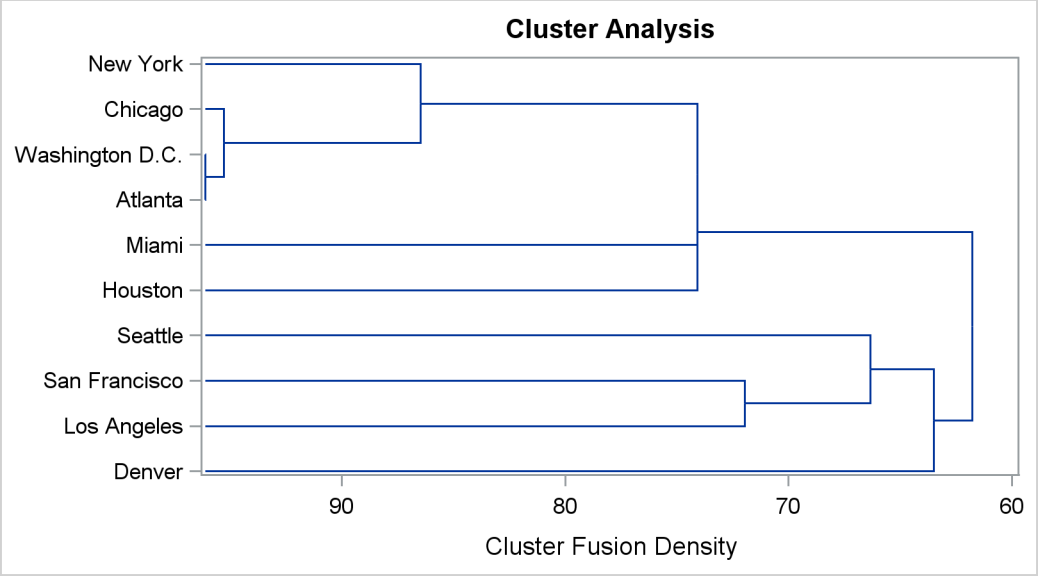
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=DENSITY K=3

The CLUSTER Procedure
Density Linkage Cluster Analysis

Cluster History

Number of Clusters	Clusters Joined		Freq	Normalized Fusion Density		Maximum Density in Each Cluster Lesser	Greater	Tie
9	Atlanta	Washington D.C.	2	96.106		92.5043	100.0	
8	CL9	Chicago	3	95.263		90.9548	100.0	
7	CL8	New York	4	86.465		76.1571	100.0	
6	CL7	Miami	5	74.079		58.8299	100.0	T
5	CL6	Houston	6	74.079		61.7747	100.0	
4	Los Angeles	San Francisco	2	71.968		65.3430	80.0885	
3	CL4	Seattle	3	66.341		56.6215	80.0885	
2	CL3	Denver	4	63.509		61.7747	80.0885	
1	CL5	CL2	10	61.775	*	80.0885	100.0	

Output 33.1.7 Dendrogram Using METHOD=DENSITY K=3



A partial listing from the following statements include Output 33.1.8 and Output 33.1.9:

```
title2 'Using METHOD=SINGLE';
proc cluster data=sashelp.mileages(type=distance) method=single;
   id City;
run;
```

Output 33.1.8 Cluster History Using METHOD=SINGLE

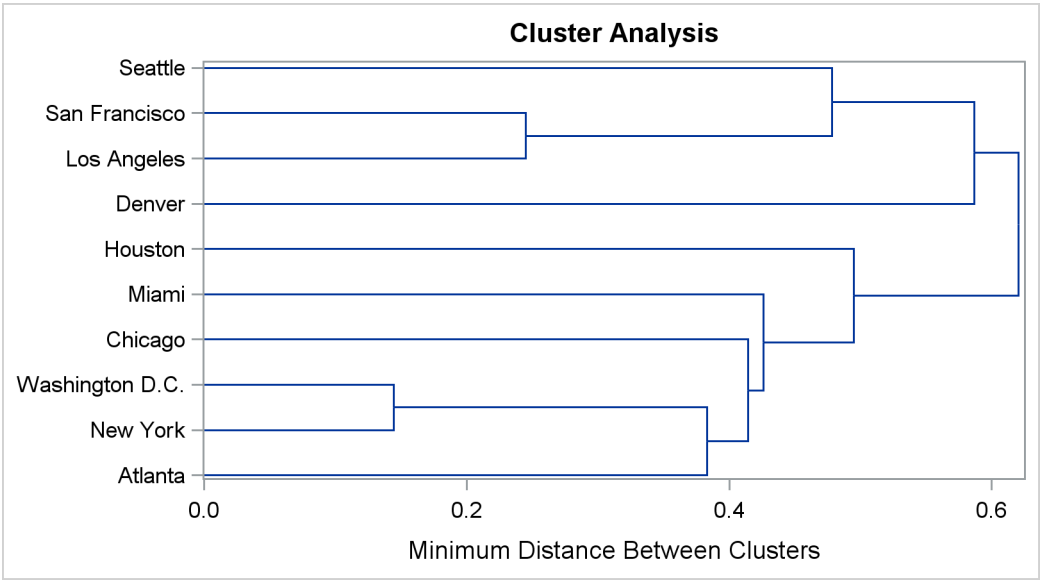
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=SINGLE

The CLUSTER Procedure
Single Linkage Cluster Analysis

Cluster History

Number of Clusters	Clusters Joined		Freq	Norm Minimum Distance	Tie
9	New York	Washington D.C.	2	0.1447	
8	Los Angeles	San Francisco	2	0.2449	
7	Atlanta	CL9	3	0.3832	
6	CL7	Chicago	4	0.4142	
5	CL6	Miami	5	0.4262	
4	CL8	Seattle	3	0.4784	
3	CL5	Houston	6	0.4947	
2	Denver	CL4	4	0.5864	
1	CL3	CL2	10	0.6203	

Output 33.1.9 Dendrogram Using METHOD=SINGLE



A partial listing from the following statements include Output 33.1.10 and Output 33.1.11:

```
title2 'Using METHOD=TWOSTAGE K=3';
proc cluster data=sashelp.mileages(type=distance) method=twostage k=3;
   id City;
run;
```

Output 33.1.10 Cluster History Using METHOD=TWOSTAGE K=3

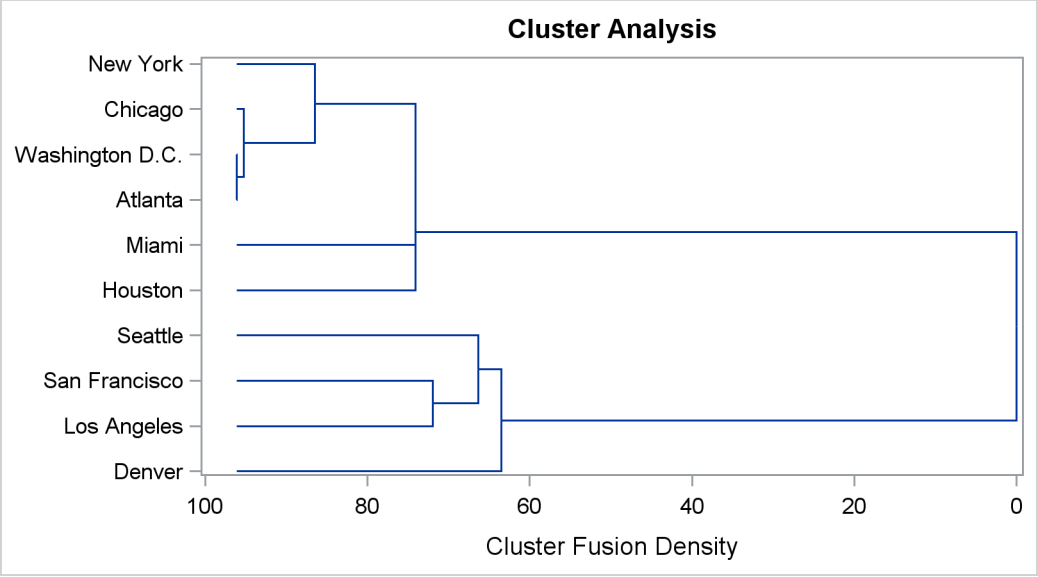
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=TWOSTAGE K=3

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Cluster History

Number of Clusters	Clusters Joined		Freq	Normalized Fusion Density	Maximum Density in Each Cluster Lesser	Greater	Tie
9	Atlanta	Washington D.C.	2	96.106	92.5043	100.0	
8	CL9	Chicago	3	95.263	90.9548	100.0	
7	CL8	New York	4	86.465	76.1571	100.0	
6	CL7	Miami	5	74.079	58.8299	100.0	T
5	CL6	Houston	6	74.079	61.7747	100.0	
4	Los Angeles	San Francisco	2	71.968	65.3430	80.0885	
3	CL4	Seattle	3	66.341	56.6215	80.0885	
2	CL3	Denver	4	63.509	61.7747	80.0885	
1	CL5	CL2	10	61.775	80.0885	100.0	

Output 33.1.11 Dendrogram Using METHOD=TWOSTAGE K=3



A partial listing from the following statements include Output 33.1.12 and Output 33.1.13:

```
title2 'Using METHOD=WARD';
proc cluster data=sashelp.mileages(type=distance) method=ward pseudo;
   id City;
run;
```

Output 33.1.12 Cluster History Using METHOD=WARD

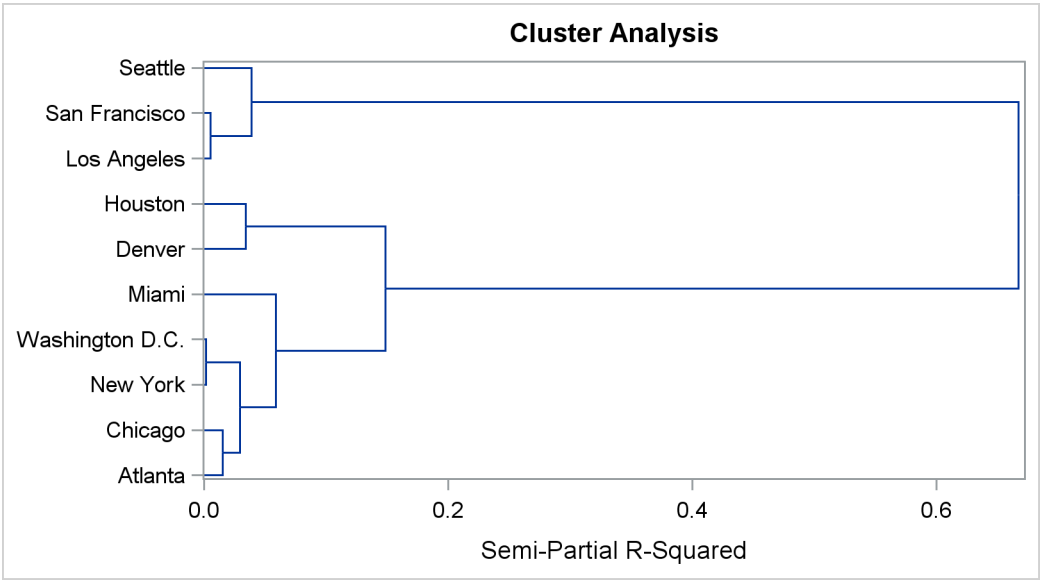
Cluster Analysis of Flying Mileages Between 10 American Cities Using METHOD=WARD

The CLUSTER Procedure
Ward's Minimum Variance Cluster Analysis

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Pseudo F Statistic	Pseudo t-Squared	Tie
9	New York	Washington D.C.	2	0.0019	.998	66.7	.	
8	Los Angeles	San Francisco	2	0.0054	.993	39.2	.	
7	Atlanta	Chicago	2	0.0153	.977	21.7	.	
6	CL7	CL9	4	0.0296	.948	14.5	3.4	
5	Denver	Houston	2	0.0344	.913	13.2	.	
4	CL8	Seattle	3	0.0391	.874	13.9	7.3	
3	CL6	Miami	5	0.0586	.816	15.5	3.8	
2	CL3	CL5	7	0.1488	.667	16.0	5.3	
1	CL2	CL4	10	0.6669	.000	.	16.0	

Output 33.1.13 Dendrogram Using METHOD=WARD



Example 33.2: Crude Birth and Death Rates

This example uses the SAS data set Poverty created in the section "Getting Started: CLUSTER Procedure" on page 2007. The data, from Rouncefield (1995), are birth rates, death rates, and infant death rates for 97 countries. Six cluster analyses are performed with eight methods. Scatter plots showing cluster membership at selected levels are produced instead of tree diagrams.

Each cluster analysis is performed by a macro called ANALYZE. The macro takes two arguments. The first, &METHOD, specifies the value of the METHOD= option to be used in the PROC CLUSTER statement. The second, &NCL, must be specified as a list of integers, separated by blanks, indicating the number of clusters desired in each scatter plot. For example, the first invocation of ANALYZE specifies the AVERAGE method and requests plots of three and eight clusters. When two-stage density linkage is used, the K= and R= options are specified as part of the first argument.

The ANALYZE macro first invokes the CLUSTER procedure with METHOD=&METHOD, where &METHOD represents the value of the first argument to ANALYZE. This part of the macro produces the PROC CLUSTER output shown.

The %DO loop processes &NCL, the list of numbers of clusters to plot. The macro variable &K is a counter that indexes the numbers within &NCL. The %SCAN function picks out the *k*th number in &NCL, which is then assigned to the macro variable &N. When &K exceeds the number of numbers in &NCL, %SCAN returns a null string. Thus, the %DO loop executes while &N is not equal to a null string. In the %WHILE condition, a null string is indicated by the absence of any nonblank characters between the comparison operator (NE) and the right parenthesis that terminates the condition.

Within the %DO loop, the TREE procedure creates an output data set containing &N clusters. The SGPLOT procedure then produces a scatter plot in which each observation is identified by the number of the cluster to which it belongs. The TITLE2 statement uses double quotes so that &N and &METHOD can be used within the title. At the end of the loop, &K is incremented by 1, and the next number is extracted from &NCL by %SCAN.

```
title 'Cluster Analysis of Birth and Death Rates';
ods graphics on;

%macro analyze(method,ncl);
   proc cluster data=poverty outtree=tree method=&method print=15 ccc pseudo;
      var birth death;
      title2;
   run;

   %let k=1;
   %let n=%scan(&ncl,&k);
   %do %while(&n NE);

      proc tree data=tree noprint out=out ncl=&n;
         copy birth death;
      run;
```

```
      proc sgplot;
         scatter y=death x=birth / group=cluster;
         title2 "Plot of &n Clusters from METHOD=&METHOD";
      run;

      %let k=%eval(&k+1);
      %let n=%scan(&ncl,&k);
   %end;
%mend;
```

The following statement produces Output 33.2.1, Output 33.2.3, and Output 33.2.4:

```
%analyze(average, 3 8)
```

For average linkage, the CCC has peaks at three, eight, ten, and twelve clusters, but the three-cluster peak is lower than the eight-cluster peak. The pseudo F statistic has peaks at three, eight, and twelve clusters. The pseudo t^2 statistic drops sharply at three clusters, continues to fall at four clusters, and has a particularly low value at twelve clusters. However, there are not enough data to seriously consider as many as twelve clusters. Scatter plots are given for three and eight clusters. The results are shown in Output 33.2.1 through Output 33.2.4. In Output 33.2.4, the eighth cluster consists of the two outlying observations, Mexico and Korea.

Output 33.2.1 Cluster Analysis for Birth and Death Rates: METHOD=AVERAGE

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Average Linkage Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

Root-Mean-Square Total-Sample Standard Deviation	10.127

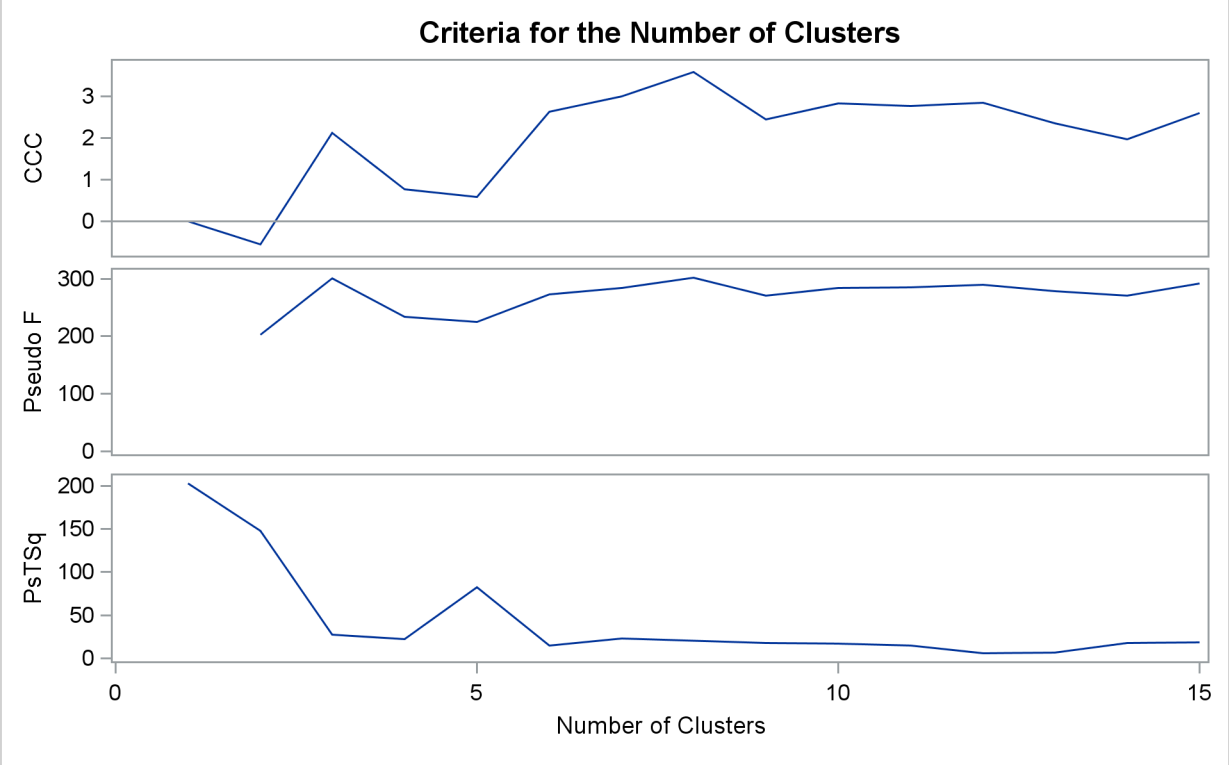
Root-Mean-Square Distance Between Observations	20.25399

Output 33.2.1 *continued*

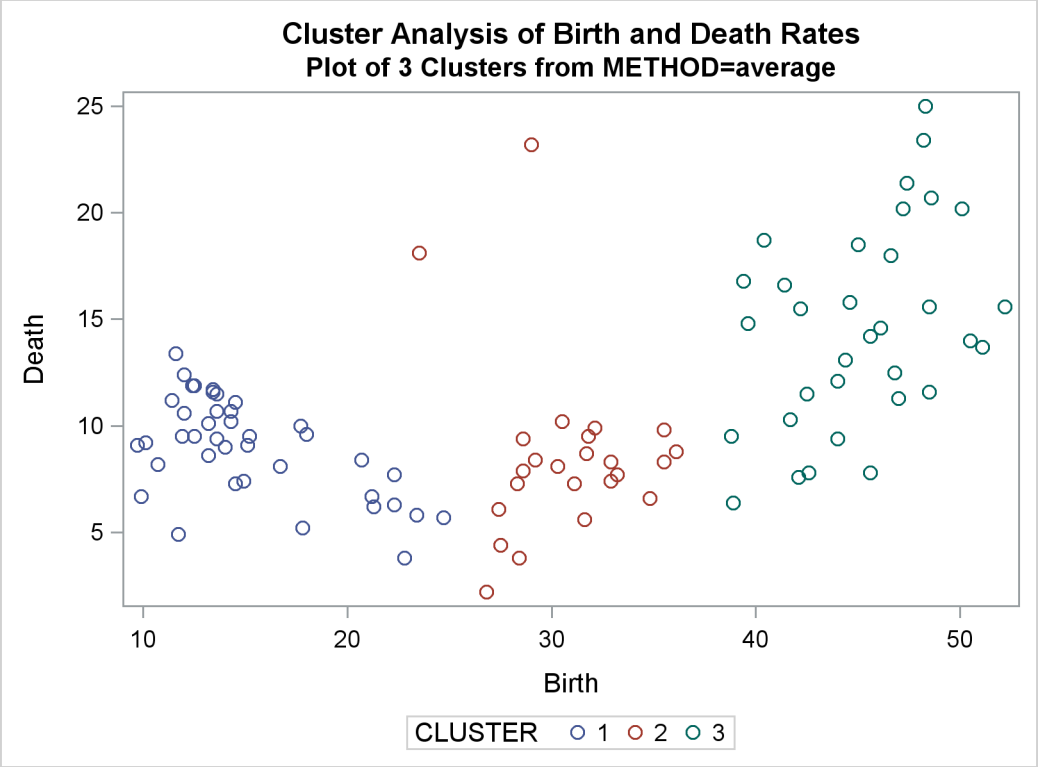
Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Norm RMS Distance	Tie
15	CL27	CL20	18	0.0035	.980	.975	2.61	292	18.6	0.2325	
14	CL23	CL17	28	0.0034	.977	.972	1.97	271	17.7	0.2358	
13	CL18	CL54	8	0.0015	.975	.969	2.35	279	7.1	0.2432	
12	CL21	CL26	8	0.0015	.974	.966	2.85	290	6.1	0.2493	
11	CL19	CL24	12	0.0033	.971	.962	2.78	285	14.8	0.2767	
10	CL22	CL16	12	0.0036	.967	.957	2.84	284	17.4	0.2858	
9	CL15	CL28	22	0.0061	.961	.951	2.45	271	17.5	0.3353	
8	OB23	OB61	2	0.0014	.960	.943	3.59	302	.	0.3703	
7	CL25	CL11	17	0.0098	.950	.933	3.01	284	23.3	0.4033	
6	CL7	CL12	25	0.0122	.938	.920	2.63	273	14.8	0.4132	
5	CL10	CL14	40	0.0303	.907	.902	0.59	225	82.7	0.4584	
4	CL13	CL6	33	0.0244	.883	.875	0.77	234	22.2	0.5194	
3	CL9	CL8	24	0.0182	.865	.827	2.13	300	27.7	0.735	
2	CL5	CL3	64	0.1836	.681	.697	-.55	203	148	0.8402	
1	CL2	CL4	97	0.6810	.000	.000	0.00	.	203	1.3348	

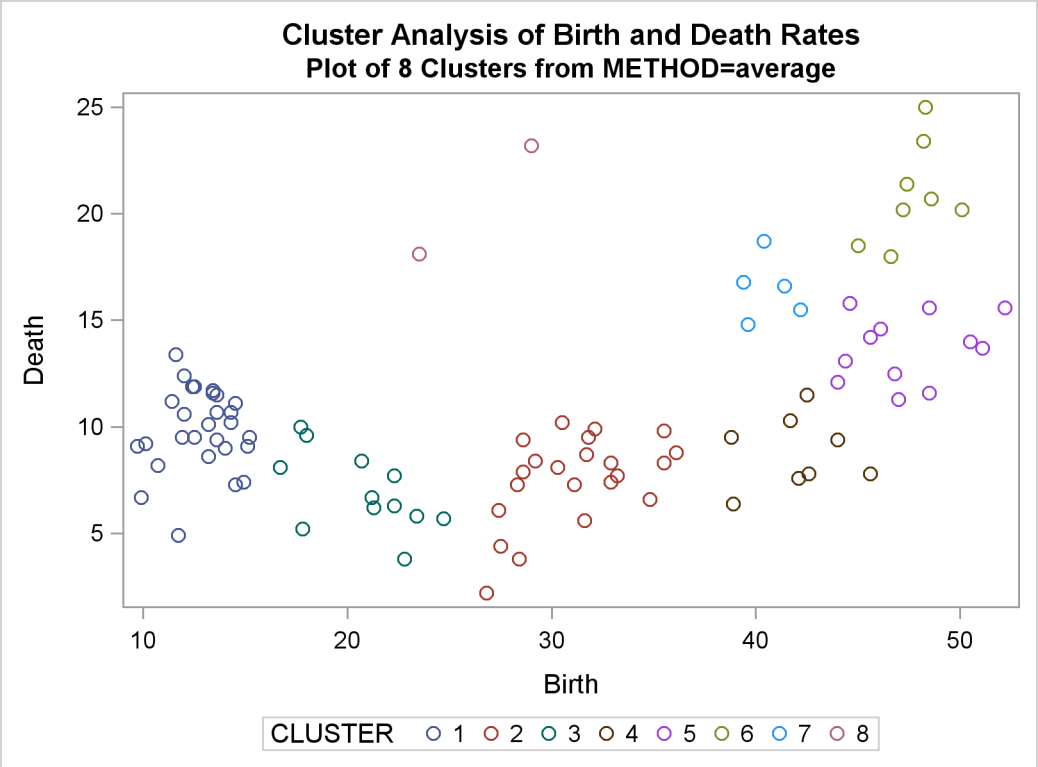
Output 33.2.2 Criteria for the Number of Clusters: METHOD=AVERAGE



Output 33.2.3 Plot of Three Clusters: METHOD=AVERAGE



Output 33.2.4 Plot of Eight Clusters: METHOD=AVERAGE



The following statement produces Output 33.2.5 and Output 33.2.7:

```
%analyze(complete, 3)
```

Complete linkage shows CCC peaks at three, eight and twelve clusters. The pseudo F statistic peaks at three and twelve clusters. The pseudo t^2 statistic indicates three clusters.

The scatter plot for three clusters is shown.

Output 33.2.5 Cluster History for Birth and Death Rates: METHOD=COMPLETE

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Complete Linkage Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

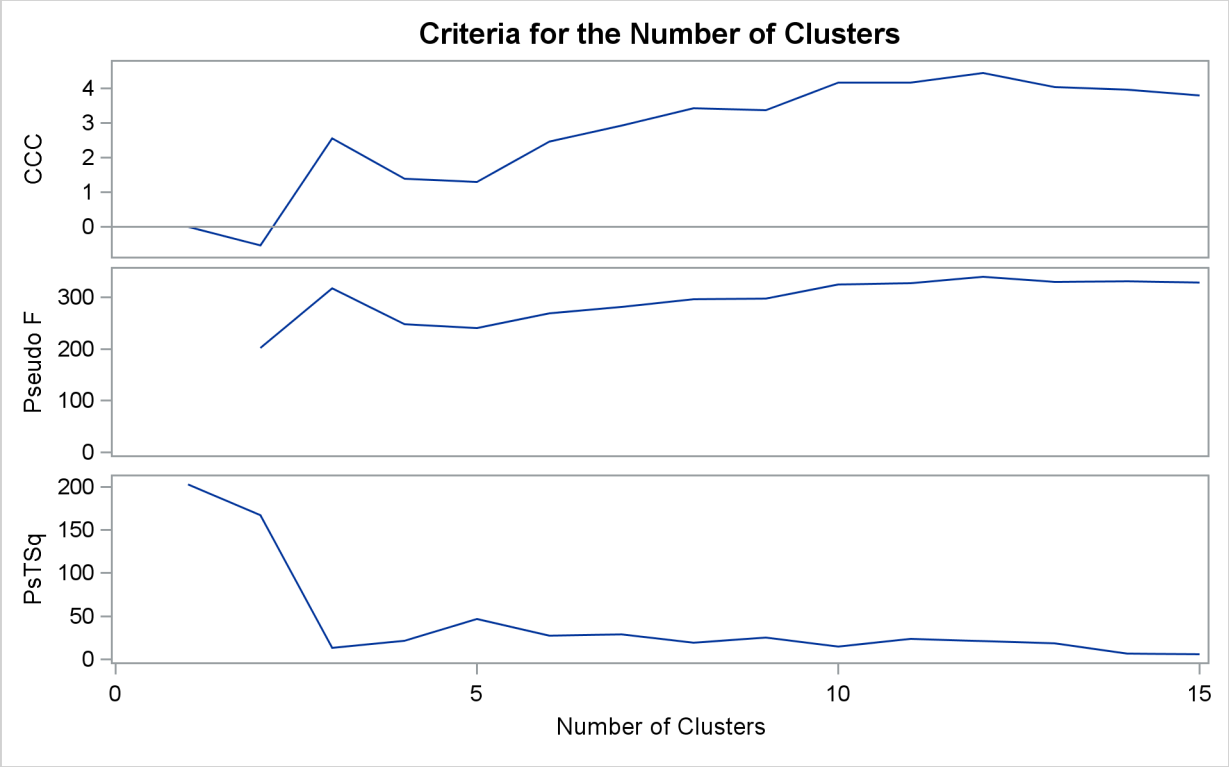
Root-Mean-Square Total-Sample Standard Deviation 10.127

Mean Distance Between Observations 17.13099

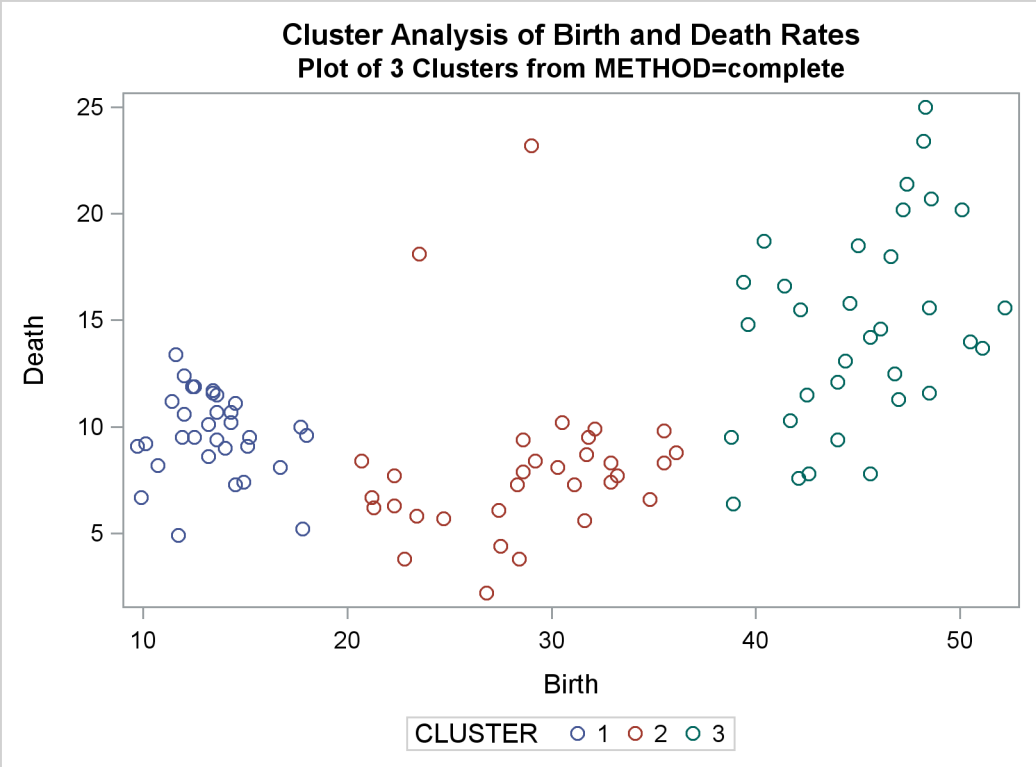
Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Norm Maximum Distance	Tie
15	CL22	CL33	8	0.0015	.983	.975	3.80	329	6.1	0.4092	
14	CL56	CL18	8	0.0014	.981	.972	3.97	331	6.6	0.4255	
13	CL30	CL44	8	0.0019	.979	.969	4.04	330	19.0	0.4332	
12	OB23	OB61	2	0.0014	.978	.966	4.45	340	.	0.4378	
11	CL19	CL24	24	0.0034	.974	.962	4.17	327	24.1	0.4962	
10	CL17	CL28	12	0.0033	.971	.957	4.18	325	14.8	0.5204	
9	CL20	CL13	16	0.0067	.964	.951	3.38	297	25.2	0.5236	
8	CL11	CL21	32	0.0054	.959	.943	3.44	297	19.7	0.6001	
7	CL26	CL15	13	0.0096	.949	.933	2.93	282	28.9	0.7233	
6	CL14	CL10	20	0.0128	.937	.920	2.46	269	27.7	0.8033	
5	CL9	CL16	30	0.0237	.913	.902	1.29	241	47.1	0.8993	
4	CL6	CL7	33	0.0240	.889	.875	1.38	248	21.7	1.2165	
3	CL5	CL12	32	0.0178	.871	.827	2.56	317	13.6	1.2326	
2	CL3	CL8	64	0.1900	.681	.697	-.55	203	167	1.5412	
1	CL2	CL4	97	0.6810	.000	.000	0.00	.	203	2.5233	

Output 33.2.6 Criteria for the Number of Clusters: METHOD=COMPLETE



Output 33.2.7 Plot of Clusters for METHOD=COMPLETE



The following statement produces Output 33.2.8 and Output 33.2.10:

```
%analyze(single, 7 10)
```

The CCC and pseudo F statistics are not appropriate for use with single linkage because of the method's tendency to chop off tails of distributions. The pseudo t^2 statistic can be used by looking for *large* values and taking the number of clusters to be one greater than the level at which the large pseudo t^2 value is displayed. For these data, there are large values at levels 6 and 9, suggesting seven or ten clusters.

The scatter plots for seven and ten clusters are shown.

Output 33.2.8 Cluster History for Birth and Death Rates: METHOD=SINGLE

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Single Linkage Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

Root-Mean-Square Total-Sample Standard Deviation 10.127

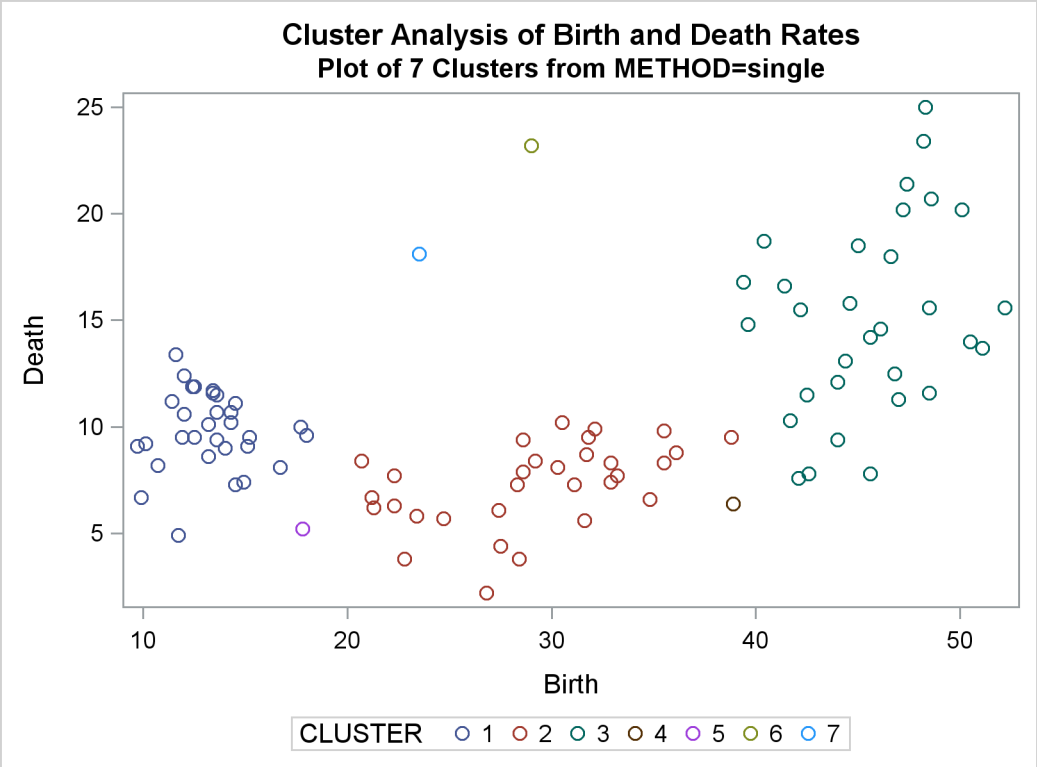
Mean Distance Between Observations 17.13099

Cluster History

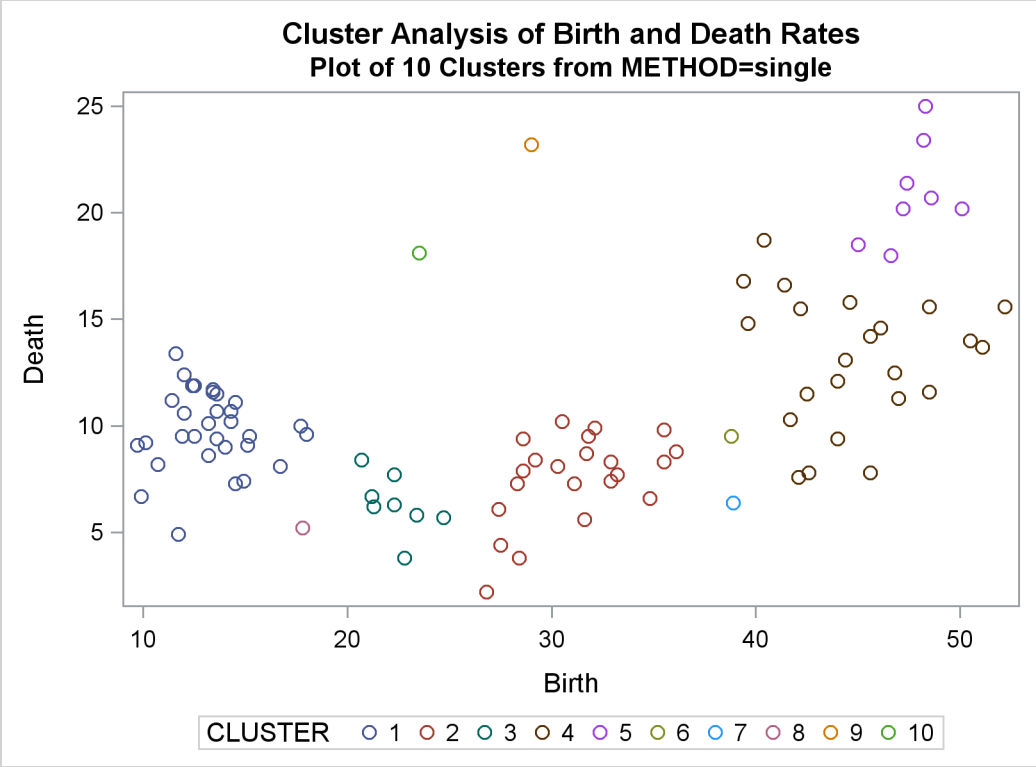
Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Norm Minimum Distance	Tie
15	CL37	CL19	8	0.0014	.968	.975	-2.3	178	6.6	0.1331	
14	CL20	CL23	15	0.0059	.962	.972	-3.1	162	18.7	0.1412	
13	CL14	CL16	19	0.0054	.957	.969	-3.4	155	8.8	0.1442	
12	CL26	OB58	31	0.0014	.955	.966	-2.7	165	4.0	0.1486	
11	OB86	CL18	4	0.0003	.955	.962	-1.6	183	3.8	0.1495	
10	CL13	CL11	23	0.0088	.946	.957	-2.3	170	11.3	0.1518	
9	CL22	CL17	30	0.0235	.923	.951	-4.7	131	45.7	0.1593	T
8	CL15	CL10	31	0.0210	.902	.943	-5.8	117	21.8	0.1593	
7	CL9	OB75	31	0.0052	.897	.933	-4.7	130	4.0	0.1628	
6	CL7	CL12	62	0.2023	.694	.920	-15	41.3	223	0.1725	
5	CL6	CL8	93	0.6681	.026	.902	-26	0.6	199	0.1756	
4	CL5	OB48	94	0.0056	.021	.875	-24	0.7	0.5	0.1811	T
3	CL4	OB67	95	0.0083	.012	.827	-15	0.6	0.8	0.1811	
2	OB23	OB61	2	0.0014	.011	.697	-13	1.0	.	0.4378	
1	CL3	CL2	97	0.0109	.000	.000	0.00	.	1.0	0.5815	

Output 33.2.9 Criteria for the Number of Clusters: METHOD=SINGLE

Output 33.2.10 Plot of Clusters for METHOD=SINGLE



Output 33.2.10 *continued*



The following statements produce Output 33.2.11 through Output 33.2.14:

```
%analyze(two k=10, 3)

%analyze(two k=18, 2)
```

For *k*th-nearest-neighbor density linkage, the number of modes as a function of *k* is as follows (not all of these analyses are shown):

k	Modes
3	13
4	6
5-7	4
8-15	3
16-21	2
22+	1

Thus, there is strong evidence of three modes and an indication of the possibility of two modes. Uniform-kernel density linkage gives similar results. For K=10 (10th-nearest-neighbor density linkage), the scatter plot for three clusters is shown; and for K=18, the scatter plot for two clusters is shown.

Output 33.2.11 Cluster History for Birth and Death Rates: METHOD=TWOSTAGE K=10

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

K = 10

Root-Mean-Square Total-Sample Standard Deviation	10.127

Output 33.2.11 *continued*

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Normalized Fusion Density	Maximum Density in Each Cluster		Tie
											Lesser	Greater	
15	CL16	OB94	22	0.0015	.921	.975	-11	68.4	1.4	9.2234	6.7927	15.3069	
14	CL19	OB49	28	0.0021	.919	.972	-11	72.4	1.8	8.7369	5.9334	33.4385	
13	CL15	OB52	23	0.0024	.917	.969	-10	76.9	2.3	8.5847	5.9651	15.3069	
12	CL13	OB96	24	0.0018	.915	.966	-9.3	83.0	1.6	7.9252	5.4724	15.3069	
11	CL12	OB93	25	0.0025	.912	.962	-8.5	89.5	2.2	7.8913	5.4401	15.3069	
10	CL11	OB78	26	0.0031	.909	.957	-7.7	96.9	2.5	7.787	5.4082	15.3069	
9	CL10	OB76	27	0.0026	.907	.951	-6.7	107	2.1	7.7133	5.4401	15.3069	
8	CL9	OB77	28	0.0023	.904	.943	-5.5	120	1.7	7.4256	4.9017	15.3069	
7	CL8	OB43	29	0.0022	.902	.933	-4.1	138	1.6	6.927	4.4764	15.3069	
6	CL7	OB87	30	0.0043	.898	.920	-2.7	160	3.1	4.932	2.9977	15.3069	
5	CL6	OB82	31	0.0055	.892	.902	-1.1	191	3.7	3.7331	2.1560	15.3069	
4	CL22	OB61	37	0.0079	.884	.875	0.93	237	10.6	3.1713	1.6308	100.0	
3	CL14	OB23	29	0.0126	.872	.827	2.60	320	10.4	2.0654	1.0744	33.4385	
2	CL4	CL3	66	0.2129	.659	.697	-1.3	183	172	12.409	33.4385	100.0	
1	CL2	CL5	97	0.6588	.000	.000	0.00	.	183	10.071	15.3069	100.0	

3 modal clusters have been formed.

Output 33.2.12 Cluster History for Birth and Death Rates: METHOD=TWOSTAGE K=18

Cluster Analysis of Birth and Death Rates

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	189.106588	173.101020	0.9220	0.9220
2	16.005568		0.0780	1.0000

K = 18

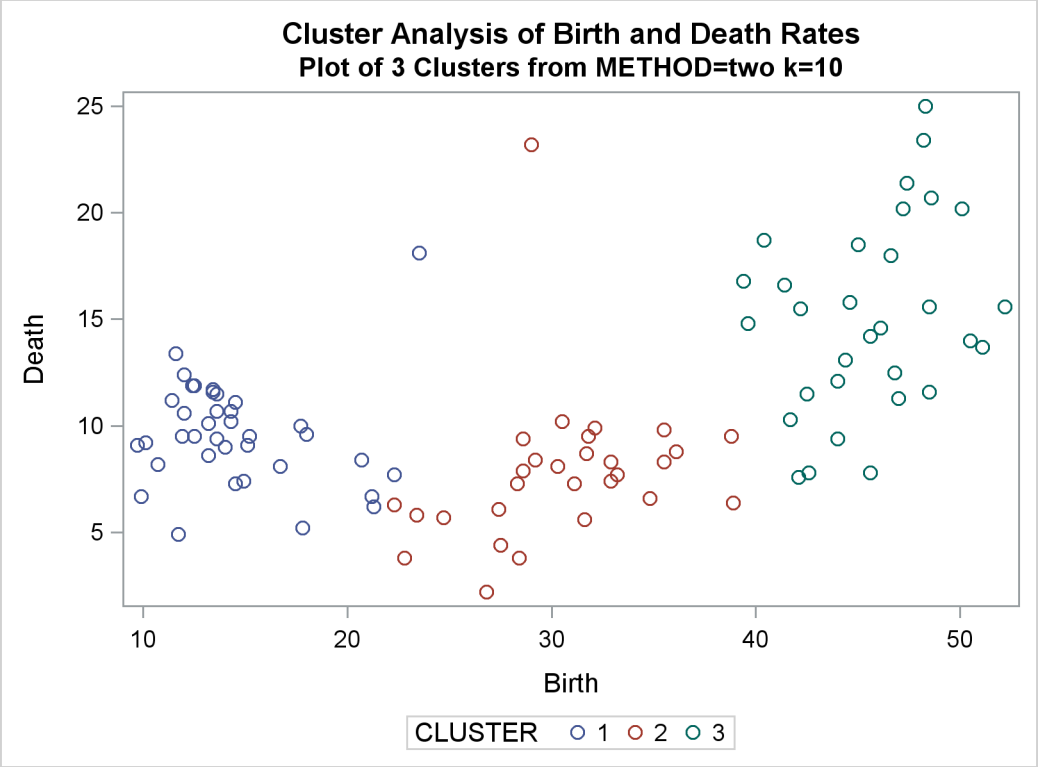
Root-Mean-Square Total-Sample Standard Deviation	10.127

Cluster History

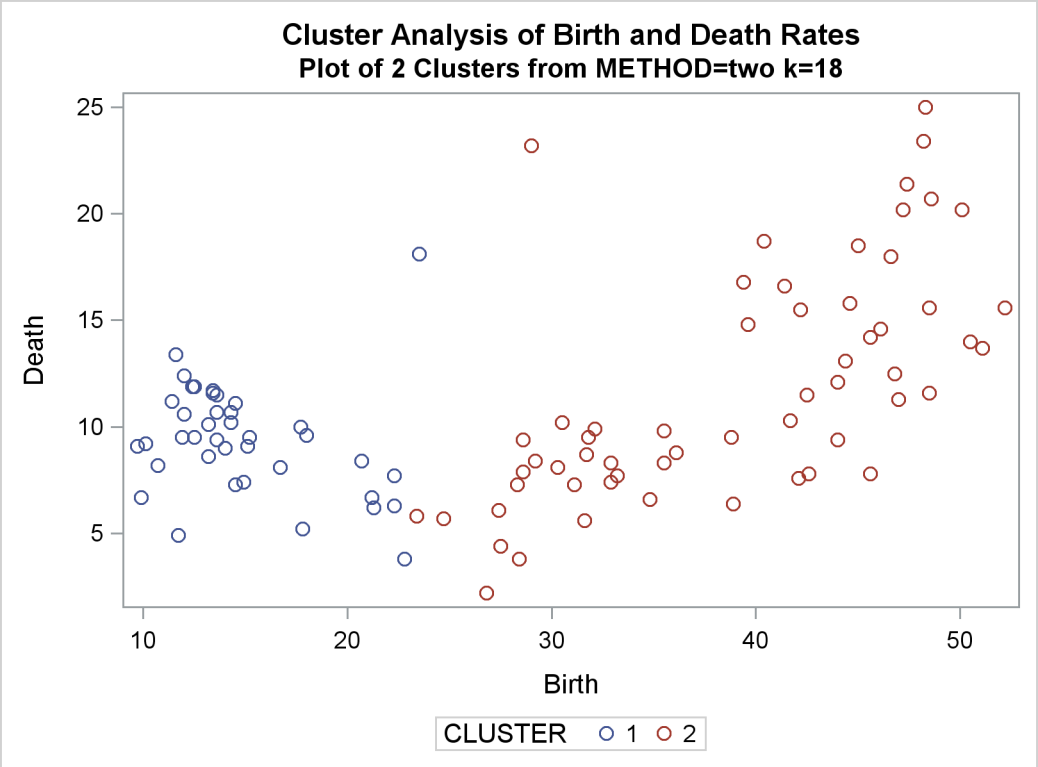
Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Normalized Fusion Density	Maximum Density in Each Cluster Lesser	Maximum Density in Each Cluster Greater	Tie
15	CL16	OB72	46	0.0107	.799	.975	-21	23.3	3.0	10.118	7.7445	23.4457	
14	CL15	OB94	47	0.0098	.789	.972	-21	23.9	2.7	9.676	7.1257	23.4457	
13	CL14	OB51	48	0.0037	.786	.969	-20	25.6	1.0	9.409	6.8398	23.4457	T
12	CL13	OB96	49	0.0099	.776	.966	-19	26.7	2.6	9.409	6.8398	23.4457	
11	CL12	OB76	50	0.0114	.764	.962	-19	27.9	2.9	8.8136	6.3138	23.4457	
10	CL11	OB77	51	0.0021	.762	.957	-18	31.0	0.5	8.6593	6.0751	23.4457	
9	CL10	OB78	52	0.0103	.752	.951	-17	33.3	2.5	8.6007	6.0976	23.4457	
8	CL9	OB43	53	0.0034	.748	.943	-16	37.8	0.8	8.4964	5.9160	23.4457	
7	CL8	OB93	54	0.0109	.737	.933	-15	42.1	2.6	8.367	5.7913	23.4457	
6	CL7	OB88	55	0.0110	.726	.920	-13	48.3	2.6	7.916	5.3679	23.4457	
5	CL6	OB87	56	0.0120	.714	.902	-12	57.5	2.7	6.6917	4.3415	23.4457	
4	CL20	OB61	39	0.0077	.707	.875	-9.8	74.7	8.3	6.2578	3.2882	100.0	
3	CL5	OB82	57	0.0138	.693	.827	-5.0	106	3.0	5.3605	3.2834	23.4457	
2	CL3	OB23	58	0.0117	.681	.697	-.54	203	2.5	3.2687	1.7568	23.4457	
1	CL2	CL4	97	0.6812	.000	.000	0.00	.	203	13.764	23.4457	100.0	

2 modal clusters have been formed.

Output 33.2.13 Plot of Clusters for METHOD=TWOSTAGE K=10



Output 33.2.14 Plot of Clusters for METHOD=TWOSTAGE K=18



In summary, most of the clustering methods indicate three or eight clusters. Most methods agree at the three-cluster level, but at the other levels, there is considerable disagreement about the composition of the clusters. The presence of numerous ties also complicates the analysis; see Example 33.4.

Example 33.3: Cluster Analysis of Fisher's Iris Data

The iris data published by Fisher (1936) have been widely used for examples in discriminant analysis and cluster analysis. The sepal length, sepal width, petal length, and petal width are measured in millimeters on 50 iris specimens from each of three species, *Iris setosa, I. versicolor,* and *I. virginica*. Mezzich and Solomon (1980) discuss a variety of cluster analyses of the iris data.

The following step displays the iris SAS data set, which is available in the Sashelp library:

```
title 'Cluster Analysis of Fisher (1936) Iris Data';

proc print data=sashelp.iris;
run;
```

The results of this step are not shown.

This example analyzes the iris data by using Ward's method and two-stage density linkage and then illustrates how the FASTCLUS procedure can be used in combination with PROC CLUSTER to analyze large data sets.

The following macro, SHOW, is used in the subsequent analyses to display cluster results. It invokes the FREQ procedure to crosstabulate clusters and species. The CANDISC procedure computes canonical variables for discriminating among the clusters, and the first two canonical variables are plotted to show cluster membership. See Chapter 31, "The CANDISC Procedure," for a canonical discriminant analysis of the iris species.

```
/*--- Define macro show ---*/
%macro show;
   proc freq;
      tables cluster*species / nopercent norow nocol plot=none;
   run;

   proc candisc noprint out=can;
      class cluster;
      var petal: sepal:;
   run;

   proc sgplot data=can;
      scatter y=can2 x=can1 / group=cluster;
   run;
%mend;
```

The first analysis clusters the iris data by using Ward's method (see Output 33.3.1) and plots the CCC and pseudo F and t^2 statistics (see Output 33.3.2). The CCC has a local peak at three clusters but a higher peak at five clusters. The pseudo F statistic indicates three clusters, while the pseudo t^2 statistic suggests three or six clusters.

The TREE procedure creates an output data set containing the three-cluster partition for use by the SHOW macro. The FREQ procedure reveals 16 misclassifications. The results are shown in Output 33.3.3.

```
title2 'By Ward''s Method';
ods graphics on;

proc cluster data=sashelp.iris method=ward print=15 ccc pseudo;
   var petal: sepal:;
   copy species;
run;

proc tree noprint ncl=3 out=out;
   copy petal: sepal: species;
run;

%show;
```

Output 33.3.1 Cluster Analysis of Fisher's Iris Data: PROC CLUSTER with METHOD=WARD

Cluster Analysis of Fisher (1936) Iris Data
By Ward's Method

The CLUSTER Procedure
Ward's Minimum Variance Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	422.824171	398.557096	0.9246	0.9246
2	24.267075	16.446125	0.0531	0.9777
3	7.820950	5.437441	0.0171	0.9948
4	2.383509		0.0052	1.0000

Root-Mean-Square Total-Sample Standard Deviation	10.69224

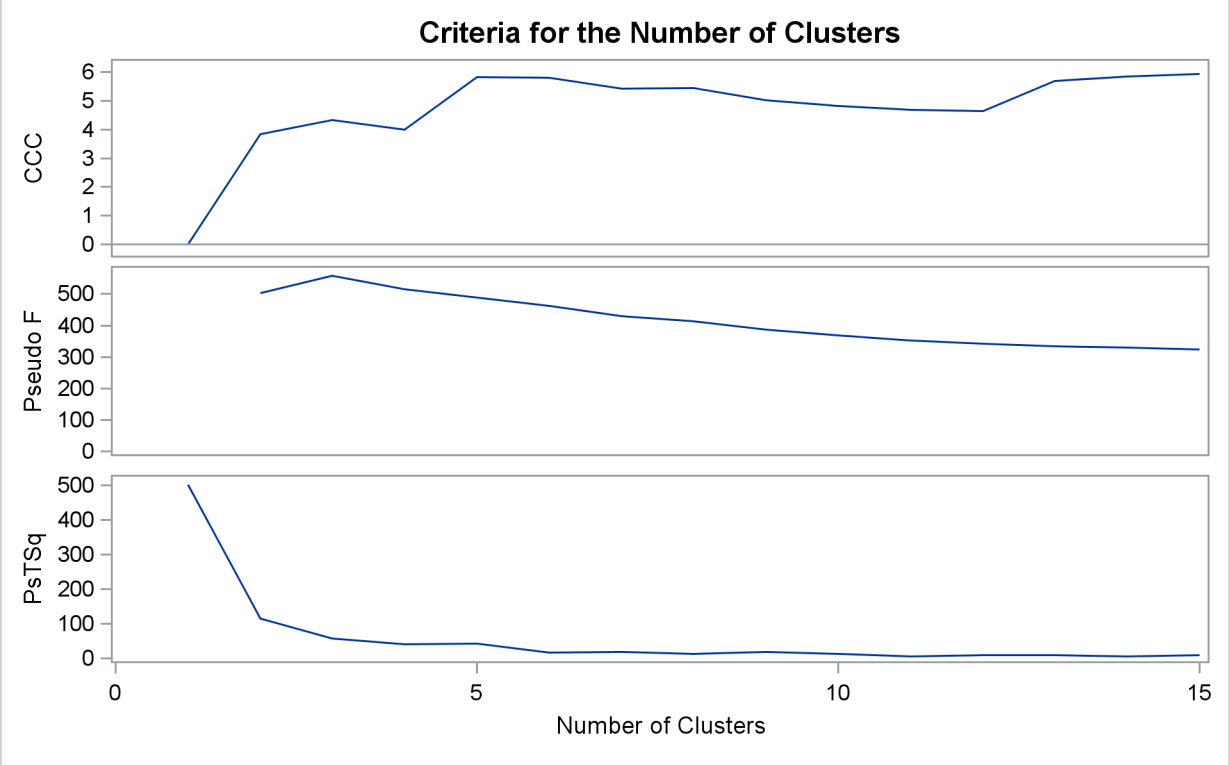
Root-Mean-Square Distance Between Observations	30.24221

Output 33.3.1 *continued*

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Tie
15	CL24	CL28	15	0.0016	.971	.958	5.93	324	9.8	
14	CL21	CL53	7	0.0019	.969	.955	5.85	329	5.1	
13	CL18	CL48	15	0.0023	.967	.953	5.69	334	8.9	
12	CL16	CL23	24	0.0023	.965	.950	4.63	342	9.6	
11	CL14	CL43	12	0.0025	.962	.946	4.67	353	5.8	
10	CL26	CL20	22	0.0027	.959	.942	4.81	368	12.9	
9	CL27	CL17	31	0.0031	.956	.936	5.02	387	17.8	
8	CL35	CL15	23	0.0031	.953	.930	5.44	414	13.8	
7	CL10	CL47	26	0.0058	.947	.921	5.43	430	19.1	
6	CL8	CL13	38	0.0060	.941	.911	5.81	463	16.3	
5	CL9	CL19	50	0.0105	.931	.895	5.82	488	43.2	
4	CL12	CL11	36	0.0172	.914	.872	3.99	515	41.0	
3	CL6	CL7	64	0.0301	.884	.827	4.33	558	57.2	
2	CL3	CL4	100	0.1110	.773	.697	3.83	503	116	
1	CL5	CL2	150	0.7726	.000	.000	0.00	.	503	

Output 33.3.2 Criteria for the Number of Clusters with METHOD=WARD



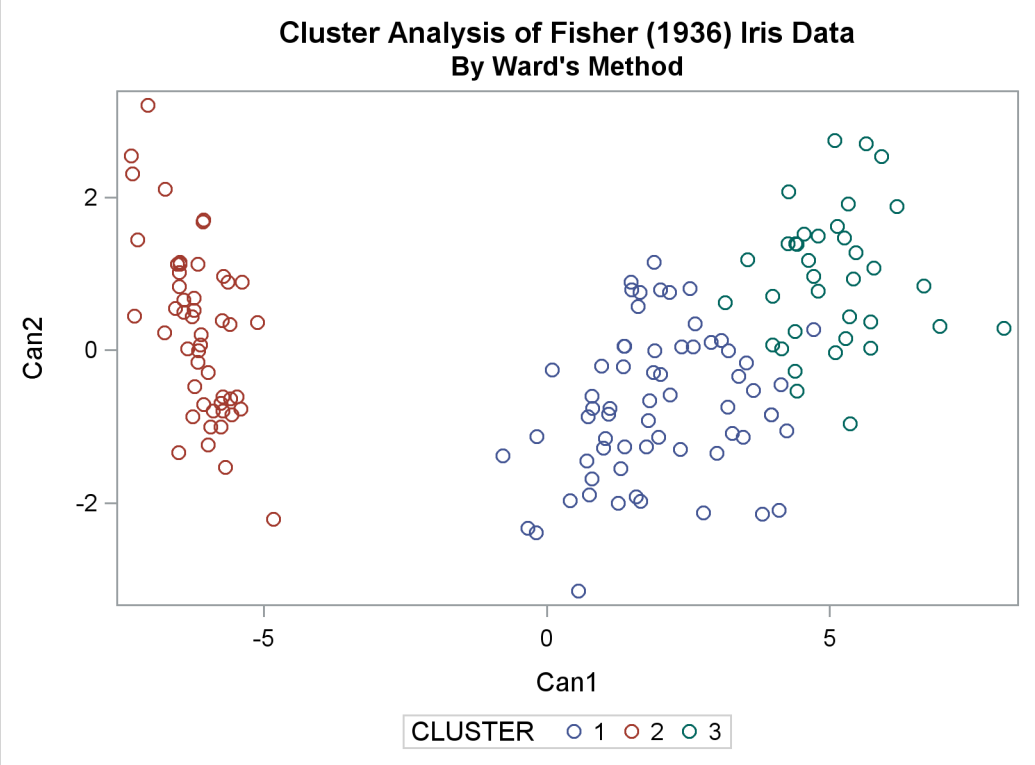
Output 33.3.3 Crosstabulation of Clusters for METHOD=WARD

Cluster Analysis of Fisher (1936) Iris Data
By Ward's Method

The FREQ Procedure

Frequency	Table of CLUSTER by Species			
	Species(Iris Species)			
CLUSTER	Setosa	Versicolor	Virginica	Total
1	0	49	15	64
2	50	0	0	50
3	0	1	35	36
Total	50	50	50	150

Output 33.3.4 Scatter Plot of Clusters for METHOD=WARD



The second analysis uses two-stage density linkage. The raw data suggest two or six modes instead of three:

k	Modes
3	12
4-6	6
7	4
8	3
9-50	2
51+	1

The following analysis uses K=8 to produce three clusters for comparison with other analyses. There are only six misclassifications. The results are shown in Output 33.3.5 and Output 33.3.6.

```
title2 'By Two-Stage Density Linkage';

proc cluster data=sashelp.iris method=twostage k=8 print=15 ccc pseudo;
   var petal: sepal:;
   copy species;
run;

proc tree noprint ncl=3 out=out;
   copy petal: sepal: species;
run;

%show;
```

Output 33.3.5 Cluster Analysis of Fisher's Iris Data: PROC CLUSTER with METHOD=TWOSTAGE

Cluster Analysis of Fisher (1936) Iris Data
By Two-Stage Density Linkage

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	422.824171	398.557096	0.9246	0.9246
2	24.267075	16.446125	0.0531	0.9777
3	7.820950	5.437441	0.0171	0.9948
4	2.383509		0.0052	1.0000

K = 8

Root-Mean-Square Total-Sample Standard Deviation	10.69224

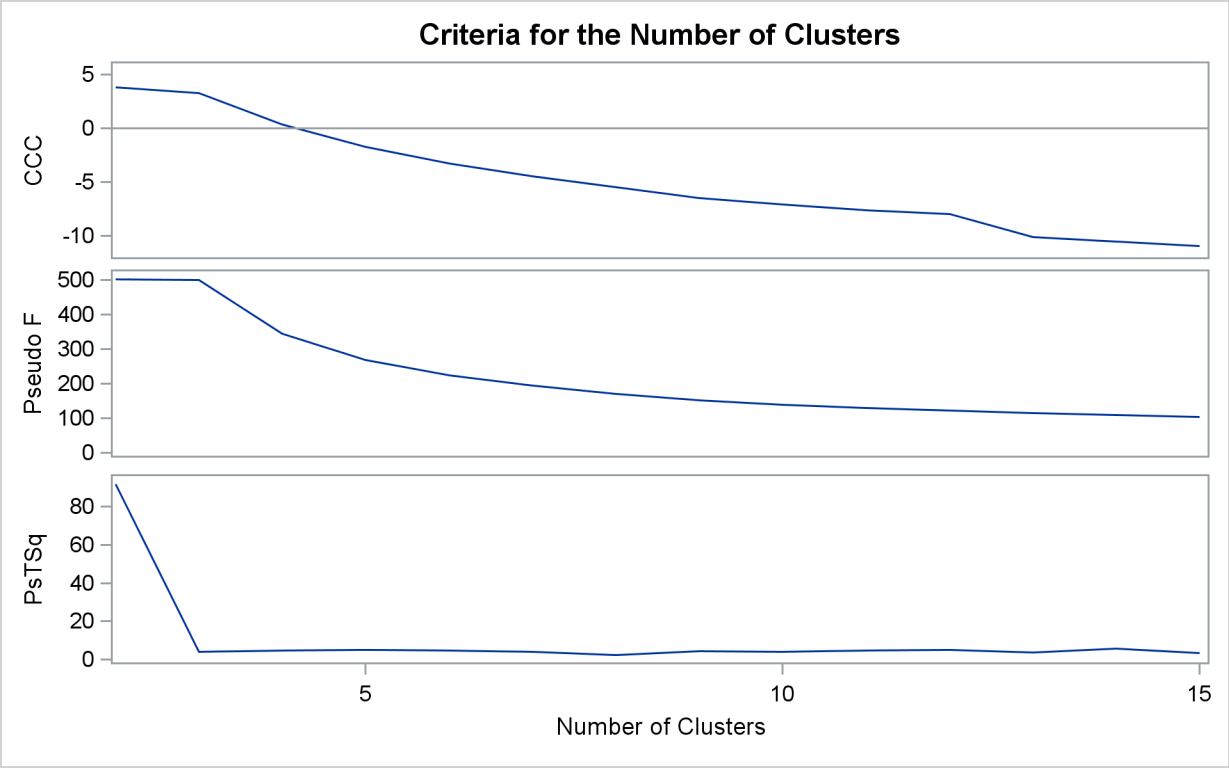
Output 33.3.5 *continued*

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Normalized Fusion Density	Maximum Density in Each Cluster Lesser	Greater	Tie
15	CL17	OB144	44	0.0025	.916	.958	-11	105	3.4	0.3903	0.2066	3.5156	
14	CL16	OB44	50	0.0023	.913	.955	-11	110	5.6	0.3637	0.1837	100.0	
13	CL15	OB127	45	0.0029	.910	.953	-10	116	3.7	0.3553	0.2130	3.5156	
12	CL28	OB66	46	0.0036	.907	.950	-8.0	122	5.2	0.3223	0.1736	8.3678	T
11	CL12	OB73	47	0.0036	.903	.946	-7.6	130	4.8	0.3223	0.1736	8.3678	
10	CL11	OB79	48	0.0033	.900	.942	-7.1	140	4.1	0.2879	0.1479	8.3678	
9	CL13	OB112	46	0.0037	.896	.936	-6.5	152	4.4	0.2802	0.2005	3.5156	
8	CL10	OB113	49	0.0019	.894	.930	-5.5	171	2.2	0.2699	0.1372	8.3678	
7	CL8	OB91	50	0.0035	.891	.921	-4.5	194	4.0	0.2586	0.1372	8.3678	
6	CL9	OB120	47	0.0042	.886	.911	-3.3	225	4.6	0.1412	0.0832	3.5156	
5	CL6	OB118	48	0.0049	.882	.895	-1.7	270	5.0	0.107	0.0605	3.5156	
4	CL5	OB110	49	0.0049	.877	.872	0.35	346	4.7	0.0969	0.0541	3.5156	
3	CL4	OB135	50	0.0047	.872	.827	3.28	500	4.1	0.0715	0.0370	3.5156	
2	CL7	CL3	100	0.0993	.773	.697	3.83	503	91.9	2.6277	3.5156	8.3678	

3 modal clusters have been formed.

Output 33.3.6 Criteria for the Number of Clusters with METHOD=TWOSTAGE



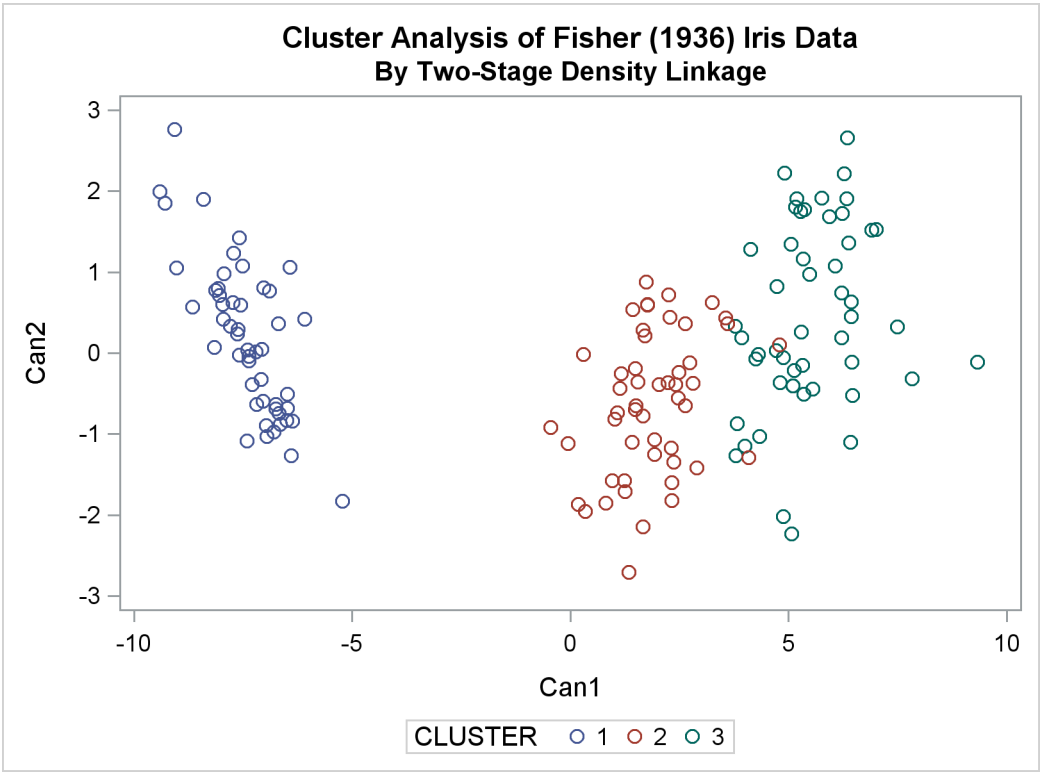
Output 33.3.7 Crosstabulation of Clusters for METHOD=TWOSTAGE

Cluster Analysis of Fisher (1936) Iris Data
By Two-Stage Density Linkage

The FREQ Procedure

Frequency	Table of CLUSTER by Species			
		Species(Iris Species)		
CLUSTER	Setosa	Versicolor	Virginica	Total
1	50	0	0	50
2	0	47	3	50
3	0	3	47	50
Total	50	50	50	150

Output 33.3.8 Scatter Plot of Clusters for METHOD=TWOSTAGE



The CLUSTER procedure is not practical for very large data sets because, with most methods, the CPU time is roughly proportional to the square or cube of the number of observations. The FASTCLUS procedure requires time proportional to the number of observations and can therefore be used with much larger data sets than PROC CLUSTER. If you want to hierarchically cluster a very large data set, you can use PROC FASTCLUS for a preliminary cluster analysis to produce a large number of clusters and then use PROC CLUSTER to hierarchically cluster the preliminary clusters.

FASTCLUS automatically creates the variables _FREQ_ and _RMSSTD_ in the MEAN= output data set. These variables are then automatically used by PROC CLUSTER in the computation of various statistics.

The following SAS code uses the iris data to illustrate the process of clustering clusters. In the preliminary analysis, PROC FASTCLUS produces ten clusters, which are then crosstabulated with species. The data set containing the preliminary clusters is sorted in preparation for later merges. The results are shown in Output 33.3.9 and Output 33.3.10.

```
title2 'Preliminary Analysis by FASTCLUS';
proc fastclus data=sashelp.iris summary maxc=10 maxiter=99 converge=0
              mean=mean out=prelim cluster=preclus;
   var petal: sepal:;
run;

proc freq;
   tables preclus*species / nopercent norow nocol plot=none;
run;

proc sort data=prelim;
   by preclus;
run;
```

Output 33.3.9 Preliminary Analysis of Fisher's Iris Data: FASTCLUS Procedure

Cluster Analysis of Fisher (1936) Iris Data
Preliminary Analysis by FASTCLUS

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=10 Maxiter=99 Converge=0

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 2.1271

Output 33.3.9 *continued*

Cluster Summary

Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster	Distance Between Cluster Centroids
1	14	2.3258	6.6047		10	5.6068
2	16	2.0402	6.7373		3	6.2977
3	23	1.6115	6.3775		8	5.4185
4	24	2.4329	8.3178		6	9.3274
5	10	3.1829	7.9517		4	12.4281
6	18	2.2628	7.1135		7	8.2685
7	12	1.9824	7.0833		1	7.6733
8	11	1.7123	7.0435		3	5.4185
9	10	2.5155	6.1335		10	8.4783
10	12	2.0207	7.9390		1	5.6068

Pseudo F Statistic = 374.89

Observed Over-All R-Squared = 0.96016

Approximate Expected Over-All R-Squared = 0.82928

Cubic Clustering Criterion = 27.285

WARNING: The two values above are invalid for correlated variables.

Output 33.3.10 Crosstabulation of Species and Cluster From the FASTCLUS Procedure

Cluster Analysis of Fisher (1936) Iris Data
Preliminary Analysis by FASTCLUS

The FREQ Procedure

Frequency — **Table of preclus by Species**

	Species(Iris Species)			
preclus(Cluster)	**Setosa**	**Versicolor**	**Virginica**	**Total**
1	0	14	0	14
2	16	0	0	16
3	23	0	0	23
4	0	0	24	24
5	0	0	10	10
6	0	3	15	18
7	0	12	0	12
8	11	0	0	11
9	0	10	0	10
10	0	11	1	12
Total	50	50	50	150

The following macro, CLUS, clusters the preliminary clusters. There is one argument to choose the METHOD= specification to be used by PROC CLUSTER. The TREE procedure creates an output data set containing the three-cluster partition, which is sorted and merged with the OUT= data set from PROC FASTCLUS to determine which cluster each of the original 150 observations belongs to. The SHOW macro is then used to display the results. In this example, the CLUS macro is invoked using Ward's method, which produces 16 misclassifications, and Wong's hybrid method, which produces 22 misclassifications.

```
/*--- Define macro clus ---*/
%macro clus(method);
   proc cluster data=mean method=&method ccc pseudo;
      var petal: sepal:;
      copy preclus;
   run;

   proc tree noprint ncl=3 out=out;
      copy petal: sepal: preclus;
   run;

   proc sort data=out;
      by preclus;
   run;

   data clus;
      merge out prelim;
      by preclus;
   run;

   %show;
%mend;
```

The following statements produce Output 33.3.11 through Output 33.3.14.

```
title2 'Clustering Clusters by Ward''s Method';
%clus(ward);
```

Output 33.3.11 Clustering Clusters by Ward's Method

Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Ward's Method

The CLUSTER Procedure
Ward's Minimum Variance Cluster Analysis

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	417.301104	398.455363	0.9504	0.9504
2	18.845742	16.244505	0.0429	0.9933
3	2.601236	2.272553	0.0059	0.9993
4	0.328684		0.0007	1.0000

Root-Mean-Square Total-Sample Standard Deviation	10.69224

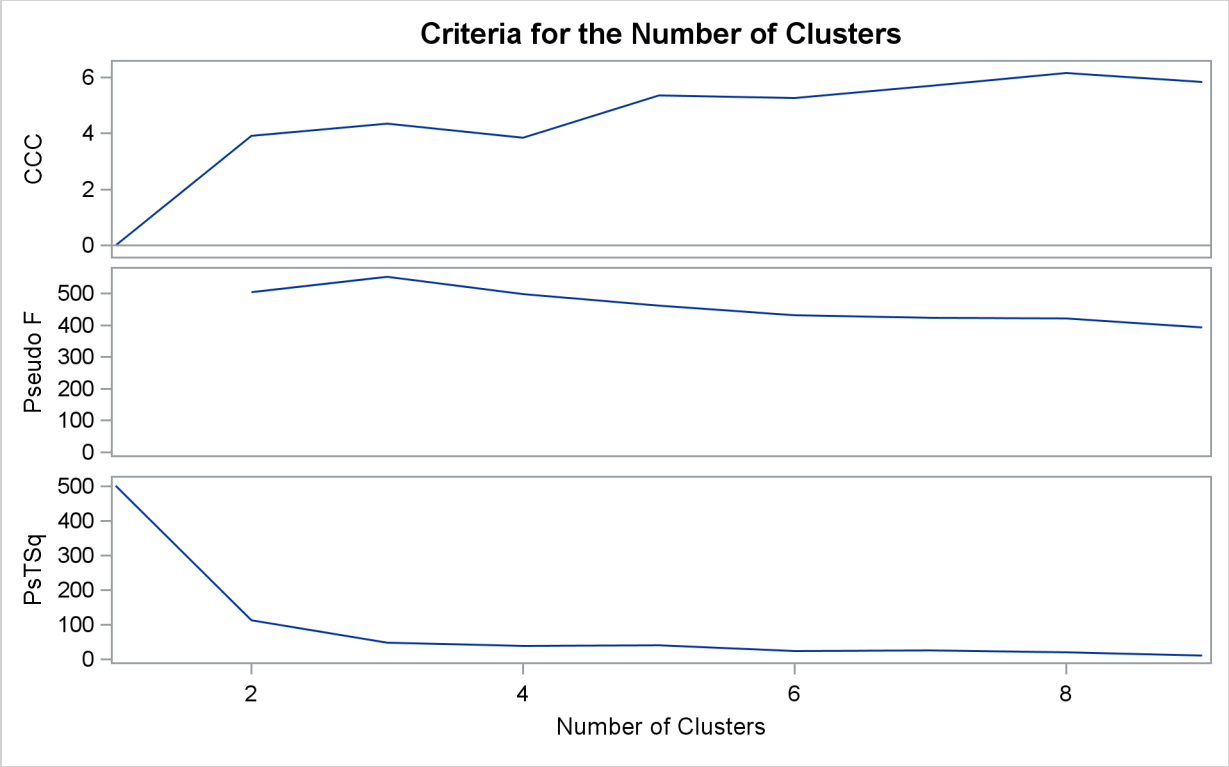
Root-Mean-Square Distance Between Observations	30.24221

Output 33.3.11 *continued*

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Tie
9	OB1	OB10	26	0.0030	.957	.934	5.84	394	10.6	
8	OB3	OB8	34	0.0032	.954	.927	6.16	420	20.2	
7	OB6	OB7	30	0.0072	.947	.919	5.70	424	26.5	
6	CL9	OB9	36	0.0094	.937	.908	5.26	431	24.5	
5	OB2	CL8	50	0.0103	.927	.893	5.36	461	41.3	
4	OB4	OB5	34	0.0160	.911	.870	3.84	498	38.4	
3	CL6	CL7	66	0.0285	.883	.825	4.36	552	48.8	
2	CL3	CL4	100	0.1099	.773	.695	3.91	503	113	
1	CL2	CL5	150	0.7726	.000	.000	0.00	.	503	

Output 33.3.12 Criteria for the Number of Clusters for Clustering Clusters from Ward's Method



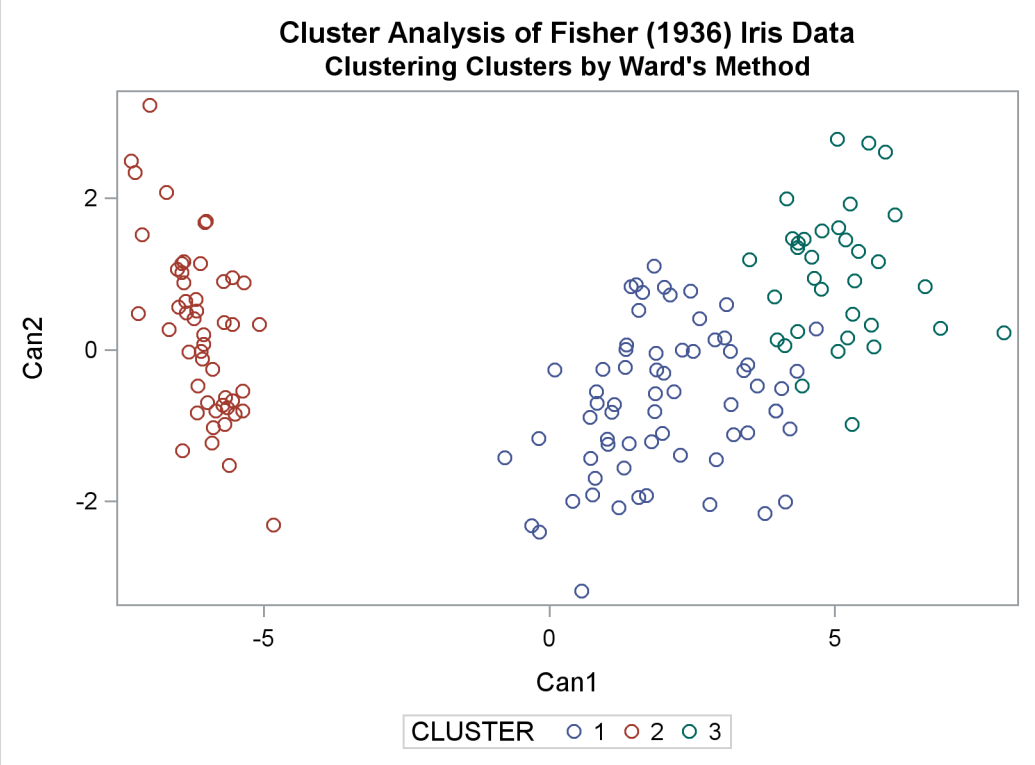
Output 33.3.13 Crosstabulation for Clustering Clusters from Ward's Method

Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Ward's Method

The FREQ Procedure

Frequency	Table of CLUSTER by Species			
	Species(Iris Species)			
CLUSTER	Setosa	Versicolor	Virginica	Total
1	0	50	16	66
2	50	0	0	50
3	0	0	34	34
Total	50	50	50	150

Output 33.3.14 Scatter Plot for Clustering Clusters using Ward's Method



The following statements produce Output 33.3.15 through Output 33.3.17.

```
title2 "Clustering Clusters by Wong's Hybrid Method";
%clus(twostage hybrid);
```

Output 33.3.15 Clustering Clusters by Wong's Hybrid Method

Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Wong's Hybrid Method

The CLUSTER Procedure
Two-Stage Density Linkage Clustering

Eigenvalues of the Covariance Matrix

	Eigenvalue	Difference	Proportion	Cumulative
1	417.301104	398.455363	0.9504	0.9504
2	18.845742	16.244505	0.0429	0.9933
3	2.601236	2.272553	0.0059	0.9993
4	0.328684		0.0007	1.0000

Root-Mean-Square Total-Sample Standard Deviation	10.69224

Cluster History

Number of Clusters	Clusters Joined		Freq	Semipartial R-Square	R-Square	Approximate Expected R-Square	Cubic Clustering Criterion	Pseudo F Statistic	Pseudo t-Squared	Normalized Fusion Density	Maximum Density in Each Cluster Lesser	Greater	Tie
9	OB3	OB8	34	0.0032	.957	.934	5.77	392	20.2	47.595	41.5390	100.0	
8	CL9	OB2	50	0.0103	.947	.927	4.19	360	41.3	34.03	28.1852	100.0	
7	OB1	OB10	26	0.0030	.944	.919	4.94	399	10.6	17.044	14.8854	22.9763	
6	OB6	OB7	30	0.0072	.936	.908	5.07	424	26.5	10.842	20.6497	24.8051	
5	CL6	OB4	54	0.0169	.920	.893	4.00	415	38.4	9.7472	20.0098	24.8051	
4	CL7	OB9	36	0.0094	.910	.870	3.74	493	24.5	7.0911	8.2711	22.9763	
3	CL5	OB5	64	0.0347	.875	.825	3.72	517	47.7	3.4164	3.2270	24.8051	
2	CL3	CL4	100	0.1029	.773	.695	3.91	503	98.5	10.77	22.9763	24.8051	
1	CL2	CL8	150	0.7726	.000	.000	0.00	.	503	0.5153	24.8051	100.0	

3 modal clusters have been formed.

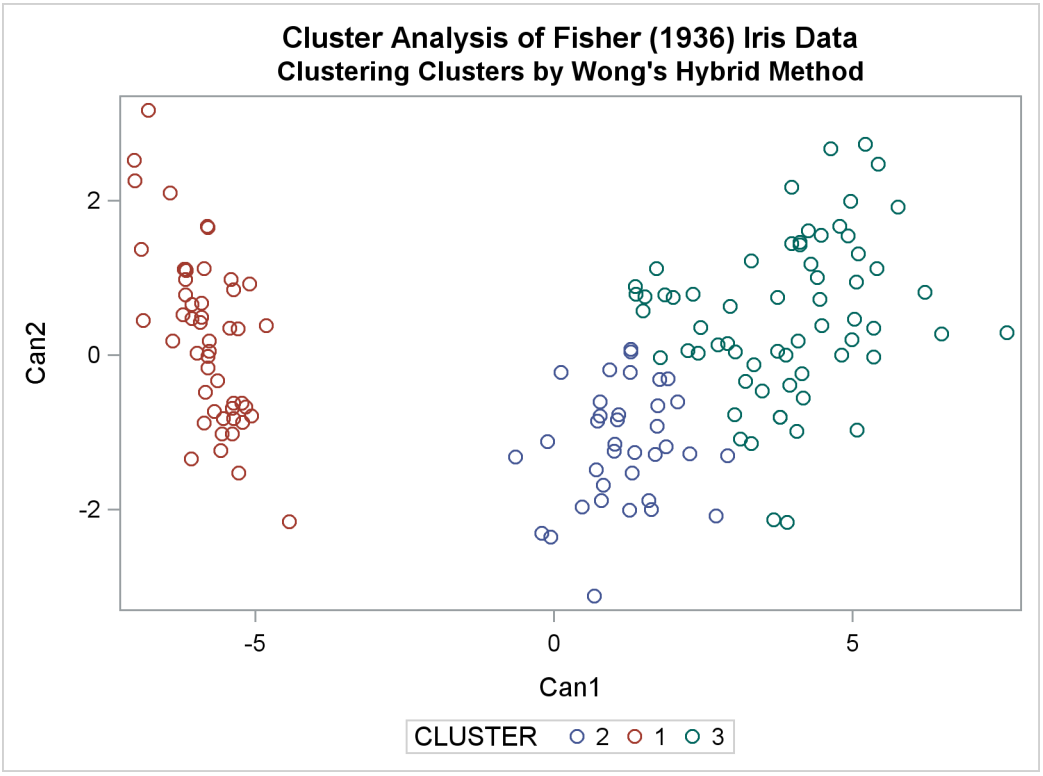
Output 33.3.16 Crosstabulation for Clustering Clusters from Wong's Hybrid Method

Cluster Analysis of Fisher (1936) Iris Data
Clustering Clusters by Wong's Hybrid Method

The FREQ Procedure

Frequency	Table of CLUSTER by Species			
	Species(Iris Species)			
CLUSTER	Setosa	Versicolor	Virginica	Total
1	50	0	0	50
2	0	35	1	36
3	0	15	49	64
Total	50	50	50	150

Output 33.3.17 Scatter Plot for Clustering Clusters using Wong's Hybrid Method



Example 33.4: Evaluating the Effects of Ties

If, at some level of the cluster history, there is a tie for minimum distance between clusters, then one or more levels of the sample cluster tree are not uniquely determined. This example shows how the degree of indeterminacy can be assessed.

Mammals have four kinds of teeth: incisors, canines, premolars, and molars. The following data set gives the number of teeth of each kind on one side of the top and bottom jaws for 32 mammals.

Since all eight variables are measured in the same units, it is not strictly necessary to rescale the data. However, the canines have much less variance than the other kinds of teeth and, therefore, have little effect on the analysis if the variables are not standardized. An average linkage cluster analysis is run with and without standardization to enable comparison of the results.

```
title 'Hierarchical Cluster Analysis of Mammals'' Teeth Data';
title2 'Evaluating the Effects of Ties';
data teeth;
   input Mammal & $16. v1-v8 @@;
   label v1='Top incisors'
         v2='Bottom incisors'
         v3='Top canines'
         v4='Bottom canines'
         v5='Top premolars'
         v6='Bottom premolars'
         v7='Top molars'
         v8='Bottom molars';
   datalines;
Brown Bat         2 3 1 1 3 3 3 3   Mole              3 2 1 0 3 3 3 3
Silver Hair Bat   2 3 1 1 2 3 3 3   Pigmy Bat         2 3 1 1 2 2 3 3
House Bat         2 3 1 1 1 2 3 3   Red Bat           1 3 1 1 2 2 3 3
Pika              2 1 0 0 2 2 3 3   Rabbit            2 1 0 0 3 2 3 3
Beaver            1 1 0 0 2 1 3 3   Groundhog         1 1 0 0 2 1 3 3
Gray Squirrel     1 1 0 0 1 1 3 3   House Mouse       1 1 0 0 0 0 3 3
Porcupine         1 1 0 0 1 1 3 3   Wolf              3 3 1 1 4 4 2 3
Bear              3 3 1 1 4 4 2 3   Raccoon           3 3 1 1 4 4 3 2
Marten            3 3 1 1 4 4 1 2   Weasel            3 3 1 1 3 3 1 2
Wolverine         3 3 1 1 4 4 1 2   Badger            3 3 1 1 3 3 1 2
River Otter       3 3 1 1 4 3 1 2   Sea Otter         3 2 1 1 3 3 1 2
Jaguar            3 3 1 1 3 2 1 1   Cougar            3 3 1 1 3 2 1 1
Fur Seal          3 2 1 1 4 4 1 1   Sea Lion          3 2 1 1 4 4 1 1
Grey Seal         3 2 1 1 3 3 2 2   Elephant Seal     2 1 1 1 4 4 1 1
Reindeer          0 4 1 0 3 3 3 3   Elk               0 4 1 0 3 3 3 3
Deer              0 4 0 0 3 3 3 3   Moose             0 4 0 0 3 3 3 3
;
```

The following statements produce Output 33.4.1:

```
title3 'Raw Data';
proc cluster data=teeth method=average nonorm noeigen;
   var v1-v8;
   id mammal;
run;
```

Output 33.4.1 Average Linkage Analysis of Mammals' Teeth Data: Raw Data

Hierarchical Cluster Analysis of Mammals' Teeth Data
Evaluating the Effects of Ties
Raw Data

The CLUSTER Procedure
Average Linkage Cluster Analysis

Root-Mean-Square Total-Sample Standard Deviation	0.898027

Cluster History

Number of Clusters	Clusters Joined		Freq	RMS Distance	Tie
31	Beaver	Groundhog	2	0	T
30	Gray Squirrel	Porcupine	2	0	T
29	Wolf	Bear	2	0	T
28	Marten	Wolverine	2	0	T
27	Weasel	Badger	2	0	T
26	Jaguar	Cougar	2	0	T
25	Fur Seal	Sea Lion	2	0	T
24	Reindeer	Elk	2	0	T
23	Deer	Moose	2	0	
22	Brown Bat	Silver Hair Bat	2	1	T
21	Pigmy Bat	House Bat	2	1	T
20	Pika	Rabbit	2	1	T
19	CL31	CL30	4	1	T
18	CL28	River Otter	3	1	T
17	CL27	Sea Otter	3	1	T
16	CL24	CL23	4	1	
15	CL21	Red Bat	3	1.2247	
14	CL17	Grey Seal	4	1.291	
13	CL29	Raccoon	3	1.4142	T
12	CL25	Elephant Seal	3	1.4142	
11	CL18	CL14	7	1.5546	
10	CL22	CL15	5	1.5811	
9	CL20	CL19	6	1.8708	T
8	CL11	CL26	9	1.9272	
7	CL8	CL12	12	2.2278	
6	Mole	CL13	4	2.2361	
5	CL9	House Mouse	7	2.4833	
4	CL6	CL7	16	2.5658	
3	CL10	CL16	9	2.8107	
2	CL3	CL5	16	3.7054	
1	CL2	CL4	32	4.2939	

The following statements produce Output 33.4.2:

```
title3 'Standardized Data';
proc cluster data=teeth std method=average nonorm noeigen;
   var v1-v8;
   id mammal;
run;
```

Output 33.4.2 Average Linkage Analysis of Mammals' Teeth Data: Standardized Data

Hierarchical Cluster Analysis of Mammals' Teeth Data
Evaluating the Effects of Ties
Standardized Data

The CLUSTER Procedure
Average Linkage Cluster Analysis

The data have been standardized to mean 0 and variance 1

Root-Mean-Square Total-Sample Standard Deviation	1

Output 33.4.2 *continued*

Cluster History

Number of Clusters	Clusters Joined		Freq	RMS Distance	Tie
31	Beaver	Groundhog	2	0	T
30	Gray Squirrel	Porcupine	2	0	T
29	Wolf	Bear	2	0	T
28	Marten	Wolverine	2	0	T
27	Weasel	Badger	2	0	T
26	Jaguar	Cougar	2	0	T
25	Fur Seal	Sea Lion	2	0	T
24	Reindeer	Elk	2	0	T
23	Deer	Moose	2	0	
22	Pigmy Bat	Red Bat	2	0.9157	
21	CL28	River Otter	3	0.9169	
20	CL31	CL30	4	0.9428	T
19	Brown Bat	Silver Hair Bat	2	0.9428	T
18	Pika	Rabbit	2	0.9428	
17	CL27	Sea Otter	3	0.9847	
16	CL22	House Bat	3	1.1437	
15	CL21	CL17	6	1.3314	
14	CL25	Elephant Seal	3	1.3447	
13	CL19	CL16	5	1.4688	
12	CL15	Grey Seal	7	1.6314	
11	CL29	Raccoon	3	1.692	
10	CL18	CL20	6	1.7357	
9	CL12	CL26	9	2.0285	
8	CL24	CL23	4	2.1891	
7	CL9	CL14	12	2.2674	
6	CL10	House Mouse	7	2.317	
5	CL11	CL7	15	2.6484	
4	CL13	Mole	6	2.8624	
3	CL4	CL8	10	3.5194	
2	CL3	CL6	17	4.1265	
1	CL2	CL5	32	4.7753	

There are ties at 16 levels for the raw data but at only 10 levels for the standardized data. There are more ties for the raw data because the increments between successive values are the same for all of the raw variables but different for the standardized variables.

One way to assess the importance of the ties in the analysis is to repeat the analysis on several random permutations of the observations and then to see to what extent the results are consistent at the interesting levels of the cluster history. Three macros are presented to facilitate this process, as follows.

```
/* ---------------------------------------------------------- */
/*                                                            */
/* The macro CLUSPERM randomly permutes observations and      */
/* does a cluster analysis for each permutation.              */
/* The arguments are as follows:                              */
/*                                                            */
/*    data    data set name                                   */
/*    var     list of variables to cluster                    */
/*    id      id variable for proc cluster                    */
/*    method  clustering method (and possibly other options)  */
/*    nperm   number of random permutations.                  */
/*                                                            */
/* ---------------------------------------------------------- */
%macro CLUSPERM(data,var,id,method,nperm);

   /* ------CREATE TEMPORARY DATA SET WITH RANDOM NUMBERS------ */
   data _temp_;
      set &data;
      array _random_ _ran_1-_ran_&nperm;
      do over _random_;
         _random_=ranuni(835297461);
      end;
   run;

   /* ------PERMUTE AND CLUSTER THE DATA----------------------- */
   %do n=1 %to &nperm;
      proc sort data=_temp_(keep=_ran_&n &var &id) out=_perm_;
         by _ran_&n;
      run;

      proc cluster method=&method noprint outtree=_tree_&n;
         var &var;
         id &id;
      run;
   %end;
%mend;
```

```
/* ---------------------------------------------------------- */
/*                                                            */
/* The macro PLOTPERM plots various cluster statistics        */
/* against the number of clusters for each permutation.       */
/* The arguments are as follows:                              */
/*                                                            */
/*    nclus   maximum number of clusters to be plotted        */
/*    nperm   number of random permutations.                  */
/*                                                            */
/* ---------------------------------------------------------- */
%macro PLOTPERM(nclus,nperm);

   /* ---CONCATENATE TREE DATA SETS FOR 20 OR FEWER CLUSTERS--- */
   data _plot_;
      set %do n=1 %to &nperm; _tree_&n(in=_in_&n) %end;;
      if _ncl_<=&nclus;
      %do n=1 %to &nperm;
         if _in_&n then _perm_=&n;
      %end;
      label _perm_='permutation number';
      keep _ncl_ _psf_ _pst2_ _ccc_ _perm_;
   run;

   /* ---PLOT THE REQUESTED STATISTICS BY NUMBER OF CLUSTERS--- */
   proc sgscatter;
      compare y=(_ccc_ _psf_ _pst2_) x=_ncl_ /group=_perm_;
      label _ccc_ = 'CCC' _psf_ = 'Pseudo F' _pst2_ = 'Pseudo T-Squared';
   run;
%mend;

/* ---------------------------------------------------------- */
/*                                                            */
/* The macro TABPERM generates cluster-membership variables   */
/* for a specified number of clusters for each permutation.   */
/* PROC TABULATE gives the frequencies and means.             */
/* The arguments are as follows:                              */
/*                                                            */
/*    var     list of variables to cluster                    */
/*            (no "-" or ":" allowed)                         */
/*    id      id variable for proc cluster                    */
/*    meanfmt format for printing means in PROC TABULATE      */
/*    nclus   number of clusters desired                      */
/*    nperm   number of random permutations.                  */
/*                                                            */
/* ---------------------------------------------------------- */
%macro TABPERM(var,id,meanfmt,nclus,nperm);

   /* ------CREATE DATA SETS GIVING CLUSTER MEMBERSHIP--------- */
   %do n=1 %to &nperm;
      proc tree data=_tree_&n noprint n=&nclus
                out=_out_&n(drop=clusname
                            rename=(cluster=_clus_&n));
         copy &var;
         id &id;
      run;
```

```
      proc sort;
         by &id &var;
      run;
   %end;

   /* ------MERGE THE CLUSTER VARIABLES---------------------- */
   data _merge_;
      merge
         %do n=1 %to &nperm;
            _out_&n
         %end;;
      by &id &var;
      length all_clus $ %eval(3*&nperm);
      %do n=1 %to &nperm;
         substr( all_clus, %eval(1+(&n-1)*3), 3) =
            put( _clus_&n, 3.);
      %end;
   run;

   /* ------ TABULATE CLUSTER COMBINATIONS------------ */
   proc sort;
      by _clus_:;
   run;
   proc tabulate order=data formchar='           ';
      class all_clus;
      var &var;
      table all_clus, n='FREQ'*f=5. mean*f=&meanfmt*(&var) /
         rts=%eval(&nperm*3+1);
   run;
%mend;
```

To use these macros, it is first convenient to define a macro variable, VLIST, listing the teeth variables, since the forms V1-V8 or V: cannot be used with the TABULATE procedure in the TABPERM macro:

```
/* -TABULATE does not accept hyphens or colons in VAR lists- */
%let vlist=v1 v2 v3 v4 v5 v6 v7 v8;
```

The CLUSPERM macro is then called to analyze 10 random permutations. The PLOTPERM macro plots the pseudo F and t^2 statistics and the cubic clustering criterion. Since the data are discrete, the pseudo F statistic and the cubic clustering criterion can be expected to increase as the number of clusters increases, so local maxima or large jumps in these statistics are more relevant than the global maximum in determining the number of clusters. For the raw data, only the pseudo t^2 statistic indicates the possible presence of clusters, with the four-cluster level being suggested. Hence, the macros are used as follows to analyze the results at the four-cluster level:

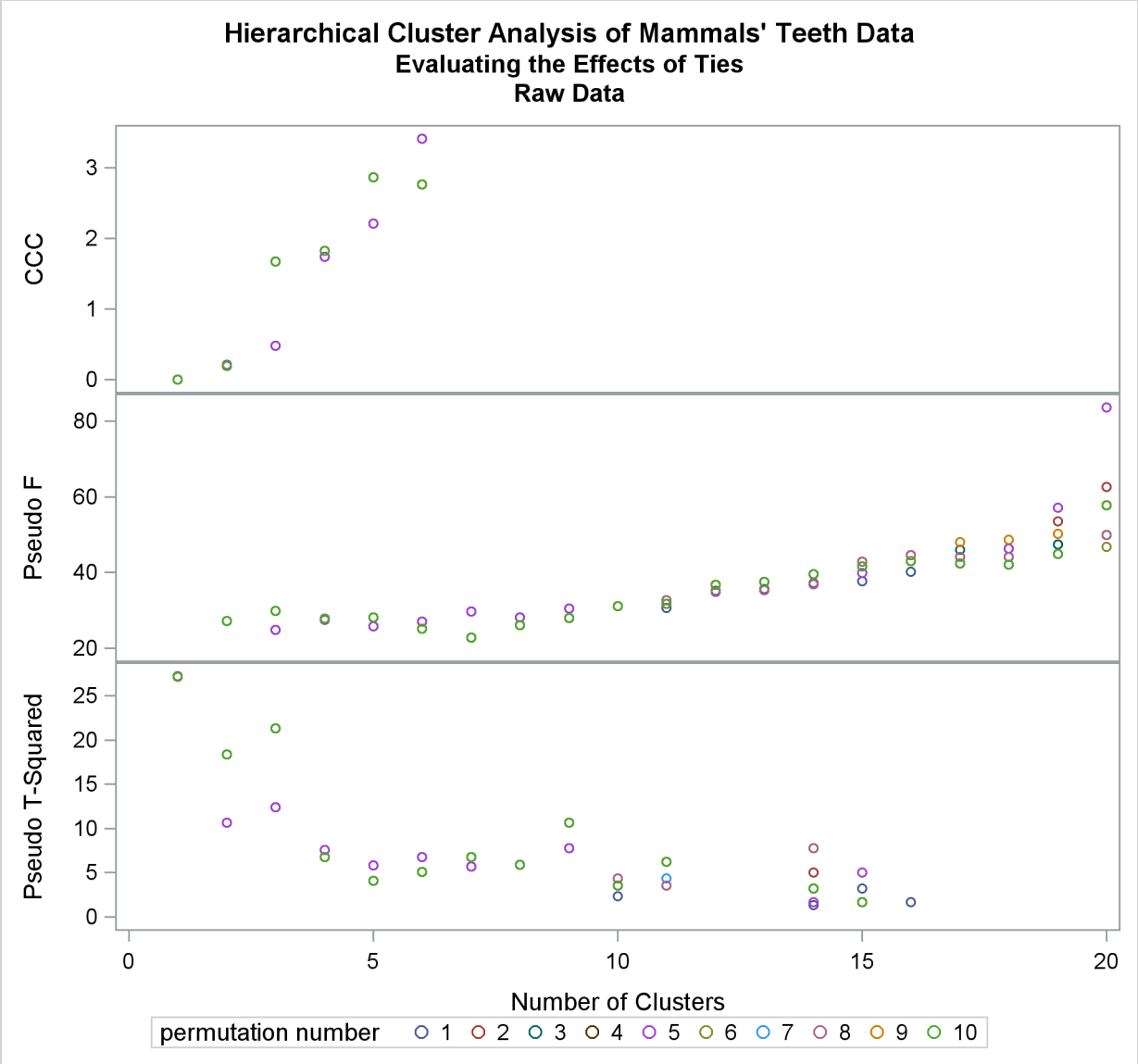
```
title3 'Raw Data';

/* ------CLUSTER RAW DATA WITH AVERAGE LINKAGE-------------- */
%clusperm( teeth, &vlist, mammal, average, 10);
```

The following statements produce Output 33.4.3.

```
/* -----PLOT STATISTICS FOR THE LAST 20 LEVELS-------------- */
%plotperm(20, 10);
```

Output 33.4.3 Analysis of 10 Random Permutations of Raw Mammals' Teeth Data



The following statements produce Output 33.4.4.

```
/* ------ANALYZE THE 4-CLUSTER LEVEL----------------------- */
%tabperm( &vlist, mammal, 9.1, 4, 10);
```

Output 33.4.4 Raw Mammals' Teeth Data: Indeterminacy at the Four-Cluster Level

Hierarchical Cluster Analysis of Mammals' Teeth Data
Evaluating the Effects of Ties
Raw Data

		Mean							
	FREQ	Top incisors	Bottom incisors	Top canines	Bottom canines	Top premolars	Bottom premolars	Top molars	Bottom molars
all_clus									
1 3 1 1 1 3 3 3 2 3	4	0.0	4.0	0.5	0.0	3.0	3.0	3.0	3.0
2 2 2 2 2 2 1 2 1 1	15	2.9	2.6	1.0	1.0	3.6	3.4	1.3	1.8
2 4 2 2 4 2 1 2 1 1	1	3.0	2.0	1.0	0.0	3.0	3.0	3.0	3.0
3 1 3 3 3 1 2 1 3 2	5	1.0	1.0	0.0	0.0	1.2	0.8	3.0	3.0
3 4 3 3 4 1 2 1 3 2	2	2.0	1.0	0.0	0.0	2.5	2.0	3.0	3.0
4 4 4 4 4 4 4 4 4 4	5	1.8	3.0	1.0	1.0	2.0	2.4	3.0	3.0

From the TABULATE output, you can see that two types of clustering are obtained. In one case, the mole is grouped with the carnivores, while the pika and rabbit are grouped with the rodents. In the other case, both the mole and the lagomorphs are grouped with the bats.

Next, the analysis is repeated with the standardized data as shown in the following statements. The pseudo F and t^2 statistics indicate three or four clusters, while the cubic clustering criterion shows a sharp rise up to four clusters and then levels off up to six clusters. So the TABPERM macro is used again at the four-cluster level. In this case, there is no indeterminacy, because the same four clusters are obtained with every permutation, although in different orders. It must be emphasized, however, that lack of indeterminacy in no way indicates validity.

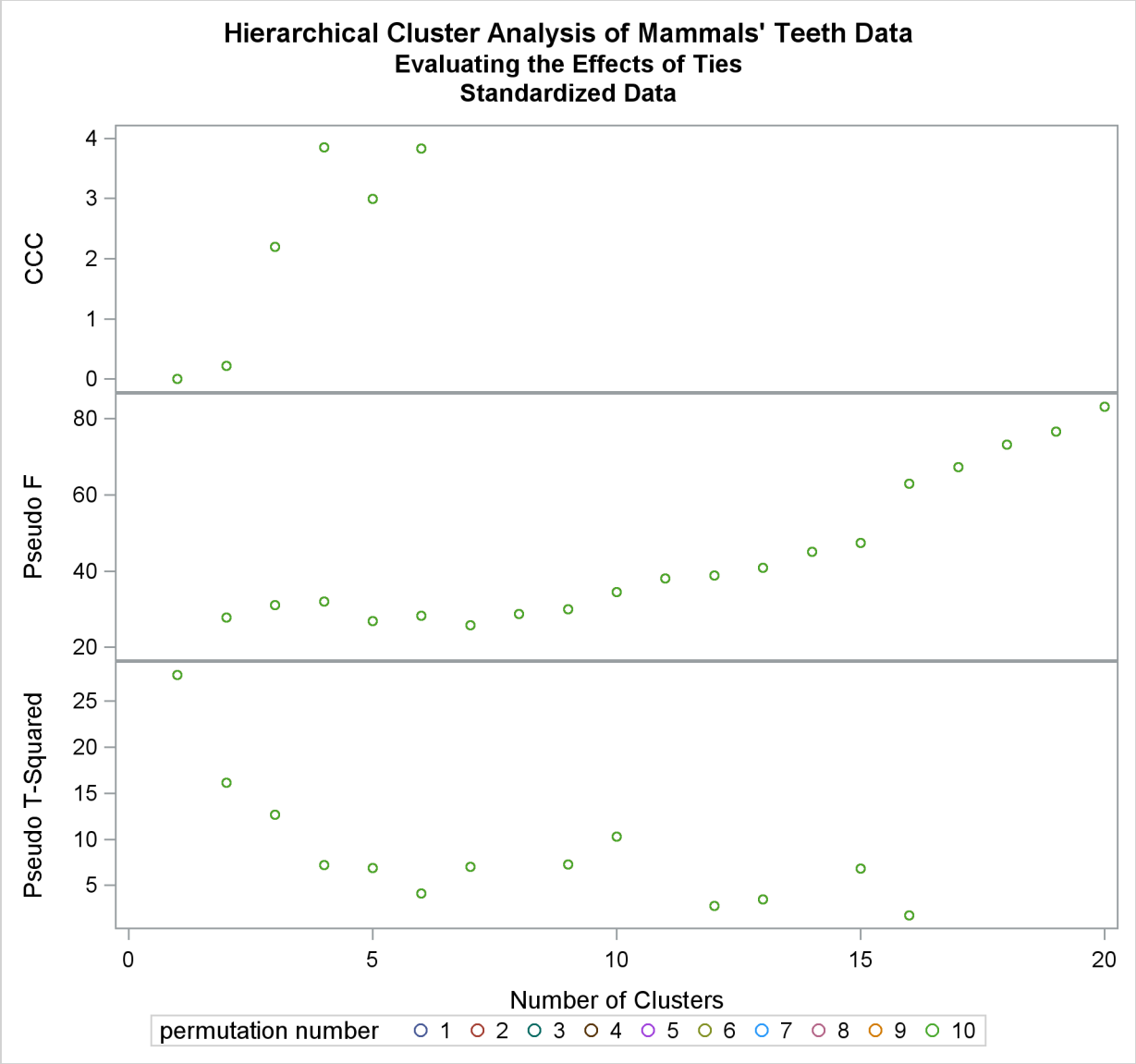
```
title3 'Standardized Data';

/*------CLUSTER STANDARDIZED DATA WITH AVERAGE LINKAGE------*/
%clusperm( teeth, &vlist, mammal, average std, 10);
```

The following statements produce Output 33.4.5.

```
/* -----PLOT STATISTICS FOR THE LAST 20 LEVELS-------------- */
%plotperm(20, 10);
```

Output 33.4.5 Analysis of 10 Random Permutations of Standardized Mammals' Teeth Data



The following statements produce Output 33.4.6.

```
/* ------ANALYZE THE 4-CLUSTER LEVEL---------------------- */
%tabperm( &vlist, mammal, 9.1, 4, 10);
```

Output 33.4.6 Standardized Mammals' Teeth Data: No Indeterminacy at the Four-Cluster Level

Hierarchical Cluster Analysis of Mammals' Teeth Data
Evaluating the Effects of Ties
Standardized Data

		Mean							
	FREQ	Top incisors	Bottom incisors	Top canines	Bottom canines	Top premolars	Bottom premolars	Top molars	Bottom molars
all_clus									
1 3 1 1 1 3 3 3 2 3	4	0.0	4.0	0.5	0.0	3.0	3.0	3.0	3.0
2 2 2 2 2 2 1 2 1 1	15	2.9	2.6	1.0	1.0	3.6	3.4	1.3	1.8
3 1 3 3 3 1 2 1 3 2	7	1.3	1.0	0.0	0.0	1.6	1.1	3.0	3.0
4 4 4 4 4 4 4 4 4 4	6	2.0	2.8	1.0	0.8	2.2	2.5	3.0	3.0

References

Anderberg, M. R. (1973), *Cluster Analysis for Applications*, New York: Academic Press.

Batagelj, V. (1981), "Note on Ultrametric Hierarchical Clustering Algorithms," *Psychometrika*, 46, 351–352.

Blackith, R. E. and Reyment, R. A. (1971), *Multivariate Morphometrics*, London: Academic Press.

Blashfield, R. K. and Aldenderfer, M. S. (1978), "The Literature on Cluster Analysis," *Multivariate Behavioral Research*, 13, 271–295.

Caliński, T. and Harabasz, J. (1974), "A Dendrite Method for Cluster Analysis," *Communications in Statistics—Theory and Methods*, 3, 1–27.

Cooper, M. C. and Milligan, G. W. (1988), "The Effect of Error on Determining the Number of Clusters," in W. Gaul and M. Schrader, eds., *Data, Expert Knowledge, and Decisions*, 319–328, London: Springer-Verlag.

Duda, R. O. and Hart, P. E. (1973), *Pattern Classification and Scene Analysis*, New York: John Wiley & Sons.

Everitt, B. S. (1980), *Cluster Analysis*, 2nd Edition, London: Heineman Educational Books.

Fisher, L. and Van Ness, J. W. (1971), "Admissible Clustering Procedures," *Biometrika*, 58, 91–104.

Fisher, R. A. (1936), "The Use of Multiple Measurements in Taxonomic Problems," *Annals of Eugenics*, 7, 179–188.

Florek, K., Lukaszewicz, J., Perkal, J., and Zubrzycki, S. (1951a), "Sur la liaison et la division des points d'un ensemble fini," *Colloquium Mathematicae*, 2, 282–285.

Florek, K., Lukaszewicz, J., Perkal, J., and Zubrzycki, S. (1951b), "Taksonomia Wroclawska," *Przeglad Antropologiczny*, 17, 193–211.

Gower, J. C. (1967), "A Comparison of Some Methods of Cluster Analysis," *Biometrics*, 23, 623–637.

Hamer, R. M. and Cunningham, J. W. (1981), "Cluster Analyzing Profile Data with Interrater Differences: A Comparison of Profile Association Measures," *Applied Psychological Measurement*, 5, 63–72.

Hartigan, J. A. (1975), *Clustering Algorithms*, New York: John Wiley & Sons.

Hartigan, J. A. (1977), "Distribution Problems in Clustering," in J. V. Ryzin, ed., *Classification and Clustering*, New York: Academic Press.

Hartigan, J. A. (1981), "Consistency of Single Linkage for High-Density Clusters," *Journal of the American Statistical Association*, 76, 388–394.

Hawkins, D. M., Muller, M. W., and ten Krooden, J. A. (1982), "Cluster Analysis," in D. M. Hawkins, ed., *Topics in Applied Multivariate Analysis*, Cambridge: Cambridge University Press.

Jardine, N. and Sibson, R. (1971), *Mathematical Taxonomy*, New York: John Wiley & Sons.

Johnson, S. C. (1967), "Hierarchical Clustering Schemes," *Psychometrika*, 32, 241–254.

Lance, G. N. and Williams, W. T. (1967), "A General Theory of Classificatory Sorting Strategies, Part I: Hierarchical Systems," *Computer Journal*, 9, 373–380.

Massart, D. L. and Kaufman, L. (1983), *The Interpretation of Analytical Chemical Data by the Use of Cluster Analysis*, New York: John Wiley & Sons.

McQuitty, L. L. (1957), "Elementary Linkage Analysis for Isolating Orthogonal and Oblique Types and Typal Relevancies," *Educational and Psychological Measurement*, 17, 207–229.

McQuitty, L. L. (1966), "Similarity Analysis by Reciprocal Pairs for Discrete and Continuous Data," *Educational and Psychological Measurement*, 26, 825–831.

Mezzich, J. E. and Solomon, H. (1980), *Taxonomy and Behavioral Science*, New York: Academic Press.

Milligan, G. W. (1979), "Ultrametric Hierarchical Clustering Algorithms," *Psychometrika*, 44, 343–346.

Milligan, G. W. (1980), "An Examination of the Effect of Six Types of Error Perturbation on Fifteen Clustering Algorithms," *Psychometrika*, 45, 325–342.

Milligan, G. W. (1987), "A Study of the Beta-Flexible Clustering Method," College of Administrative Science Working Paper Series, No. 87-61, Ohio State University.

Milligan, G. W. and Cooper, M. C. (1985), "An Examination of Procedures for Determining the Number of Clusters in a Data Set," *Psychometrika*, 50, 159–179.

Milligan, G. W. and Cooper, M. C. (1987), "A Study of Variable Standardization," College of Administrative Science Working Paper Series, No. 87-63.

Rouncefield, M. (1995), "The Statistics of Poverty and Inequality," Journal of Statistics Education Data Archive, accessed May 22, 2009.
URL http://www.amstat.org/publications/jse/v3n2/datasets.rouncefield.html

Sarle, W. S. (1983), *Cubic Clustering Criterion*, Technical Report A-108, SAS Institute Inc.

Silverman, B. W. (1986), *Density Estimation for Statistics and Data Analysis*, New York: Chapman & Hall.

Sneath, P. H. A. (1957), "The Application of Computers to Taxonomy," *Journal of General Microbiology*, 17, 201–226.

Sneath, P. H. A. and Sokal, R. R. (1973), *Numerical Taxonomy*, San Francisco: W. H. Freeman.

Sokal, R. R. and Michener, C. D. (1958), "A Statistical Method for Evaluating Systematic Relationships," *University of Kansas Science Bulletin*, 38, 1409–1438.

Sørensen, T. (1948), "A Method of Establishing Groups of Equal Amplitude in Plant Sociology Based on Similarity of Species Content and Its Application to Analyses of the Vegetation on Danish Commons," *Biologiske Skrifter*, 5, 1–34.

Spath, H. (1980), *Cluster Analysis Algorithms*, Chichester, UK: Ellis Horwood.

Symons, M. J. (1981), "Clustering Criteria and Multivariate Normal Mixtures," *Biometrics*, 37, 35–43.

Ward, J. H. (1963), "Hierarchical Grouping to Optimize an Objective Function," *Journal of the American Statistical Association*, 58, 236–244.

Wishart, D. (1969), "Mode Analysis: A Generalisation of Nearest Neighbour Which Reduces Chaining Effects," in A. J. Cole, ed., *Numerical Taxonomy*, London: Academic Press.

Wong, M. A. (1982), "A Hybrid Clustering Method for Identifying High-Density Clusters," *Journal of the American Statistical Association*, 77, 841–847.

Wong, M. A. and Lane, T. (1983), "A *k*th Nearest Neighbor Clustering Procedure," *Journal of the Royal Statistical Society, Series B*, 45, 362–368.

Wong, M. A. and Schaack, C. (1982), "Using the *k*th Nearest Neighbor Clustering Procedure to Determine the Number of Subpopulations," *American Statistical Association Proceedings of the Statistical Computing Section*, 40–48.

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