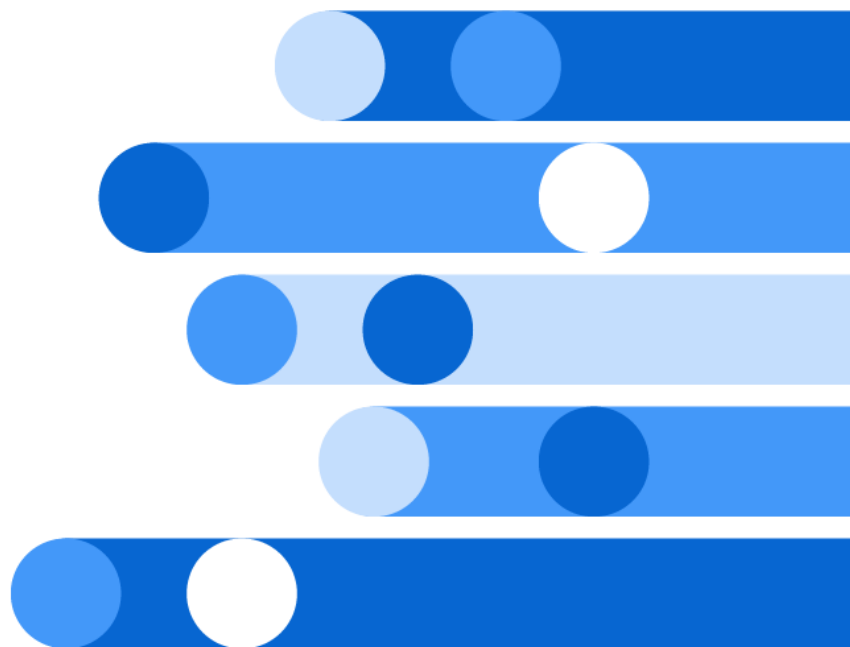




# SAS/STAT 15.3<sup>®</sup> User's Guide The FASTCLUS Procedure



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### **SAS/STAT® 15.3 User's Guide**

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# Chapter 45

## The FASTCLUS Procedure

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## Overview: FASTCLUS Procedure

The FASTCLUS procedure performs a disjoint cluster analysis on the basis of distances computed from one or more quantitative variables. The observations are divided into clusters such that every observation belongs to one and only one cluster; the clusters do not form a tree structure as they do in the CLUSTER procedure. If you want separate analyses for different numbers of clusters, you can run PROC FASTCLUS once for each analysis. Alternatively, to do hierarchical clustering on a large data set, use PROC FASTCLUS to find initial clusters, and then use those initial clusters as input to PROC CLUSTER.

By default, the FASTCLUS procedure uses Euclidean distances, so the cluster centers are based on least squares estimation. This kind of clustering method is often called a *k-means model*, since the cluster centers are the means of the observations assigned to each cluster when the algorithm is run to complete convergence. Each iteration reduces the least squares criterion until convergence is achieved.

Often there is no need to run the FASTCLUS procedure to convergence. PROC FASTCLUS is designed to find good clusters (but not necessarily the best possible clusters) with only two or three passes through the data set. The initialization method of PROC FASTCLUS guarantees that, if there exist clusters such that all distances between observations in the same cluster are less than all distances between observations in different clusters, and if you tell PROC FASTCLUS the correct number of clusters to find, it can always find such a clustering without iterating. Even with clusters that are not as well separated, PROC FASTCLUS usually finds initial seeds that are sufficiently good that few iterations are required. Hence, by default, PROC FASTCLUS performs only one iteration.

The initialization method used by the FASTCLUS procedure makes it sensitive to outliers. PROC FASTCLUS can be an effective procedure for detecting outliers because outliers often appear as clusters with only one member.

The FASTCLUS procedure can use an  $L_p$  (least  $p$ th powers) clustering criterion (Spath 1985, pp. 62–63) instead of the least squares ( $L_2$ ) criterion used in *k-means* clustering methods. The LEAST= $p$  option specifies the power  $p$  to be used. Using the LEAST= option increases execution time since more iterations are usually required, and the default iteration limit is increased when you specify LEAST= $p$ . Values of  $p$  less than 2 reduce the effect of outliers on the cluster centers compared with least squares methods; values of  $p$  greater than 2 increase the effect of outliers.

The FASTCLUS procedure is intended for use with large data sets, with 100 or more observations. With small data sets, the results can be highly sensitive to the order of the observations in the data set.

PROC FASTCLUS uses algorithms that place a larger influence on variables with larger variance, so it might be necessary to standardize the variables before performing the cluster analysis. See the “Using PROC FASTCLUS” section for standardization details.

PROC FASTCLUS produces brief summaries of the clusters it finds. For more extensive examination of the clusters, you can request an output data set containing a cluster membership variable.

---

## Background

The FASTCLUS procedure combines an effective method for finding initial clusters with a standard iterative algorithm for minimizing the sum of squared distances from the cluster means. The result is an efficient procedure for disjoint clustering of large data sets. PROC FASTCLUS was directly inspired by the Hartigan (1975) *leader algorithm* and the MacQueen (1967) *k-means algorithm*. PROC FASTCLUS uses a method that Anderberg (1973) calls *nearest centroid sorting*. A set of points called *cluster seeds* is selected as a first guess of the means of the clusters. Each observation is assigned to the nearest seed to form temporary clusters. The seeds are then replaced by the means of the temporary clusters, and the process is repeated until no further changes occur in the clusters. Similar techniques are described in most references on clustering (Anderberg 1973; Hartigan 1975; Everitt 1980; Spath 1980).

The FASTCLUS procedure differs from other nearest centroid sorting methods in the way the initial cluster seeds are selected. The importance of initial seed selection is demonstrated by Milligan (1980).

The clustering is done on the basis of Euclidean distances computed from one or more numeric variables. If there are missing values, PROC FASTCLUS computes an adjusted distance by using the nonmissing values. Observations that are very close to each other are usually assigned to the same cluster, while observations that are far apart are in different clusters.

The FASTCLUS procedure operates in four steps:

1. Observations called *cluster seeds* are selected.
2. If you specify the DRIFT option, temporary clusters are formed by assigning each observation to the cluster with the nearest seed. Each time an observation is assigned, the cluster seed is updated as the current mean of the cluster. This method is sometimes called *incremental*, *on-line*, or *adaptive* training.
3. If the maximum number of iterations is greater than zero, clusters are formed by assigning each observation to the nearest seed. After all observations are assigned, the cluster seeds are replaced by either the cluster means or other location estimates (cluster centers) appropriate to the LEAST= $p$  option. This step can be repeated until the changes in the cluster seeds become small or zero (MAXITER= $n \geq 1$ ).
4. Final clusters are formed by assigning each observation to the nearest seed.

If PROC FASTCLUS runs to complete convergence, the final cluster seeds will equal the cluster means or cluster centers. If PROC FASTCLUS terminates before complete convergence, which often happens with the default settings, the final cluster seeds might not equal the cluster means or cluster centers. If you want complete convergence, specify CONVERGE=0 and a large value for the MAXITER= option.

The initial cluster seeds must be observations with no missing values. You can specify the maximum number of seeds (and, hence, clusters) by using the MAXCLUSTERS= option. You can also specify a minimum distance by which the seeds must be separated by using the RADIUS= option.

PROC FASTCLUS always selects the first complete (no missing values) observation as the first seed. The next complete observation that is separated from the first seed by at least the distance specified in the RADIUS= option becomes the second seed. Later observations are selected as new seeds if they are separated from all previous seeds by at least the radius, as long as the maximum number of seeds is not exceeded.

If an observation is complete but fails to qualify as a new seed, PROC FASTCLUS considers using it to replace one of the old seeds. Two tests are made to see if the observation can qualify as a new seed.

First, an old seed is replaced if the distance between the observation and the closest seed is greater than the minimum distance between seeds. The seed that is replaced is selected from the two seeds that are closest to each other. The seed that is replaced is the one of these two with the shortest distance to the closest of the remaining seeds when the other seed is replaced by the current observation.

If the observation fails the first test for seed replacement, a second test is made. The observation replaces the nearest seed if the smallest distance from the observation to all seeds other than the nearest one is greater than the shortest distance from the nearest seed to all other seeds. If the observation fails this test, PROC FASTCLUS goes on to the next observation.

You can specify the REPLACE= option to limit seed replacement. You can omit the second test for seed replacement (REPLACE=PART), causing PROC FASTCLUS to run faster, but the seeds selected might not be as widely separated as those obtained by the default method. You can also suppress seed replacement entirely by specifying REPLACE=NONE. In this case, PROC FASTCLUS runs much faster, but you must choose a good value for the RADIUS= option in order to get good clusters. This method is similar to the Hartigan (1975, pp. 74–78) leader algorithm and the *simple cluster seeking algorithm* described by Tou and Gonzalez (1974, pp. 90–92).

---

## Getting Started: FASTCLUS Procedure

The following example demonstrates how to use the FASTCLUS procedure to compute disjoint clusters of observations in a SAS data set.

The data in this example are measurements taken on 159 freshwater fish caught from the same lake (Laengelmaevesi) near Tampere in Finland. This data set is available from Puranen.

The species (bream, parkki, pike, perch, roach, smelt, and whitefish), weight, three different length measurements (measured from the nose of the fish to the beginning of its tail, the notch of its tail, and the end of its tail), height, and width of each fish are tallied. The height and width are recorded as percentages of the third length variable.

Suppose that you want to group empirically the fish measurements into clusters and that you want to associate the clusters with the species. You can use the FASTCLUS procedure to perform a cluster analysis.

The following DATA step creates the SAS data set Fish:

```
proc format;
  value specfmt
    1='Bream'
    2='Roach'
    3='Whitefish'
    4='Parkki'
    5='Perch'
    6='Pike'
    7='Smelt';
run;
```

```

data fish (drop=HtPct WidthPct);
  title 'Fish Measurement Data';
  input Species Weight Length1 Length2 Length3 HtPct WidthPct @@;

  *** transform variables;
  if Weight <= 0 or Weight =. then delete;
  Weight3=Weight**(1/3);
  Height=HtPct*Length3/(Weight3*100);
  Width=WidthPct*Length3/(Weight3*100);
  Length1=Length1/Weight3;
  Length2=Length2/Weight3;
  Length3=Length3/Weight3;
  logLengthRatio=log(Length3/Length1);

  format Species specfmt.;
  symbol = put(Species, specfmt2.);
  datalines;
1 242.0 23.2 25.4 30.0 38.4 13.4 1 290.0 24.0 26.3 31.2 40.0 13.8
1 340.0 23.9 26.5 31.1 39.8 15.1 1 363.0 26.3 29.0 33.5 38.0 13.3
1 430.0 26.5 29.0 34.0 36.6 15.1 1 450.0 26.8 29.7 34.7 39.2 14.2
1 500.0 26.8 29.7 34.5 41.1 15.3 1 390.0 27.6 30.0 35.0 36.2 13.4
1 450.0 27.6 30.0 35.1 39.9 13.8 1 500.0 28.5 30.7 36.2 39.3 13.7
1 475.0 28.4 31.0 36.2 39.4 14.1 1 500.0 28.7 31.0 36.2 39.7 13.3
1 500.0 29.1 31.5 36.4 37.8 12.0 1 . 29.5 32.0 37.3 37.3 13.6
1 600.0 29.4 32.0 37.2 40.2 13.9 1 600.0 29.4 32.0 37.2 41.5 15.0
1 700.0 30.4 33.0 38.3 38.8 13.8 1 700.0 30.4 33.0 38.5 38.8 13.5

  ... more lines ...

7 19.7 13.2 14.3 15.2 18.9 13.6 7 19.9 13.8 15.0 16.2 18.1 11.6
;

```

The double trailing at sign (@@) in the INPUT statement specifies that observations are input from each line until all values are read. The variables are rescaled in order to adjust for dimensionality. Because the new variables Weight3–logLengthRatio depend on the variable Weight, observations with missing values for Weight are not added to the data set. Consequently, there are 157 observations in the SAS data set Fish.

In the Fish data set, the variables are not measured in the same units and cannot be assumed to have equal variance. Therefore, it is necessary to standardize the variables before performing the cluster analysis.

The following statements standardize the variables and perform a cluster analysis on the standardized data:

```

proc stdize data=Fish out=Stand method=std;
  var Length1 logLengthRatio Height Width Weight3;
run;

proc fastclus data=Stand out=Clust
  maxclusters=7 maxiter=100;
  var Length1 logLengthRatio Height Width Weight3;
run;

```

The STDIZE procedure is first used to standardize all the analysis variables to a mean of 0 and standard deviation of 1. The procedure creates the output data set Stand to contain the transformed variables (for detailed information, see Chapter 115, “The STDIZE Procedure”).

The FASTCLUS procedure then uses the data set `Stand` as input and creates the data set `Clust`. This output data set contains the original variables and two new variables, `Cluster` and `Distance`. The variable `Cluster` contains the cluster number to which each observation has been assigned. The variable `Distance` gives the distance from the observation to its cluster seed.

It is usually desirable to try several values of the `MAXCLUSTERS=` option. A reasonable beginning for this example is to use `MAXCLUSTERS=7`, since there are seven species of fish represented in the data set `Fish`.

The `VAR` statement specifies the variables used in the cluster analysis.

The results from this analysis are displayed in the following figures.

**Figure 45.1** Initial Seeds Used in the FASTCLUS Procedure

**Fish Measurement Data**

**The FASTCLUS Procedure**  
**Replace=FULL Radius=0 Maxclusters=7 Maxiter=100 Converge=0.02**

Initial Seeds					
Cluster	Length1	logLengthRatio	Height	Width	Weight3
1	1.388338414	-0.979577858	-1.594561848	-2.254050655	2.103447062
2	-1.117178039	-0.877218192	-0.336166276	2.528114070	1.170706464
3	2.393997461	-0.662642015	-0.930738701	-2.073879107	-1.839325419
4	-0.495085516	-0.964041012	-0.265106856	-0.028245072	1.536846394
5	-0.728772773	0.540096664	1.130501398	-1.207930053	-1.107018207
6	-0.506924177	0.748211648	1.762482687	0.211507596	1.368987826
7	1.573996573	-0.796593995	-0.824217424	1.561715851	-1.607942726

Criterion Based on Final Seeds = 0.3979

the [Figure 45.1](#) displays the table of initial seeds used for each variable and cluster. The first line in the figure displays the option settings for `REPLACE`, `RADIUS`, `MAXCLUSTERS`, and `MAXITER`. These options, with the exception of `MAXCLUSTERS` and `MAXITER`, are set at their respective default values (`REPLACE=FULL`, `RADIUS=0`). Both the `MAXCLUSTERS=` and `MAXITER=` options are set in the `PROC FASTCLUS` statement.

Next, `PROC FASTCLUS` produces a table of summary statistics for the clusters. [Figure 45.2](#) displays the number of observations in the cluster (frequency) and the root mean squared standard deviation. The next two columns display the largest Euclidean distance from the cluster seed to any observation within the cluster and the number of the nearest cluster.

The last column of the table displays the distance between the centroid of the nearest cluster and the centroid of the current cluster. A centroid is the point having coordinates that are the means of all the observations in the cluster.



**Figure 45.2** Cluster Summary Table from the FASTCLUS Procedure

Cluster Summary						
Cluster	Frequency	RMS Std Deviation	Maximum Distance		Nearest Cluster	Distance Between Cluster Centroids
			from Seed to Observation	Radius Exceeded		
1	17	0.5064	1.7781		4	2.5106
2	19	0.3696	1.5007		4	1.5510
3	13	0.3803	1.7135		1	2.6704
4	13	0.4161	1.3976		7	1.4266
5	11	0.2466	0.6966		6	1.7301
6	34	0.3563	1.5443		5	1.7301
7	50	0.4447	2.3915		4	1.4266

Figure 45.3 displays the table of statistics for the variables. The table lists for each variable the total standard deviation, the pooled within-cluster standard deviation and the R-square value for predicting the variable from the cluster. The ratio of between-cluster variance to within-cluster variance ( $R^2$  to  $1 - R^2$ ) appears in the last column.

**Figure 45.3** Statistics for Variables Used in the FASTCLUS Procedure

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
Length1	1.00000	0.31428	0.905030	9.529606
logLengthRatio	1.00000	0.39276	0.851676	5.741989
Height	1.00000	0.20917	0.957929	22.769295
Width	1.00000	0.55558	0.703200	2.369270
Weight3	1.00000	0.47251	0.785323	3.658162
OVER-ALL	1.00000	0.40712	0.840631	5.274764

Pseudo F Statistic = 131.87

Approximate Expected Over-All R-Squared = 0.57420

Cubic Clustering Criterion = 37.808

The pseudo  $F$  statistic, approximate expected overall R square, and cubic clustering criterion (CCC) are listed at the bottom of the figure. You can compare values of these statistics by running PROC FASTCLUS with different values for the MAXCLUSTERS= option. The R square and CCC values are not valid for correlated variables.

Values of the cubic clustering criterion greater than 2 or 3 indicate good clusters. Values between 0 and 2 indicate potential clusters, but they should be taken with caution; large negative values can indicate outliers.

PROC FASTCLUS next produces the within-cluster means and standard deviations of the variables, displayed in Figure 45.4.

**Figure 45.4** Cluster Means and Standard Deviations from the FASTCLUS Procedure

Cluster Means					
Cluster	Length1	logLengthRatio	Height	Width	Weight3
1	1.747808245	-0.868605685	-1.327226832	-1.128760946	0.806373599
2	-0.405231510	-0.979113021	-0.281064162	1.463094486	1.060450065
3	2.006796315	-0.652725165	-1.053213440	-1.224020795	-1.826752838
4	-0.136820952	-1.039312574	-0.446429482	0.162596336	0.278560318
5	-0.850130601	0.550190242	1.245156076	-0.836585750	-0.567022647
6	-0.843912827	1.522291347	1.511408739	-0.380323563	0.763114370
7	-0.165570970	-0.048881276	-0.353723615	0.546442064	-0.668780782

Cluster Standard Deviations					
Cluster	Length1	logLengthRatio	Height	Width	Weight3
1	0.3418476428	0.3544065543	0.1666302451	0.6172880027	0.7944227150
2	0.3129902863	0.3592350778	0.1369052680	0.5467406493	0.3720119097
3	0.2962504486	0.1740941675	0.1736086707	0.7528475622	0.0905232968
4	0.3254364840	0.2836681149	0.1884592934	0.4543390702	0.6612055341
5	0.1781837609	0.0745984121	0.2056932592	0.2784540794	0.3832002850
6	0.2273744242	0.3385584051	0.2046010964	0.5143496067	0.4025849044
7	0.3734733622	0.5275768119	0.2551130680	0.5721303628	0.4223181710

It is useful to study further the clusters calculated by the FASTCLUS procedure. One method is to look at a frequency tabulation of the clusters with other classification variables. The following statements invoke the FREQ procedure to crosstabulate the empirical clusters with the variable Species:

```
proc freq data=Clust;
  tables Species*Cluster;
run;
```

Figure 45.5 displays the marked division between clusters.

**Figure 45.5** Frequency Table of Cluster versus Species**Fish Measurement Data****The FREQ Procedure**

Frequency Percent Row Pct Col Pct	Table of Species by CLUSTER								
	Species	CLUSTER(Cluster)							Total
		1	2	3	4	5	6	7	
<b>Bream</b>	0	0	0	0	0	34	0	34	
	0.00	0.00	0.00	0.00	0.00	21.66	0.00	21.66	
	0.00	0.00	0.00	0.00	0.00	100.00	0.00		
	0.00	0.00	0.00	0.00	0.00	100.00	0.00		
<b>Roach</b>	0	0	0	0	0	0	19	19	
	0.00	0.00	0.00	0.00	0.00	0.00	12.10	12.10	
	0.00	0.00	0.00	0.00	0.00	0.00	100.00		
	0.00	0.00	0.00	0.00	0.00	0.00	38.00		
<b>Whitefish</b>	0	2	0	1	0	0	3	6	
	0.00	1.27	0.00	0.64	0.00	0.00	1.91	3.82	
	0.00	33.33	0.00	16.67	0.00	0.00	50.00		
	0.00	10.53	0.00	7.69	0.00	0.00	6.00		
<b>Parkki</b>	0	0	0	0	11	0	0	11	
	0.00	0.00	0.00	0.00	7.01	0.00	0.00	7.01	
	0.00	0.00	0.00	0.00	100.00	0.00	0.00		
	0.00	0.00	0.00	0.00	100.00	0.00	0.00		
<b>Perch</b>	0	17	0	12	0	0	27	56	
	0.00	10.83	0.00	7.64	0.00	0.00	17.20	35.67	
	0.00	30.36	0.00	21.43	0.00	0.00	48.21		
	0.00	89.47	0.00	92.31	0.00	0.00	54.00		
<b>Pike</b>	17	0	0	0	0	0	0	17	
	10.83	0.00	0.00	0.00	0.00	0.00	0.00	10.83	
	100.00	0.00	0.00	0.00	0.00	0.00	0.00		
	100.00	0.00	0.00	0.00	0.00	0.00	0.00		
<b>Smelt</b>	0	0	13	0	0	0	1	14	
	0.00	0.00	8.28	0.00	0.00	0.00	0.64	8.92	
	0.00	0.00	92.86	0.00	0.00	0.00	7.14		
	0.00	0.00	100.00	0.00	0.00	0.00	2.00		
<b>Total</b>	17	19	13	13	11	34	50	157	
	10.83	12.10	8.28	8.28	7.01	21.66	31.85	100.00	

For cases in which you have three or more clusters, you can use the CANDISC and SGPLOT procedures to obtain a graphical check on the distribution of the clusters. In the following statements, the CANDISC and SGPLOT procedures are used to compute canonical variables and plot the clusters:

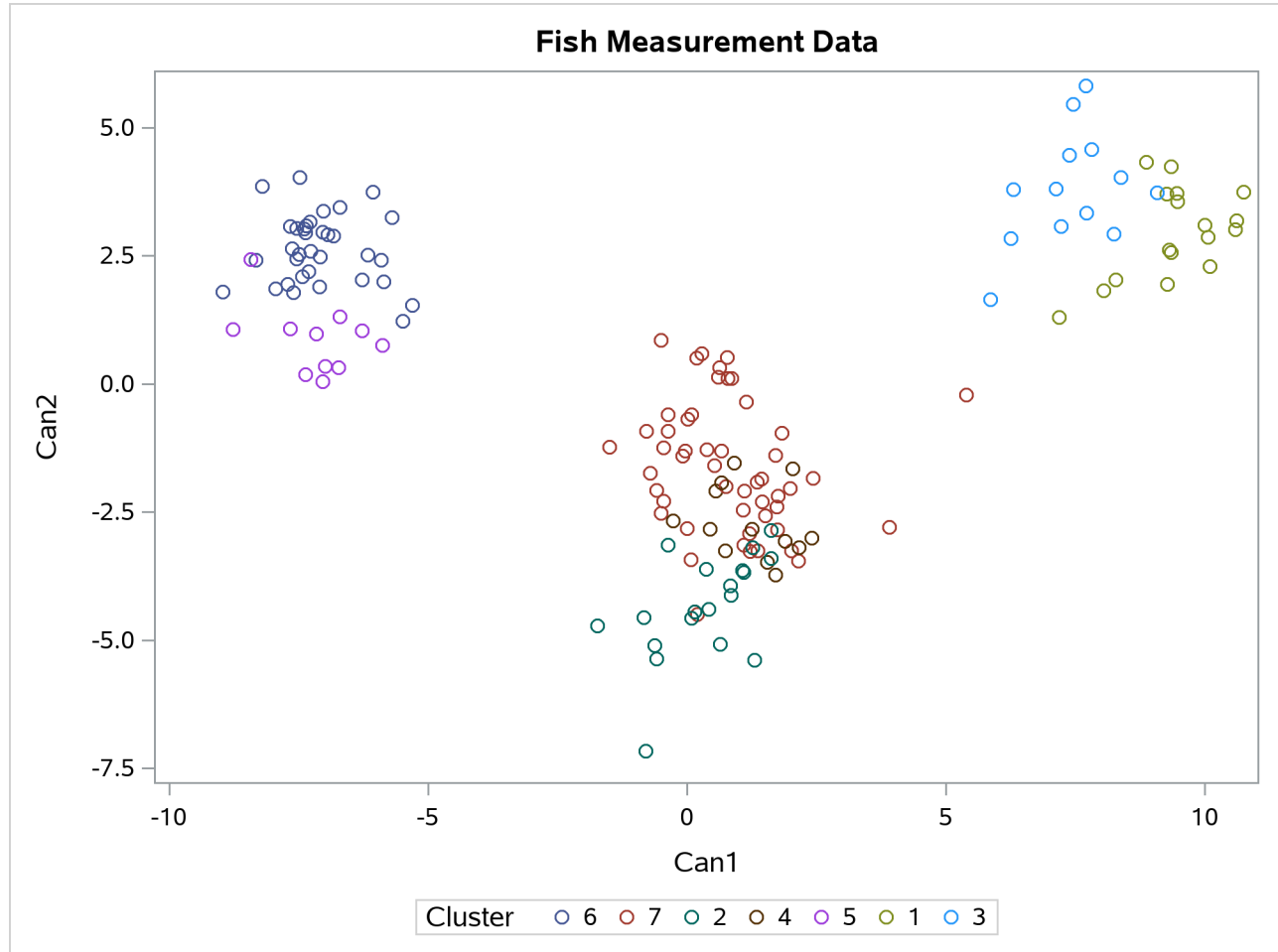
```
proc candisc data=Clust out=Can noprint;
  class Cluster;
  var Length1 logLengthRatio Height Width Weight3;
run;

proc sgplot data=Can;
  scatter y=Can2 x=Can1 / group=Cluster;
run;
```

First, the CANDISC procedure is invoked to perform a canonical discriminant analysis by using the data set Clust and creating the output SAS data set Can. The NOPRINT option suppresses display of the output. The CLASS statement specifies the variable Cluster to define groups for the analysis. The VAR statement specifies the variables used in the analysis.

Next, the SGPLOT procedure plots the two canonical variables from PROC CANDISC, Can1 and Can2. The SCATTER statement specifies the variable Cluster as the group identification variable. The resulting plot (Figure 45.6) illustrates the spatial separation of the clusters calculated in the FASTCLUS procedure.

**Figure 45.6** Plot of Canonical Variables and Cluster Value



## Syntax: FASTCLUS Procedure

The following statements are available in the FASTCLUS procedure:

```
PROC FASTCLUS < MAXCLUSTERS=n> < RADIUS=t> < options> ;
  VAR variables ;
  ID variables ;
  FREQ variable ;
  WEIGHT variable ;
  BY variables ;
```

Usually you need only the VAR statement in addition to the PROC FASTCLUS statement. The BY, FREQ, ID, VAR, and WEIGHT statements are described in alphabetical order after the PROC FASTCLUS statement.

### PROC FASTCLUS Statement

```
PROC FASTCLUS < MAXCLUSTERS=n> < RADIUS=t> < options> ;
```

The PROC FASTCLUS statement invokes the FASTCLUS procedure. You must specify the MAXCLUSTERS= option or RADIUS= option or both in the PROC FASTCLUS statement.

#### **MAXCLUSTERS**=*n*

##### **MAXC**=*n*

specifies the maximum number of clusters permitted. If you omit the MAXCLUSTERS= option, a value of 100 is assumed.

#### **RADIUS**=*t*

##### **R**=*t*

establishes the minimum distance criterion for selecting new seeds. No observation is considered as a new seed unless its minimum distance to previous seeds exceeds the value given by the RADIUS= option. The default value is 0. If you specify the REPLACE=RANDOM option, the RADIUS= option is ignored.

You can specify the following options in the PROC FASTCLUS statement. [Table 45.1](#) summarizes the options available in the PROC FASTCLUS statement.

**Table 45.1** PROC FASTCLUS Statement Options

Option	Description
<b>Specify Input and Output Data Sets</b>	
<b>DATA</b> =	Specifies input data set
<b>INSTAT</b> =	Specifies input SAS data set previously created by the OUTSTAT= option
<b>SEED</b> =	Specifies input SAS data set for selecting initial cluster seeds
<b>VARDEF</b> =	Specifies divisor for variances

Table 45.1 continued

Option	Description
<b>Output Data Processing</b>	
CLUSTER=	Specifies name for cluster membership variable in OUTSEED= and OUT= data sets
CLUSTERLABEL=	Specifies label for cluster membership variable in OUTSEED= and OUT= data sets
OUT=	Specifies output SAS data set containing original data and cluster assignments
OUTITER	Specifies writing to OUTSEED= data set on every iteration
OUTSEED= or MEAN=	Specifies output SAS data set containing cluster centers
OUTSTAT=	Specifies output SAS data set containing statistics
<b>Initial Clusters</b>	
DRIFT	Permits cluster to seeds to drift during initialization
MAXCLUSTERS=	Specifies maximum number of clusters
RADIUS=	Specifies minimum distance for selecting new seeds
RANDOM=	Specifies seed to initialize pseudo-random number generator
REPLACE=	Specifies seed replacement method
<b>Clustering Methods</b>	
CONVERGE=	Specifies convergence criterion
DELETE=	Deletes cluster seeds with few observations
LEAST=	Optimizes an $L_p$ criterion, where $1 \leq p \leq \infty$
MAXITER=	Specifies maximum number of iterations
STRICT	Prevents an observation from being assigned to a cluster if its distance to the nearest cluster seed is large
<b>Arcane Algorithmic Options</b>	
BINS=	Specifies number of bins used for computing medians for LEAST=1
HC=	Specifies criterion for updating the homotopy parameter
HP=	Specifies initial value of the homotopy parameter
IRLS	Uses an iteratively reweighted least squares method instead of the modified Eklom-Newton method for $1 < p < 2$
<b>Missing Values</b>	
IMPUTE	Imputes missing values after final cluster assignment
NOMISS	Excludes observations with missing values
<b>Control Displayed Output</b>	
DISTANCE	Displays distances between cluster centers
LIST	Displays cluster assignments for all observations
NOPRINT	Suppresses displayed output
SHORT	Suppresses display of large matrices
SUMMARY	Suppresses display of all results except for the cluster summary
VARIABLESAREUNCORRELATED	Suppresses warning in output

The following list provides details on these options. The list is in alphabetical order.

**BINS=*n***

specifies the number of bins used in the bin-sort algorithm for computing medians for LEAST=1. By default, PROC FASTCLUS uses from 10 to 100 bins, depending on the amount of memory available. Larger values use more memory and make each iteration somewhat slower, but they can reduce the number of iterations. Smaller values have the opposite effect. The minimum value of *n* is 5.

**CLUSTER=*name***

specifies a name for the variable in the OUTSEED= and OUT= data sets that indicates cluster membership. The default name for this variable is CLUSTER.

**CLUSTERLABEL=*name***

specifies a label for the variable CLUSTER in the OUTSEED= and OUT= data sets. By default this variable has no label.

**CONVERGE=*c*****CONV=*c***

specifies the convergence criterion. Any nonnegative value is permitted. The default value is 0.0001 for all values of *p* if LEAST=*p* is explicitly specified; otherwise, the default value is 0.02. Iterations stop when the maximum relative change in the cluster seeds is less than or equal to the convergence criterion and additional conditions on the homotopy parameter, if any, are satisfied (see the HP= option). The relative change in a cluster seed is the distance between the old seed and the new seed divided by a scaling factor. If you do not specify the LEAST= option, the scaling factor is the minimum distance between the initial seeds. If you specify the LEAST= option, the scaling factor is an  $L_1$  scale estimate and is recomputed on each iteration. Specify the CONVERGE= option only if you specify a MAXITER= value greater than 1.

**DATA=*SAS-data-set***

specifies the input data set containing observations to be clustered. If you omit the DATA= option, the most recently created SAS data set is used. The data must be coordinates, not distances, similarities, or correlations.

**DELETE=*n***

deletes cluster seeds to which *n* or fewer observations are assigned. Deletion occurs after processing for the DRIFT option is completed and after each iteration specified by the MAXITER= option. Cluster seeds are not deleted after the final assignment of observations to clusters, so in rare cases a final cluster might not have more than *n* members. The DELETE= option is ineffective if you specify MAXITER=0 and do not specify the DRIFT option. By default, no cluster seeds are deleted.

**DISTANCE | DIST**

computes distances between the cluster means.

**DRIFT**

executes the second of the four steps described in the section “[Background](#)” on page 2883. After initial seed selection, each observation is assigned to the cluster with the nearest seed. After an observation is processed, the seed of the cluster to which it is assigned is recalculated as the mean of the observations currently assigned to the cluster. Thus, the cluster seeds drift about rather than remaining fixed for the duration of the pass.

**HC=c****HP= $p_1$  <  $p_2$  >**

pertains to the homotopy parameter for LEAST= $p$ , where  $1 < p < 2$ . You should specify these options only if you encounter convergence problems when you use the default values.

For  $1 < p < 2$ , PROC FASTCLUS tries to optimize a perturbed variant of the  $L_p$  clustering criterion (Gonin and Money 1989, pp. 5–6).

When the homotopy parameter is 0, the optimization criterion is equivalent to the clustering criterion. For a large homotopy parameter, the optimization criterion approaches the least squares criterion and is therefore easy to optimize. Beginning with a large homotopy parameter, PROC FASTCLUS gradually decreases it by a factor in the range [0.01,0.5] over the course of the iterations. When both the homotopy parameter and the convergence measure are sufficiently small, the optimization process is declared to have converged.

If the initial homotopy parameter is too large or if it is decreased too slowly, the optimization can require many iterations. If the initial homotopy parameter is too small or if it is decreased too quickly, convergence to a local optimum is likely. The following list gives details on setting the homotopy parameter.

**HC=c** specifies the criterion for updating the homotopy parameter. The homotopy parameter is updated when the maximum relative change in the cluster seeds is less than or equal to  $c$ . The default is the minimum of 0.01 and 100 times the value of the CONVERGE= option.

**HP= $p_1$**  specifies  $p_1$  as the initial value of the homotopy parameter. The default is 0.05 if the modified Eklblom-Newton method is used; otherwise, it is 0.25.

**HP= $p_1$   $p_2$**  also specifies  $p_2$  as the minimum value for the homotopy parameter, which must be reached for convergence. The default is the minimum of  $p_1$  and 0.01 times the value of the CONVERGE= option.

**IMPUTE**

requests imputation of missing values after the final assignment of observations to clusters. If an observation that is assigned (or would have been assigned) to a cluster has a missing value for variables used in the cluster analysis, the missing value is replaced by the corresponding value in the cluster seed to which the observation is assigned (or would have been assigned). If the observation cannot be assigned to a cluster, missing value replacement depends on whether or not the NOMISS option is specified. If NOMISS is not specified, missing values are replaced by the mean of all observations in the DATA= data set having a value for that variable. If NOMISS is specified, missing values are replaced by the mean of only observations used in the analysis. (A weighted mean is used if a variable is specified in the WEIGHT statement.) For information about cluster assignment see the section “OUT= Data Set” on page 2901. If you specify the IMPUTE option, the imputed values are not used in computing cluster statistics.

If you also request an OUT= data set, it contains the imputed values.



**INSTAT=SAS-data-set**

reads a SAS data set previously created with the FASTCLUS procedure by using the OUTSTAT= option. If you specify the INSTAT= option, no clustering iterations are performed and no output is displayed. Only cluster assignment and imputation are performed as an OUT= data set is created.

**IRLS**

causes PROC FASTCLUS to use an iteratively reweighted least squares method instead of the modified Eklblom-Newton method. If you specify the IRLS option, you must also specify LEAST= $p$ , where  $1 < p < 2$ . Use the IRLS option only if you encounter convergence problems with the default method.

**LEAST= $p$  | MAX****L= $p$  | MAX**

causes PROC FASTCLUS to optimize an  $L_p$  criterion, where  $1 \leq p \leq \infty$  (Spath 1985, pp. 62–63). Infinity is indicated by LEAST=MAX. The value of this clustering criterion is displayed in the iteration history.

If you do not specify the LEAST= option, PROC FASTCLUS uses the least squares ( $L_2$ ) criterion. However, the default number of iterations is only 1 if you omit the LEAST= option, so the optimization of the criterion is generally not completed. If you specify the LEAST= option, the maximum number of iterations is increased to permit the optimization process a chance to converge. See the MAXITER= $n$  option for details.

Specifying the LEAST= option also changes the default convergence criterion from 0.02 to 0.0001. See the CONVERGE= $c$  for details.

When LEAST=2, PROC FASTCLUS tries to minimize the root mean squared difference between the data and the corresponding cluster means.

When LEAST=1, PROC FASTCLUS tries to minimize the mean absolute difference between the data and the corresponding cluster medians.

When LEAST=MAX, PROC FASTCLUS tries to minimize the maximum absolute difference between the data and the corresponding cluster midranges.

For general values of  $p$ , PROC FASTCLUS tries to minimize the  $p$ th root of the mean of the  $p$ th powers of the absolute differences between the data and the corresponding cluster seeds. Large values of  $p$  may cause floating-point underflow or overflow.

The divisor in the clustering criterion is either the number of nonmissing data used in the analysis or, if there is a WEIGHT statement, the sum of the weights corresponding to all the nonmissing data used in the analysis (that is, an observation with  $n$  nonmissing data contributes  $n$  times the observation weight to the divisor). The divisor is not adjusted for degrees of freedom.

The method for updating cluster seeds during iteration depends on the LEAST= option, as follows (Gonin and Money 1989).

LEAST= $p$	Algorithm for Computing Cluster Seeds
$p = 1$	Bin sort for median
$1 < p < 2$	Modified Merle-Spath if you specify IRLS; otherwise modified Eklblom-Newton
$p = 2$	Arithmetic mean
$2 < p < \infty$	Newton
$p = \infty$	Midrange

During the final pass, a modified Merle-Spath step is taken to compute the cluster centers for  $1 \leq p < 2$  or  $2 < p < \infty$ .

If you specify the LEAST= $p$  option with a value other than 2, PROC FASTCLUS computes pooled scale estimates analogous to the root mean squared standard deviation but based on  $p$ th power deviations instead of squared deviations.

LEAST= $p$	Scale Estimate
$p = 1$	Mean absolute deviation
$1 < p < \infty$	Root mean $p$ th-power absolute deviation
$p = \infty$	Maximum absolute deviation

The divisors for computing the mean absolute deviation or the root mean  $p$ th-power absolute deviation are adjusted for degrees of freedom just like the divisors for computing standard deviations. This adjustment can be suppressed by the VARDEF= option.

#### LIST

lists all observations, giving the value of the ID variable (if any), the number of the cluster to which the observation is assigned, and the distance between the observation and the final cluster seed.

#### MAXITER= $n$

specifies the maximum number of iterations for recomputing cluster seeds. When the value of the MAXITER= option is greater than zero, PROC FASTCLUS executes the third of the four steps described in the section “Background” on page 2883. In each iteration, each observation is assigned to the nearest seed, and the seeds are recomputed as the means of the clusters.

The default value of the MAXITER= option depends on the LEAST= $p$  option.

LEAST= $p$	MAXITER=
Not specified	1
$p = 1$	20
$1 < p < 1.5$	50
$1.5 \leq p < 2$	20
$p = 2$	10
$2 < p \leq \infty$	20

#### MEAN=SAS-data-set

creates an output data set to contain the cluster means and other statistics for each cluster. 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 Programmers Guide: Essentials*.

#### NOMISS

excludes observations with missing values from the analysis. However, if you also specify the IMPUTE option, observations with missing values are included in the final cluster assignments.

**NOPRINT**

suppresses the display of all output. Note that this option temporarily disables the Output Delivery System (ODS). For more information, see Chapter 23, “Using the Output Delivery System.”

**OUT=SAS-data-set**

creates an output data set to contain all the original data, plus the new variables CLUSTER and DISTANCE. 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 Programmers Guide: Essentials*.

**OUTITER**

outputs information from the iteration history to the OUTSEED= data set, including the cluster seeds at each iteration.

**OUTSEED=SAS-data-set****OUTS=SAS-data-set**

is another name for the MEAN= data set, provided because the data set can contain location estimates other than means. The MEAN= option is still accepted.

**OUTSTAT=SAS-data-set**

creates an output data set to contain various statistics, especially those not included in the OUTSEED= data set. Unlike the OUTSEED= data set, the OUTSTAT= data set is not suitable for use as a SEED= data set in a subsequent PROC FASTCLUS step.

**RANDOM=n**

specifies a positive integer as a starting value for the pseudo-random number generator for use with REPLACE=RANDOM. If you do not specify the RANDOM= option, the time of day is used to initialize the pseudo-random number sequence.

**REPLACE=FULL | PART | NONE | RANDOM**

specifies how seed replacement is performed, as follows:

<b>FULL</b>	requests default seed replacement as described in the section “Background” on page 2883.
<b>PART</b>	requests seed replacement only when the distance between the observation and the closest seed is greater than the minimum distance between seeds.
<b>NONE</b>	suppresses seed replacement.
<b>RANDOM</b>	selects a simple pseudo-random sample of complete observations as initial cluster seeds.

**SEED=SAS-data-set**

specifies an input data set from which initial cluster seeds are to be selected. If you do not specify the SEED= option, initial seeds are selected from the DATA= data set. The SEED= data set must contain the same variables that are used in the data analysis.

**SHORT**

suppresses the display of the initial cluster seeds, cluster means, and standard deviations.

**STRICT****STRICT=*s***

prevents an observation from being assigned to a cluster if its distance to the nearest cluster seed exceeds the value of the STRICT= option. If you specify the STRICT option without a numeric value, you must also specify the RADIUS= option, and its value is used instead. In the OUT= data set, observations that are not assigned due to the STRICT= option are given a negative cluster number, the absolute value of which indicates the cluster with the nearest seed.

**SUMMARY**

suppresses the display of the initial cluster seeds, statistics for variables, cluster means, and standard deviations.

**VARDEF=DF | N | WDF | WEIGHT | WGT**

specifies the divisor to be used in the calculation of variances and covariances. The default value is VARDEF=DF. The possible values of the VARDEF= option and associated divisors are as follows.

Value	Description	Divisor
DF	Error degrees of freedom	$n - c$
N	Number of observations	$n$
WDF	Sum of weights DF	$(\sum_i w_i) - c$
WEIGHT   WGT	Sum of weights	$\sum_i w_i$

In the preceding definitions,  $c$  represents the number of clusters.

**VARIABLESAREUNCORRELATED**

suppresses the warning, displayed in the listing when there are two or more VAR variables, concerning the validity of the Approximate Expected Over-All R-Squared and the Cubic Clustering Criterion when the variables used in clustering are correlated. Note that the FASTCLUS procedure does not compute correlations; the warning is for a potential problem.

---

**BY Statement**

**BY** *variables* ;

You can specify a BY statement in PROC FASTCLUS 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 in the FASTCLUS 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).

If you specify the SEED= option and the SEED= data set does not contain any of the BY variables, then the entire SEED= data set is used to obtain initial cluster seeds for each BY group in the DATA= data set.

If the SEED= data set contains some but not all of the BY variables, or if some BY variables do not have the same type or length in the SEED= data set as in the DATA= data set, then PROC FASTCLUS displays an error message and stops.

If all the BY variables appear in the SEED= data set with the same type and length as in the DATA= data set, then each BY group in the SEED= data set is used to obtain initial cluster seeds for the corresponding BY group in the DATA= data set. All BY groups in the DATA= data set must also appear in the SEED= data set. The BY groups in the SEED= data set must be in the same order as in the DATA= data set. If you specify the NOTSORTED option in the BY statement, both data sets must contain exactly the same BY groups in the same order. If you do not specify NOTSORTED, some BY groups can appear in the SEED= data set but not in the DATA= data set; such BY groups are not used in the analysis.

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*.

---

## FREQ Statement

**FREQ** *variable* ;

If a variable in the data set represents the frequency of occurrence for the other values in the observation, include the variable's name in a FREQ statement. The procedure then treats the data set as if each observation appears  $n$  times, where  $n$  is the value of the FREQ variable for the observation.

If the value of the FREQ variable is missing or less than or equal to zero, the observation is not used in the analysis. The exact values of the FREQ variable are used in computations: frequency values are not truncated to integers. The total number of observations is considered to be equal to the sum of the FREQ variable when the procedure determines degrees of freedom for significance probabilities.

The WEIGHT and FREQ statements have a similar effect, except in determining the number of observations for significance tests.

---

## ID Statement

**ID** *variable* ;

The ID variable, which can be character or numeric, identifies observations on the output when you specify the LIST option.

---

## VAR Statement

**VAR** *variables* ;

The VAR statement lists the 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.

---

## WEIGHT Statement

**WEIGHT** *variable* ;

The values of the WEIGHT variable are used to compute weighted cluster means. The WEIGHT and FREQ statements have a similar effect, except the WEIGHT statement does not alter the degrees of freedom or the number of observations. The WEIGHT variable can take nonintegral values. An observation is used in the analysis only if the value of the WEIGHT variable is greater than zero.

---

## Details: FASTCLUS Procedure

---

### Updates in the FASTCLUS Procedure

Some FASTCLUS procedure options and statements have changed from previous versions. The differences are as follows:

- Values of the FREQ variable are no longer truncated to integers. Noninteger variables specified in the FREQ statement produce results different from those in previous releases.
- The IMPUTE option produces different cluster standard deviations and related statistics. When you specify the IMPUTE option, imputed values are no longer used in computing cluster statistics. This change causes the cluster standard deviations and other statistics computed from the standard deviations to be different from those in previous releases.
- The INSTAT= option reads a SAS data set previously created with the FASTCLUS procedure by using the OUTSTAT= option. If you specify the INSTAT= option, no clustering iterations are performed and no output is produced. Only cluster assignment and imputation are performed as an OUT= data set is created.

- The OUTSTAT= data set contains additional information used for imputation. `_TYPE_=SEED` corresponds to values that are cluster seeds. Observations previously designated `_TYPE_='SCALE'` are now `_TYPE_='DISPERSION'`.

---

## Missing Values

Observations with all missing values are excluded from the analysis. If you specify the NOMISS option, observations with any missing values are excluded. Observations with missing values cannot be cluster seeds.

The distance between an observation with missing values and a cluster seed is obtained by computing the squared distance based on the nonmissing values, multiplying by the ratio of the number of variables,  $n$ , to the number of variables having nonmissing values,  $m$ , and taking the square root:

$$\sqrt{\left(\frac{n}{m}\right) \sum (x_i - s_i)^2}$$

where

- $n$  = number of variables
- $m$  = number of variables with nonmissing values
- $x_i$  = value of the  $i$ th variable for the observation
- $s_i$  = value of the  $i$ th variable for the seed

If you specify the LEAST= $p$  option with a power  $p$  other than 2 (the default), the distance is computed using

$$\left(\left(\frac{n}{m}\right) \sum (x_i - s_i)^p\right)^{\frac{1}{p}}$$

The summation is taken over variables with nonmissing values.

The IMPUTE option fills in missing values in the OUT= output data set.

---

## Output Data Sets

### OUT= Data Set

The OUT= data set contains the following:

- the original variables
- a new variable indicating the cluster assignment status of each observation. The value will be less than the permitted number of clusters (see the MAXCLUSTERS= option) if the procedure detects fewer clusters than the maximum. A positive value indicates the cluster to which the observation was assigned. A negative value indicates that the observation was not assigned to a cluster (see the STRICT option), and the absolute value indicates the cluster to which the observation would have been assigned. If the value is missing, the observation cannot be assigned to any cluster. You can specify the variable name with the CLUSTER= option. The default name is CLUSTER.

- a new variable, DISTANCE, giving the distance from the observation to its cluster seed

If you specify the IMPUTE option, the OUT= data set also contains a new variable, \_IMPUTE\_, giving the number of imputed values in each observation.

### OUTSEED= Data Set

The OUTSEED= data set contains one observation for each cluster. The variables are as follows:

- the BY variables, if any
- a new variable giving the cluster number. You can specify the variable name with the CLUSTER= option. The default name is CLUSTER.
- either the FREQ variable or a new variable called \_FREQ\_ giving the number of observations in the cluster
- the WEIGHT variable, if any
- a new variable, \_RMSSTD\_, giving the root mean squared standard deviation for the cluster. See Chapter 40, “The CLUSTER Procedure,” for details.
- a new variable, \_RADIUS\_, giving the maximum distance between any observation in the cluster and the cluster seed
- a new variable, \_GAP\_, containing the distance between the current cluster mean and the nearest other cluster mean. The value is the centroid distance given in the output.
- a new variable, \_NEAR\_, specifying the cluster number of the nearest cluster
- the VAR variables giving the cluster means

If you specify the LEAST= $p$  option with a value other than 2, the \_RMSSTD\_ variable is replaced by the \_SCALE\_ variable, which contains the pooled scale estimate analogous to the root mean squared standard deviation but based on  $p$ th-power deviations instead of squared deviations:

LEAST=1	mean absolute deviation
LEAST= $p$	root mean $p$ th-power absolute deviation
LEAST=MAX	maximum absolute deviation

If you specify the OUTITER option, there is one set of observations in the OUTSEED= data set for each pass through the data set (that is, one set for initial seeds, one for each iteration, and one for the final clusters). Also, several additional variables appear:

_ITER_	is the iteration number. For the initial seeds, the value is 0. For the final cluster means or centers, the _ITER_ variable is one greater than the last iteration reported in the iteration history.
_CRIT_	is the clustering criterion as described under the LEAST= option.



- \_CHANGE\_** is the maximum over clusters of the relative change in the cluster seed from the previous iteration. The relative change in a cluster seed is the distance between the old seed and the new seed divided by a scaling factor. If you do not specify the LEAST= option, the scaling factor is the minimum distance between the initial seeds. If you specify the LEAST= option, the scaling factor is an  $L_1$  scale estimate and is recomputed on each iteration.
- \_HOMPAR\_** is the value of the homotopy parameter. This variable appears only for LEAST= $p$  with  $1 < p < 2$ .
- \_BINSIZ\_** is the maximum bin size used for estimating medians. This variable appears only for LEAST=1.

If you specify the OUTITER option, the variables **\_SCALE\_** or **\_RMSSTD\_**, **\_RADIUS\_**, **\_NEAR\_**, and **\_GAP\_** have missing values except for the last pass.

You can use the OUTSEED= data set as a SEED= input data set for a subsequent analysis.

### OUTSTAT= Data Set

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

- BY variables, if any
- a new character variable, **\_TYPE\_**, specifying the type of statistic given by other variables (see [Table 45.2](#) and [Table 45.3](#))
- a new numeric variable giving the cluster number. You can specify the variable name with the CLUSTER= option. The default name is CLUSTER.
- a new numeric variable, **OVER\_ALL**, containing statistics that apply over all of the VAR variables
- the VAR variables giving statistics for particular variables

The values of **\_TYPE\_** for all LEAST= options are given in [Table 45.2](#).

**Table 45.2** **\_TYPE\_**

<b>_TYPE_</b>	<b>Contents of VAR Variables</b>	<b>Contents of OVER_ALL</b>
INITIAL	Initial seeds	Missing
CRITERION	Missing	Optimization criterion (see the LEAST= option); this value is displayed just before the “Cluster Summary” table.
CENTER	Cluster centers (see the LEAST= option)	Missing
SEED	Cluster seeds: additional information used for imputation	

**Table 45.2** *continued*

<b>_TYPE_</b>	<b>Contents of VAR variables</b>	<b>Contents of OVER_ALL</b>
DISPERSION	Dispersion estimates for each cluster (see the LEAST= option); these values are displayed in a separate row with title depending on the LEAST= option	Dispersion estimates pooled over variables (see the LEAST= option); these values are displayed in the “Cluster Summary” table with label depending on the LEAST= option.
FREQ	Frequency of each cluster omitting observations with missing values for the VAR variable; these values are not displayed	Frequency of each cluster based on all observations with any nonmissing value; these values are displayed in the “Cluster Summary” table.
WEIGHT	Sum of weights for each cluster omitting observations with missing values for the VAR variable; these values are not displayed	Sum of weights for each cluster based on all observations with any nonmissing value; these values are displayed in the “Cluster Summary” table.

Observations with `_TYPE_='WEIGHT'` are included only if you specify the WEIGHT statement.

The `_TYPE_` values included only for least squares clustering are given [Table 45.3](#). Least squares clustering is obtained by omitting the LEAST= option or by specifying LEAST=2.

**Table 45.3** `_TYPE_`

<b>_TYPE_</b>	<b>Contents of VAR Variables</b>	<b>Contents of OVER_ALL</b>
MEAN	Mean for the total sample; this is not displayed	Missing
STD	Standard deviation for the total sample; labeled “Total STD” in the output	Standard deviation pooled over all the VAR variables; labeled “Total STD” in the output
WITHIN_STD	Pooled within-cluster standard deviation	Within cluster standard deviation pooled over clusters and all the VAR variables
RSQ	R square for predicting the variable from the clusters; labeled “R-Squared” in the output	R square pooled over all the VAR variables; labeled “R-Squared” in the output

**Table 45.3** *continued*

<b>_TYPE_</b>	<b>Contents of VAR variables</b>	<b>Contents of OVER_ALL</b>
RSQ_RATIO	$\frac{R^2}{1-R^2}$ ; labeled “RSQ/(1-RSQ)” in the output	$\frac{R^2}{1-R^2}$ ; labeled “RSQ/(1-RSQ)” in the output
PSEUDO_F	Missing	Pseudo <i>F</i> statistic
ESRQ	Missing	Approximate expected value of R square under the null hypothesis of a single uniform cluster
CCC	Missing	Cubic clustering criterion

## Computational Resources

Let

- $n$  = number of observations
- $v$  = number of variables
- $c$  = number of clusters
- $p$  = number of passes over the data set

### Memory

The memory required is approximately  $4(19v + 12cv + 10c + 2 \max(c + 1, v))$  bytes.

If you request the DISTANCE option, an additional  $4c(c + 1)$  bytes of space is needed.

### Time

The overall time required by PROC FASTCLUS is roughly proportional to  $nvc$  if  $c$  is small with respect to  $n$ .

Initial seed selection requires one pass over the data set. If the observations are in random order, the time required is roughly proportional to

$$nvc + vc^2$$

unless you specify REPLACE=NONE. In that case, a complete pass might not be necessary, and the time is roughly proportional to  $mvc$ , where  $c \leq m \leq n$ .

The DRIFT option, each iteration, and the final assignment of cluster seeds each require one pass, with time for each pass roughly proportional to *nvc*.

For greatest efficiency, you should list the variables in the VAR statement in order of decreasing variance.

---

## Using PROC FASTCLUS

Before using PROC FASTCLUS, decide whether your variables should be standardized in some way, since variables with large variances tend to have more effect on the resulting clusters than those with small variances. If all variables are measured in the same units, standardization might not be necessary. Otherwise, some form of standardization is strongly recommended. The STDIZE procedure provides a variety of standardization methods, including robust scale estimators (for detailed information, see Chapter 115, “The STDIZE Procedure”).

The FACTOR or PRINCOMP procedure can compute standardized principal component scores. The ACECLUS procedure can transform the variables according to an estimated within-cluster covariance matrix.

Nonlinear transformations of the variables can change the number of population clusters and should therefore be approached with caution. For most applications, the variables should be transformed so that equal differences are of equal practical importance. An interval scale of measurement is required. Ordinal or ranked data are generally not appropriate.

PROC FASTCLUS produces relatively little output. In most cases you should create an output data set and use another procedure such as PRINT, SGPLOT, MEANS, DISCRIM, or CANDISC to study the clusters. It is usually desirable to try several values of the MAXCLUSTERS= option. Macros are useful for running PROC FASTCLUS repeatedly with other procedures.

A simple application of PROC FASTCLUS with two variables to examine the 2- and 3-cluster solutions can proceed as follows:

```
proc stdize method=std out=stan;
    var v1 v2;
run;

proc fastclus data=stan out=clust maxclusters=2;
    var v1 v2;
run;

proc sgplot;
    scatter y=v2 x=v1 / markerchar=cluster;
run;

proc fastclus data=stan out=clust maxclusters=3;
    var v1 v2;
run;

proc sgplot;
    scatter y=v2 x=v1 / markerchar=cluster;
run;
```

If you have more than two variables, you can use the CANDISC procedure to compute canonical variables for plotting the clusters. For example:

```

proc stdize method=std out=stan;
  var v1-v10;
run;

proc fastclus data=stan out=clust maxclusters=3;
  var v1-v10;
run;

proc candisc out=can;
  var v1-v10;
  class cluster;
run;

proc sgplot;
  scatter y=can2 x=can1 / markerchar=cluster;
run;

```

If the data set is not too large, it might also be helpful to use the following to list the clusters:

```

proc sort;
  by cluster distance;
run;

proc print;
  by cluster;
run;

```

By examining the values of DISTANCE, you can determine if any observations are unusually far from their cluster seeds.

It is often advisable, especially if the data set is large or contains outliers, to make a preliminary PROC FASTCLUS run with a large number of clusters, perhaps 20 to 100. Use MAXITER=0 and OUTSEED=SAS-*data-set*. You can save time on subsequent runs if you select cluster seeds from this output data set by using the SEED= option.

You should check the preliminary clusters for outliers, which often appear as clusters with only one member. Use a DATA step to delete outliers from the data set created by the OUTSEED= option before using it as a SEED= data set in later runs. If there are severe outliers, you should specify the STRICT option in the subsequent PROC FASTCLUS runs to prevent the outliers from distorting the clusters.

You can use the OUTSEED= data set with the SGPLOT procedure to plot `_GAP_` by `_FREQ_`. An overlay of `_RADIUS_` by `_FREQ_` provides a baseline against which to compare the values of `_GAP_`. Outliers appear in the upper-left area of the plot, with large `_GAP_` values and small `_FREQ_` values. Good clusters appear in the upper-right area, with large values of both `_GAP_` and `_FREQ_`. Good potential cluster seeds appear in the lower right, as well as in the upper-right, since large `_FREQ_` values indicate high-density regions. Small `_FREQ_` values in the left part of the plot indicate poor cluster seeds because the points are in low-density regions. It often helps to remove all clusters with small frequencies even though the clusters might not be remote enough to be considered outliers. Removing points in low-density regions improves cluster separation and provides visually sharper cluster outlines in scatter plots.

## Displayed Output

Unless the SHORT or SUMMARY option is specified, PROC FASTCLUS displays the following:

- Initial Seeds, cluster seeds selected after one pass through the data
- Change in Cluster Seeds for each iteration, if you specify MAXITER= $n > 1$

If you specify the LEAST= $p$  option, with ( $1 < p < 2$ ), and you omit the IRLS option, an additional column is displayed in the Iteration History table. This column contains a character to identify the method used in each iteration. PROC FASTCLUS chooses the most efficient method to cluster the data at each iterative step, given the condition of the data. Thus, the method chosen is data dependent. The possible values are described as follows:

Value	Method
N	Newton's method
I or L	Iteratively weighted least squares (IRLS)
1	IRLS step, halved once
2	IRLS step, halved twice
3	IRLS step, halved three times

PROC FASTCLUS displays a Cluster Summary, giving the following for each cluster:

- Cluster number
- Frequency, the number of observations in the cluster
- Weight, the sum of the weights of the observations in the cluster, if you specify the WEIGHT statement
- RMS Std Deviation, the root mean squared across variables of the cluster standard deviations, which is equal to the root mean square distance between observations in the cluster
- Maximum Distance from Seed to Observation, the maximum distance from the cluster seed to any observation in the cluster
- Nearest Cluster, the number of the cluster with mean closest to the mean of the current cluster
- Centroid Distance, the distance between the centroids (means) of the current cluster and the nearest other cluster

A table of statistics for each variable is displayed unless you specify the SUMMARY option. The table contains the following:

- Total STD, the total standard deviation
- Within STD, the pooled within-cluster standard deviation
- R-Square, the R square for predicting the variable from the cluster

- $RSQ/(1 - RSQ)$ , the ratio of between-cluster variance to within-cluster variance ( $R^2/(1 - R^2)$ )
- OVER-ALL, all of the previous quantities pooled across variables

PROC FASTCLUS also displays the following:

- Pseudo  $F$  Statistic,

$$\frac{\frac{R^2}{c-1}}{\frac{1-R^2}{n-c}}$$

where  $R$  square is the observed overall  $R$  square,  $c$  is the number of clusters, and  $n$  is the number of observations. The pseudo  $F$  statistic was suggested by Caliński and Harabasz (1974). See Milligan and Cooper (1985) and Cooper and Milligan (1988) regarding the use of the pseudo  $F$  statistic in estimating the number of clusters. See [Example 40.2](#) in Chapter 40, “The CLUSTER Procedure,” for a comparison of pseudo  $F$  statistics.

- Observed Overall R-Square, if you specify the SUMMARY option
- Approximate Expected Overall R-Square, the approximate expected value of the overall  $R$  square under the uniform null hypothesis assuming that the variables are uncorrelated. The value is missing if the number of clusters is greater than one-fifth the number of observations.
- Cubic Clustering Criterion, computed under the assumption that the variables are uncorrelated. The value is missing if the number of clusters is greater than one-fifth the number of observations.

If you are interested in the approximate expected  $R$  square or the cubic clustering criterion but your variables are correlated, you should cluster principal component scores from the PRINCOMP procedure. Both of these statistics are described by Sarle (1983). The performance of the cubic clustering criterion in estimating the number of clusters is examined by Milligan and Cooper (1985) and Cooper and Milligan (1988).

- Distances Between Cluster Means, if you specify the DISTANCE option

Unless you specify the SHORT or SUMMARY option, PROC FASTCLUS displays the following:

- Cluster Means for each variable
- Cluster Standard Deviations for each variable

## ODS Table Names

PROC FASTCLUS 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 45.4. For more information on ODS, see Chapter 23, “Using the Output Delivery System.”

**Table 45.4** ODS Tables Produced by PROC FASTCLUS

ODS Table Name	Description	Statement	Option
ApproxExpOverAllRSq	Approximate expected overall R-square, single number	PROC FASTCLUS	Default
CCC	CCC, Cubic Clustering Criterion, single number	PROC FASTCLUS	Default
ClusterList	Cluster listing, obs, id, and distances	PROC FASTCLUS	LIST
ClusterSum	Cluster summary, cluster number, distances	PROC FASTCLUS	PRINTALL
ClusterCenters	Cluster centers	PROC FASTCLUS	Default
ClusterDispersion	Cluster dispersion	PROC FASTCLUS	Default
ConvergenceStatus	Convergence status	PROC FASTCLUS	PRINTALL
Criterion	Criterion based on final seeds, single number	PROC FASTCLUS	Default
DistBetweenClust	Distance between clusters	PROC FASTCLUS	Default
InitialSeeds	Initial seeds	PROC FASTCLUS	Default
IterHistory	Iteration history, various statistics for each iteration	PROC FASTCLUS	PRINTALL
MinDist	Minimum distance between initial seeds, single number	PROC FASTCLUS	PRINTALL
NumberOfBins	Number of bins	PROC FASTCLUS	Default
ObsOverAllRSquare	Observed overall R-square, single number	PROC FASTCLUS	SUMMARY
PrelScaleEst	Preliminary L(1) scale estimate, single number	PROC FASTCLUS	PRINTALL
PseudoFStat	Pseudo $F$ statistic, single number	PROC FASTCLUS	Default
SimpleStatistics	Simple statistics for input variables	PROC FASTCLUS	Default
VariableStat	Statistics for variables within clusters	PROC FASTCLUS	Default



---

## Examples: FASTCLUS Procedure

---

### Example 45.1: 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.

In this example, the FASTCLUS procedure is used to find two and then three clusters. In the following code, an output data set is created, and PROC FREQ is invoked to compare the clusters with the species classification. See [Output 45.1.1](#) and [Output 45.1.2](#) for these results.

For three clusters, you can use the CANDISC procedure to compute canonical variables for plotting the clusters. See [Output 45.1.3](#) and [Output 45.1.4](#) for the results.

```
proc format;
  value specname
    1='Setosa      '
    2='Versicolor'
    3='Virginica  ';
run;

data iris;
  title 'Fisher (1936) Iris Data';
  input SepalLength SepalWidth PetalLength PetalWidth Species @@;
  format Species specname.;
  label SepalLength='Sepal Length in mm.'
        SepalWidth  ='Sepal Width in mm.'
        PetalLength='Petal Length in mm.'
        PetalWidth  ='Petal Width in mm.';
  datalines;
50 33 14 02 1 64 28 56 22 3 65 28 46 15 2 67 31 56 24 3
63 28 51 15 3 46 34 14 03 1 69 31 51 23 3 62 22 45 15 2
59 32 48 18 2 46 36 10 02 1 61 30 46 14 2 60 27 51 16 2
65 30 52 20 3 56 25 39 11 2 65 30 55 18 3 58 27 51 19 3
68 32 59 23 3 51 33 17 05 1 57 28 45 13 2 62 34 54 23 3
77 38 67 22 3 63 33 47 16 2 67 33 57 25 3 76 30 66 21 3
49 25 45 17 3 55 35 13 02 1 67 30 52 23 3 70 32 47 14 2

... more lines ...

55 23 40 13 2 66 30 44 14 2 68 28 48 14 2 54 34 17 02 1
51 37 15 04 1 52 35 15 02 1 58 28 51 24 3 67 30 50 17 2
63 33 60 25 3 53 37 15 02 1
;

proc fastclus data=iris maxc=2 maxiter=10 out=clus;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;
```

```

proc freq;
  tables cluster*species;
run;

proc fastclus data=iris maxc=3 maxiter=10 out=clus;
  var SepalLength SepalWidth PetalLength PetalWidth;
run;

proc freq;
  tables cluster*Species;
run;

proc candisc anova out=can;
  class cluster;
  var SepalLength SepalWidth PetalLength PetalWidth;
  title2 'Canonical Discriminant Analysis of Iris Clusters';
run;

proc sgplot data=Can;
  scatter y=Can2 x=Can1 / group=Cluster;
  title2 'Plot of Canonical Variables Identified by Cluster';
run;

```

**Output 45.1.1** Fisher's Iris Data: PROC FASTCLUS with MAXC=2 and PROC FREQ

### Fisher (1936) Iris Data

The FASTCLUS Procedure  
 Replace=FULL Radius=0 Maxclusters=2 Maxiter=10 Converge=0.02

Initial Seeds				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	43.00000000	30.00000000	11.00000000	1.00000000
2	77.00000000	26.00000000	69.00000000	23.00000000

Minimum Distance Between Initial Seeds = 70.85196

Iteration History				
Iteration	Criterion	Relative Change in Cluster Seeds		
		1	2	
1	11.0638	0.1904	0.3163	
2	5.3780	0.0596	0.0264	
3	5.0718	0.0174	0.00766	

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 5.0417

**Output 45.1.1** *continued*

Cluster Summary					
Cluster	Frequency	RMS Std Deviation	Maximum Distance		Distance Between Cluster Centroids
			from Seed to Observation	Radius Exceeded	
1	53	3.7050	21.1621		39.2879
2	97	5.6779	24.6430		39.2879

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
SepalLength	8.28066	5.49313	0.562896	1.287784
SepalWidth	4.35866	3.70393	0.282710	0.394137
PetalLength	17.65298	6.80331	0.852470	5.778291
PetalWidth	7.62238	3.57200	0.781868	3.584390
OVER-ALL	10.69224	5.07291	0.776410	3.472463

Pseudo F Statistic = 513.92

Approximate Expected Over-All R-Squared = 0.51539

Cubic Clustering Criterion = 14.806

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

Cluster Means				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	50.05660377	33.69811321	15.60377358	2.90566038
2	63.01030928	28.86597938	49.58762887	16.95876289

Cluster Standard Deviations				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	3.427350930	4.396611045	4.404279486	2.105525249
2	6.336887455	3.267991438	7.800577673	4.155612484

**Fisher (1936) Iris Data**

**The FREQ Procedure**

Frequency Percent Row Pct Col Pct	Table of CLUSTER by Species				
	CLUSTER(Cluster)	Species			Total
		Setosa	Versicolor	Virginica	
	1	50	3	0	53
		33.33	2.00	0.00	35.33
		94.34	5.66	0.00	
		100.00	6.00	0.00	
	2	0	47	50	97
		0.00	31.33	33.33	64.67
		0.00	48.45	51.55	
		0.00	94.00	100.00	
	<b>Total</b>	50	50	50	150
		33.33	33.33	33.33	100.00

**Output 45.1.2** Fisher's Iris Data: PROC FASTCLUS with MAXC=3 and PROC FREQ**Fisher (1936) Iris Data****The FASTCLUS Procedure**

Replace=FULL Radius=0 Maxclusters=3 Maxiter=10 Converge=0.02

**Initial Seeds**

Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	58.00000000	40.00000000	12.00000000	2.00000000
2	77.00000000	38.00000000	67.00000000	22.00000000
3	49.00000000	25.00000000	45.00000000	17.00000000

Minimum Distance Between Initial Seeds = 38.23611

**Iteration History**

Iteration	Criterion	Relative Change in Cluster Seeds		
		1	2	3
1	6.7591	0.2652	0.3205	0.2985
2	3.7097	0	0.0459	0.0317
3	3.6427	0	0.0182	0.0124

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 3.6289

**Cluster Summary**

Cluster	Frequency	RMS Std Deviation	Maximum Distance		Nearest Cluster	Distance Between Cluster Centroids
			from Seed to Observation	Radius Exceeded		
1	50	2.7803	12.4803		3	33.5693
2	38	4.0168	14.9736		3	17.9718
3	62	4.0398	16.9272		2	17.9718

**Statistics for Variables**

Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
SepalLength	8.28066	4.39488	0.722096	2.598359
SepalWidth	4.35866	3.24816	0.452102	0.825156
PetalLength	17.65298	4.21431	0.943773	16.784895
PetalWidth	7.62238	2.45244	0.897872	8.791618
OVER-ALL	10.69224	3.66198	0.884275	7.641194

Pseudo F Statistic = 561.63

Approximate Expected Over-All R-Squared = 0.62728

Cubic Clustering Criterion = 25.021

**Output 45.1.2** *continued*

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

Cluster Means				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	50.06000000	34.28000000	14.62000000	2.46000000
2	68.50000000	30.73684211	57.42105263	20.71052632
3	59.01612903	27.48387097	43.93548387	14.33870968

Cluster Standard Deviations				
Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	3.524896872	3.790643691	1.736639965	1.053855894
2	4.941550255	2.900924461	4.885895746	2.798724562
3	4.664100551	2.962840548	5.088949673	2.974997167

**Fisher (1936) Iris Data**

**The FREQ Procedure**

Frequency Percent Row Pct Col Pct	Table of CLUSTER by Species				
	CLUSTER(Cluster)	Species			Total
		Setosa	Versicolor	Virginica	
	1	50	0	0	50
		33.33	0.00	0.00	33.33
		100.00	0.00	0.00	
		100.00	0.00	0.00	
	2	0	2	36	38
		0.00	1.33	24.00	25.33
		0.00	5.26	94.74	
		0.00	4.00	72.00	
	3	0	48	14	62
		0.00	32.00	9.33	41.33
		0.00	77.42	22.58	
		0.00	96.00	28.00	
	<b>Total</b>	50	50	50	150
		33.33	33.33	33.33	100.00

**Output 45.1.3** Fisher's Iris Data Using PROC CANDISC

**Fisher (1936) Iris Data  
Canonical Discriminant Analysis of Iris Clusters**

**The CANDISC Procedure**

Total Sample Size	150	DF Total	149
Variables	4	DF Within Classes	147
Classes	3	DF Between Classes	2

Number of Observations Read	150
Number of Observations Used	150

**Output 45.1.3** *continued*


---

Class Level Information			
Variable			
CLUSTER Name	Frequency	Weight	Proportion
1 _1	50	50.0000	0.333333
2 _2	38	38.0000	0.253333
3 _3	62	62.0000	0.413333

---

**Fisher (1936) Iris Data**  
**Canonical Discriminant Analysis of Iris Clusters**

**The CANDISC Procedure**

---

Univariate Test Statistics								
F Statistics, Num DF=2, Den DF=147								
Variable	Label	Total Standard Deviation	Pooled Standard Deviation	Between Standard Deviation	R-Square	R-Square / (1-RSq)	F Value	Pr > F
SepalLength	Sepal Length in mm.	8.2807	4.3949	8.5893	0.7221	2.5984	190.98	<.0001
SepalWidth	Sepal Width in mm.	4.3587	3.2482	3.5774	0.4521	0.8252	60.65	<.0001
PetalLength	Petal Length in mm.	17.6530	4.2143	20.9336	0.9438	16.7849	1233.69	<.0001
PetalWidth	Petal Width in mm.	7.6224	2.4524	8.8164	0.8979	8.7916	646.18	<.0001

---

Average R-Square	
Unweighted	0.7539604
Weighted by Variance	0.8842753

---



---

Multivariate Statistics and F Approximations					
S=2 M=0.5 N=71					
Statistic	Value	F Value	Num DF	Den DF	Pr > F
Wilks' Lambda	0.03222337	164.55	8	288	<.0001
Pillai's Trace	1.25669612	61.29	8	290	<.0001
Hotelling-Lawley Trace	21.06722883	377.66	8	203.4	<.0001
Roy's Greatest Root	20.63266809	747.93	4	145	<.0001

---

NOTE: F Statistic for Roy's Greatest Root is an upper bound.

NOTE: F Statistic for Wilks' Lambda is exact.

---

Output 45.1.3 continued

Fisher (1936) Iris Data  
Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

	Canonical Correlation	Adjusted Canonical Correlation	Approximate Standard Error	Squared Canonical Correlation	Eigenvalues of Inv(E)*H = CanRsq/(1-CanRsq)			
					Eigenvalue	Difference	Proportion	Cumulative
1	0.976613	0.976123	0.003787	0.953774	20.6327	20.1981	0.9794	0.9794
2	0.550384	0.543354	0.057107	0.302923	0.4346		0.0206	1.0000

Test of H0: The canonical correlations in the current row and all that follow are zero

	Likelihood Ratio	Approximate F Value	Num DF	Den DF	Pr > F
1	0.03222337	164.55	8	288	<.0001
2	0.69707749	21.00	3	145	<.0001

Fisher (1936) Iris Data  
Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

Total Canonical Structure				
Variable	Label	Can1	Can2	
SepalLength	Sepal Length in mm.	0.831965	0.452137	
SepalWidth	Sepal Width in mm.	-0.515082	0.810630	
PetalLength	Petal Length in mm.	0.993520	0.087514	
PetalWidth	Petal Width in mm.	0.966325	0.154745	

Between Canonical Structure				
Variable	Label	Can1	Can2	
SepalLength	Sepal Length in mm.	0.956160	0.292846	
SepalWidth	Sepal Width in mm.	-0.748136	0.663545	
PetalLength	Petal Length in mm.	0.998770	0.049580	
PetalWidth	Petal Width in mm.	0.995952	0.089883	

Pooled Within Canonical Structure				
Variable	Label	Can1	Can2	
SepalLength	Sepal Length in mm.	0.339314	0.716082	
SepalWidth	Sepal Width in mm.	-0.149614	0.914351	
PetalLength	Petal Length in mm.	0.900839	0.308136	
PetalWidth	Petal Width in mm.	0.650123	0.404282	

**Output 45.1.3** *continued***Fisher (1936) Iris Data  
Canonical Discriminant Analysis of Iris Clusters****The CANDISC Procedure**


---

Total-Sample Standardized Canonical Coefficients			
Variable	Label	Can1	Can2
<b>SepalLength</b>	Sepal Length in mm.	0.047747341	1.021487262
<b>SepalWidth</b>	Sepal Width in mm.	-0.577569244	0.864455153
<b>PetalLength</b>	Petal Length in mm.	3.341309573	-1.283043758
<b>PetalWidth</b>	Petal Width in mm.	0.996451144	0.900476563

---

Pooled Within-Class Standardized Canonical Coefficients			
Variable	Label	Can1	Can2
<b>SepalLength</b>	Sepal Length in mm.	0.0253414487	0.5421446856
<b>SepalWidth</b>	Sepal Width in mm.	-.4304161258	0.6442092294
<b>PetalLength</b>	Petal Length in mm.	0.7976741592	-.3063023132
<b>PetalWidth</b>	Petal Width in mm.	0.3205998034	0.2897207865

---

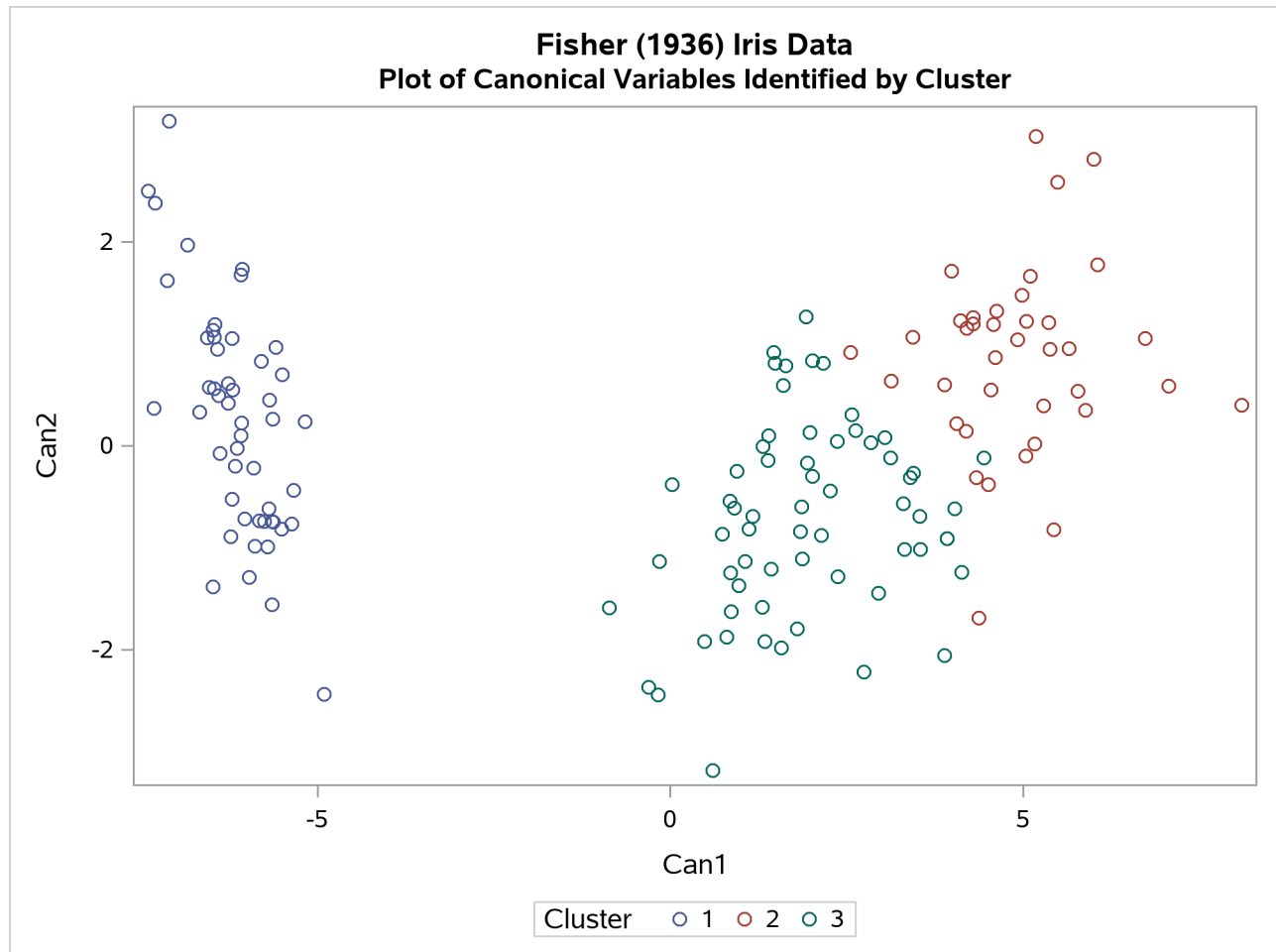
Raw Canonical Coefficients			
Variable	Label	Can1	Can2
<b>SepalLength</b>	Sepal Length in mm.	0.0057661265	0.1233581748
<b>SepalWidth</b>	Sepal Width in mm.	-.1325106494	0.1983303556
<b>PetalLength</b>	Petal Length in mm.	0.1892773419	-.0726814163
<b>PetalWidth</b>	Petal Width in mm.	0.1307270927	0.1181359305

---

Class Means on Canonical Variables		
CLUSTER	Can1	Can2
1	-6.131527227	0.244761516
2	4.931414018	0.861972277
3	1.922300462	-0.725693908

---



**Output 45.1.4** Plot of Fisher's Iris Data Using PROC CANDISC

## Example 45.2: Outliers

This example involves data artificially generated to contain two clusters and several severe outliers. A preliminary analysis specifies 20 clusters and outputs an `OUTSEED=` data set to be used for a diagnostic plot. The exact number of initial clusters is not important; similar results could be obtained with 10 or 50 initial clusters. Examination of the plot suggests that clusters with more than five (again, the exact number is not important) observations can yield good seeds for the main analysis. A `DATA` step deletes clusters with five or fewer observations, and the remaining cluster means provide seeds for the next `PROC FASTCLUS` analysis.

Two clusters are requested; the `LEAST=` option specifies the mean absolute deviation criterion (`LEAST=1`). Values of the `LEAST=` option less than 2 reduce the effect of outliers on cluster centers.

The next analysis also requests two clusters; the `STRICT=` option is specified to prevent outliers from distorting the results. The `STRICT=` value is chosen to be close to the `_GAP_` and `_RADIUS_` values of the larger clusters in the diagnostic plot; the exact value is not critical.

A final `PROC FASTCLUS` run assigns the outliers to clusters.

The following SAS statements implement these steps, and the results are displayed in [Output 45.2.3](#) through [Output 45.2.8](#). First, an artificial data set is created with two clusters and some outliers. Then PROC FASTCLUS is run with many clusters to produce an OUTSEED= data set. A diagnostic plot using the variables `_GAP_` and `_RADIUS_` is then produced using the SGSCATTER procedure. The results from these steps are shown in [Output 45.2.1](#) and [Output 45.2.2](#).

```

title 'Using PROC FASTCLUS to Analyze Data with Outliers';
data x;
  drop n;
  do n=1 to 100;
    x=rannor(12345)+2;
    y=rannor(12345);
    output;
  end;
  do n=1 to 100;
    x=rannor(12345)-2;
    y=rannor(12345);
    output;
  end;
  do n=1 to 10;
    x=10*rannor(12345);
    y=10*rannor(12345);
    output;
  end;
run;

title2 'Preliminary PROC FASTCLUS Analysis with 20 Clusters';
proc fastclus data=x outseed=mean1 maxc=20 maxiter=0 summary;
  var x y;
run;

proc sgscatter data=mean1;
  compare y=( _gap_ _radius_ ) x=_freq_;
run;

```

**Output 45.2.1** Preliminary Analysis of Data with Outliers Using PROC FASTCLUS

**Using PROC FASTCLUS to Analyze Data with Outliers  
Preliminary PROC FASTCLUS Analysis with 20 Clusters**

**The FASTCLUS Procedure  
Replace=FULL Radius=0 Maxclusters=20 Maxiter=0**

---

Criterion Based on Final Seeds = 0.6873

---

Output 45.2.1 *continued*

Cluster Summary						
Cluster	Frequency	RMS Std Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster	Distance Between Cluster Centroids
1	8	0.4753	1.1924		19	1.7205
2	1	.	0		6	6.2847
3	44	0.6252	1.6774		5	1.4386
4	1	.	0		20	5.2130
5	38	0.5603	1.4528		3	1.4386
6	2	0.0542	0.1085		2	6.2847
7	1	.	0		14	2.5094
8	2	0.6480	1.2961		1	1.8450
9	1	.	0		7	9.4534
10	1	.	0		18	4.2514
11	1	.	0		16	4.7582
12	20	0.5911	1.6291		16	1.5601
13	5	0.6682	1.4244		3	1.9553
14	1	.	0		7	2.5094
15	5	0.4074	1.2678		3	1.7609
16	22	0.4168	1.5139		19	1.4936
17	8	0.4031	1.4794		5	1.5564
18	1	.	0		10	4.2514
19	45	0.6475	1.6285		16	1.4936
20	3	0.5719	1.3642		15	1.8999

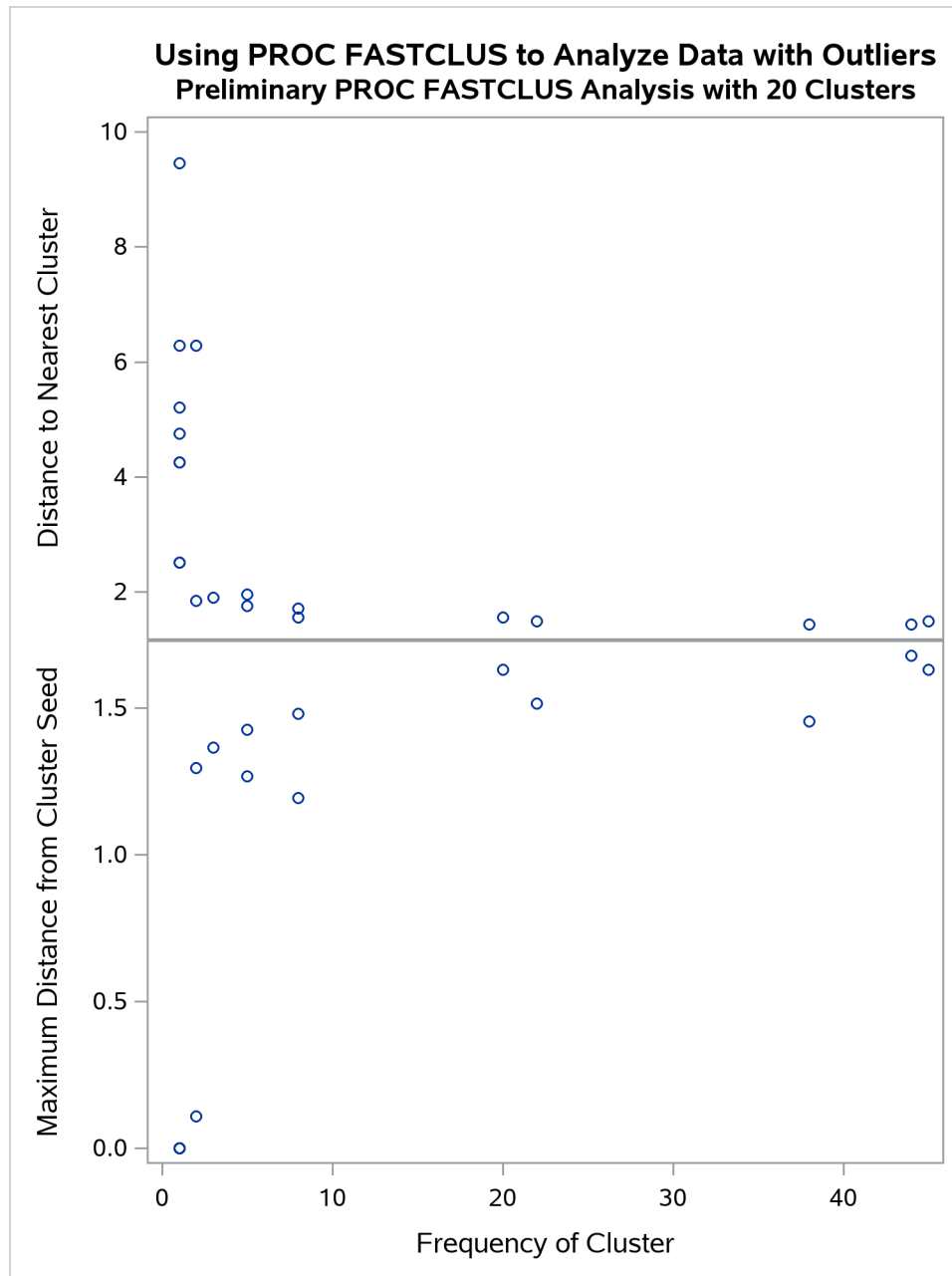
Pseudo F Statistic = 207.58

Observed Over-All R-Squared = 0.95404

Approximate Expected Over-All R-Squared = 0.96103

Cubic Clustering Criterion = -2.503

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

**Output 45.2.2** Preliminary Analysis of Data with Outliers: Plot Using PROC SGSCATTER

In the following SAS statements, a DATA step is used to remove low frequency clusters, then the FASTCLUS procedure is run again, selecting seeds from the high frequency clusters in the previous analysis using LEAST=1 clustering criterion. The results are shown in [Output 45.2.3](#) and [Output 45.2.4](#).

```

data seed;
  set mean1;
  if _freq_>5;
run;

title2 'PROC FASTCLUS Analysis Using LEAST= Clustering Criterion';

```

```

title3 'Values < 2 Reduce Effect of Outliers on Cluster Centers';
proc fastclus data=x seed=seed maxc=2 least=1 out=out;
  var x y;
run;

proc sgplot data=out;
  scatter y=y x=x / group=cluster;
run;

```

**Output 45.2.3** Analysis of Data with Outliers Using the LEAST= Option

**Using PROC FASTCLUS to Analyze Data with Outliers  
 PROC FASTCLUS Analysis Using LEAST= Clustering Criterion  
 Values < 2 Reduce Effect of Outliers on Cluster Centers**

The FASTCLUS Procedure  
 Replace=FULL Radius=0 Maxclusters=2 Maxiter=20 Converge=0.0001 Least=1

Initial Seeds		
Cluster	x	y
1	2.794174248	-0.065970836
2	-2.027300384	-2.051208579

Minimum Distance Between Initial Seeds = 6.806712

Preliminary L(1) Scale Estimate = 2.796579

Number of Bins = 100

Iteration History				
Iteration	Criterion	Maximum Bin Size	Relative Change in Cluster Seeds	
			1	2
1	1.3983	0.2263	0.4091	0.6696
2	1.0776	0.0226	0.00511	0.0452
3	1.0771	0.00226	0.00229	0.00234
4	1.0771	0.000396	0.000253	0.000144
5	1.0771	0.000396	0	0

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 1.0771

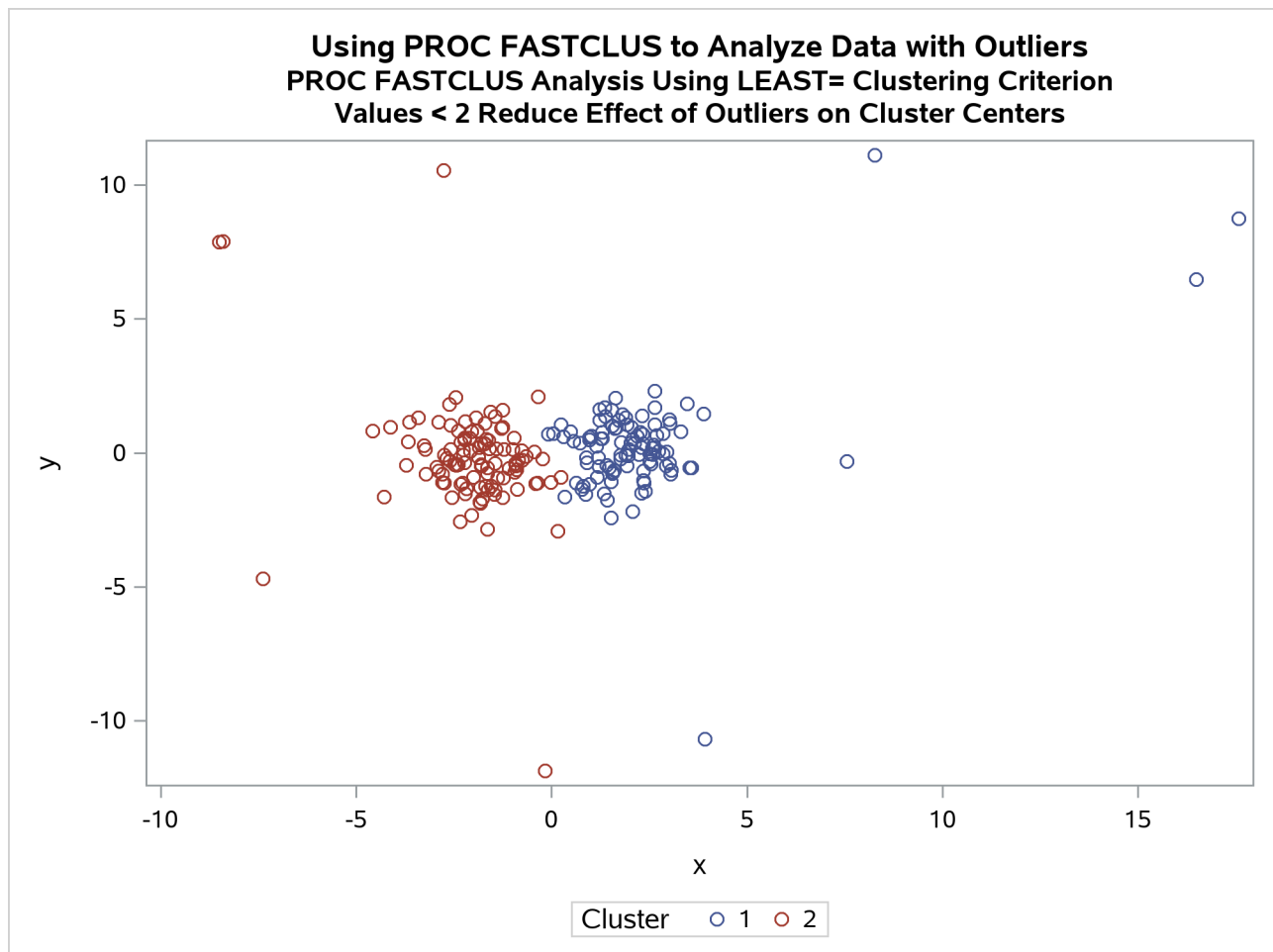
Cluster Summary						
Cluster	Frequency	Mean Maximum Distance			Nearest Cluster	Distance Between Cluster Medians
		Absolute Deviation	from Seed to Observation	Radius Exceeded		
1	102	1.1278	24.1622		2	4.2585
2	108	1.0494	14.8292		1	4.2585

**Output 45.2.3** *continued*

Cluster Medians		
Cluster	x	y
1	1.923023887	0.222482918
2	-1.826721743	-0.286253041

Mean Absolute Deviations from Final Seeds		
Cluster	x	y
1	1.113465261	1.142120480
2	0.890331835	1.208370913

**Output 45.2.4** Analysis Plot of Data with Outliers

The FASTCLUS procedure is run again, selecting seeds from high frequency clusters in the previous analysis. `STRICT=` prevents outliers from distorting the results. The results are shown in [Output 45.2.5](#) and [Output 45.2.6](#).

```

title2 'PROC FASTCLUS Analysis Using STRICT= to Omit Outliers';
proc fastclus data=x seed=seed
    maxc=2 strict=3.0 out=out outseed=mean2;
    var x y;
run;

proc sgplot data=out;
    scatter y=y x=x / group=cluster;
run;

```

**Output 45.2.5** Cluster Analysis with Outliers Omitted: PROC FASTCLUS SGPLOT

**Using PROC FASTCLUS to Analyze Data with Outliers  
PROC FASTCLUS Analysis Using STRICT= to Omit Outliers**

The FASTCLUS Procedure  
 Replace=FULL Radius=0 Strict=3 Maxclusters=2 Maxiter=1

Initial Seeds		
Cluster	x	y
1	2.794174248	-0.065970836
2	-2.027300384	-2.051208579

Criterion Based on Final Seeds = 0.9515

Cluster Summary						
Cluster	Frequency	RMS Std Deviation	Maximum Distance		Nearest Cluster	Distance Between Cluster Centroids
			from Seed to Observation	Radius Exceeded		
1	99	0.9501	2.9589		2	3.7666
2	99	0.9290	2.8011		1	3.7666

12 Observation(s) were not assigned to a cluster because the minimum distance to a cluster seed exceeded the STRICT= value.

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
x	2.06854	0.87098	0.823609	4.669219
y	1.02113	1.00352	0.039093	0.040683
OVER-ALL	1.63119	0.93959	0.669891	2.029303

Pseudo F Statistic = 397.74

Approximate Expected Over-All R-Squared = 0.60615

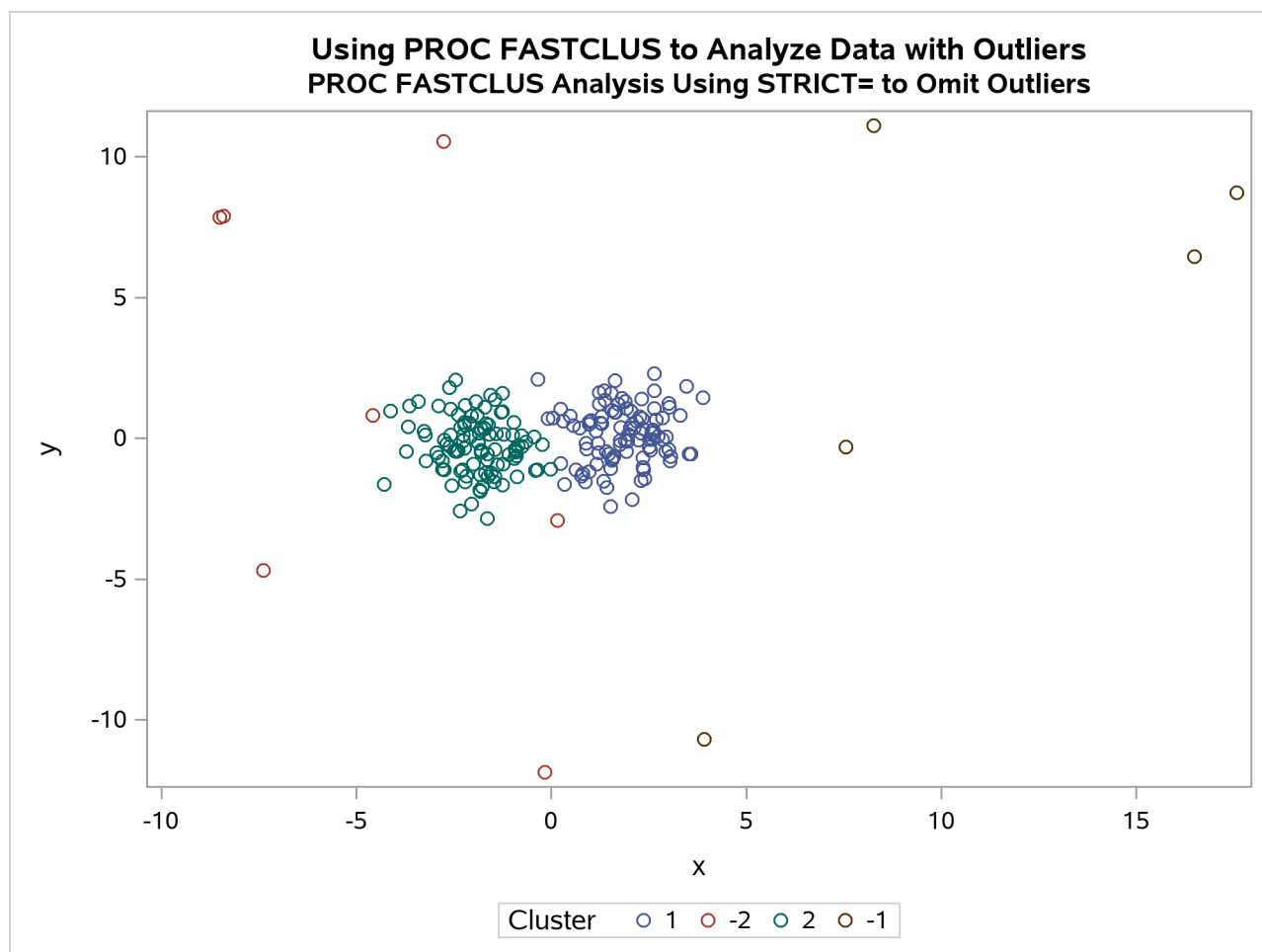
Cubic Clustering Criterion = 3.197

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

Cluster Means		
Cluster	x	y
1	1.825111432	0.141211701
2	-1.919910712	-0.261558725

**Output 45.2.5** *continued*

Cluster Standard Deviations		
Cluster	x	y
1	0.889549271	1.006965219
2	0.852000588	1.000062579

**Output 45.2.6** Cluster Analysis with Outliers Omitted: Plot Using PROC SGPLOT

Finally, the FASTCLUS procedure is run one more time with zero iterations to assign outliers and tails to clusters. The results are shown in [Output 45.2.7](#) and [Output 45.2.8](#).

```

title2 'Final PROC FASTCLUS Analysis Assigning Outliers to Clusters';
proc fastclus data=x seed=mean2 maxc=2 maxiter=0 out=out;
  var x y;
run;

proc sgplot data=out;
  scatter y=y x=x / group=cluster;
run;

```



**Output 45.2.7** Cluster Analysis with Outliers Omitted: PROC FASTCLUS

**Using PROC FASTCLUS to Analyze Data with Outliers  
Final PROC FASTCLUS Analysis Assigning Outliers to Clusters**

**The FASTCLUS Procedure**  
**Replace=FULL Radius=0 Maxclusters=2 Maxiter=0**

---

Initial Seeds		
Cluster	x	y
1	1.825111432	0.141211701
2	-1.919910712	-0.261558725

---

**Criterion Based on Final Seeds = 2.0594**

---



---

Cluster Summary						
Cluster	Frequency	RMS Std Deviation	Maximum Distance	Radius Exceeded	Nearest Cluster	Distance Between Cluster Centroids
			from Seed to Observation			
1	103	2.2569	17.9426		2	4.3753
2	107	1.8371	11.7362		1	4.3753

---



---

Statistics for Variables				
Variable	Total STD	Within STD	R-Square	RSQ/(1-RSQ)
x	2.92721	1.95529	0.555950	1.252000
y	2.15248	2.14754	0.009347	0.009435
OVER-ALL	2.56922	2.05367	0.364119	0.572621

---

**Pseudo F Statistic = 119.11**

---

**Approximate Expected Over-All R-Squared = 0.49090**

---

**Cubic Clustering Criterion = -5.338**

---

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

---

Cluster Means		
Cluster	x	y
1	2.280017469	0.263940765
2	-2.075547895	-0.151348765

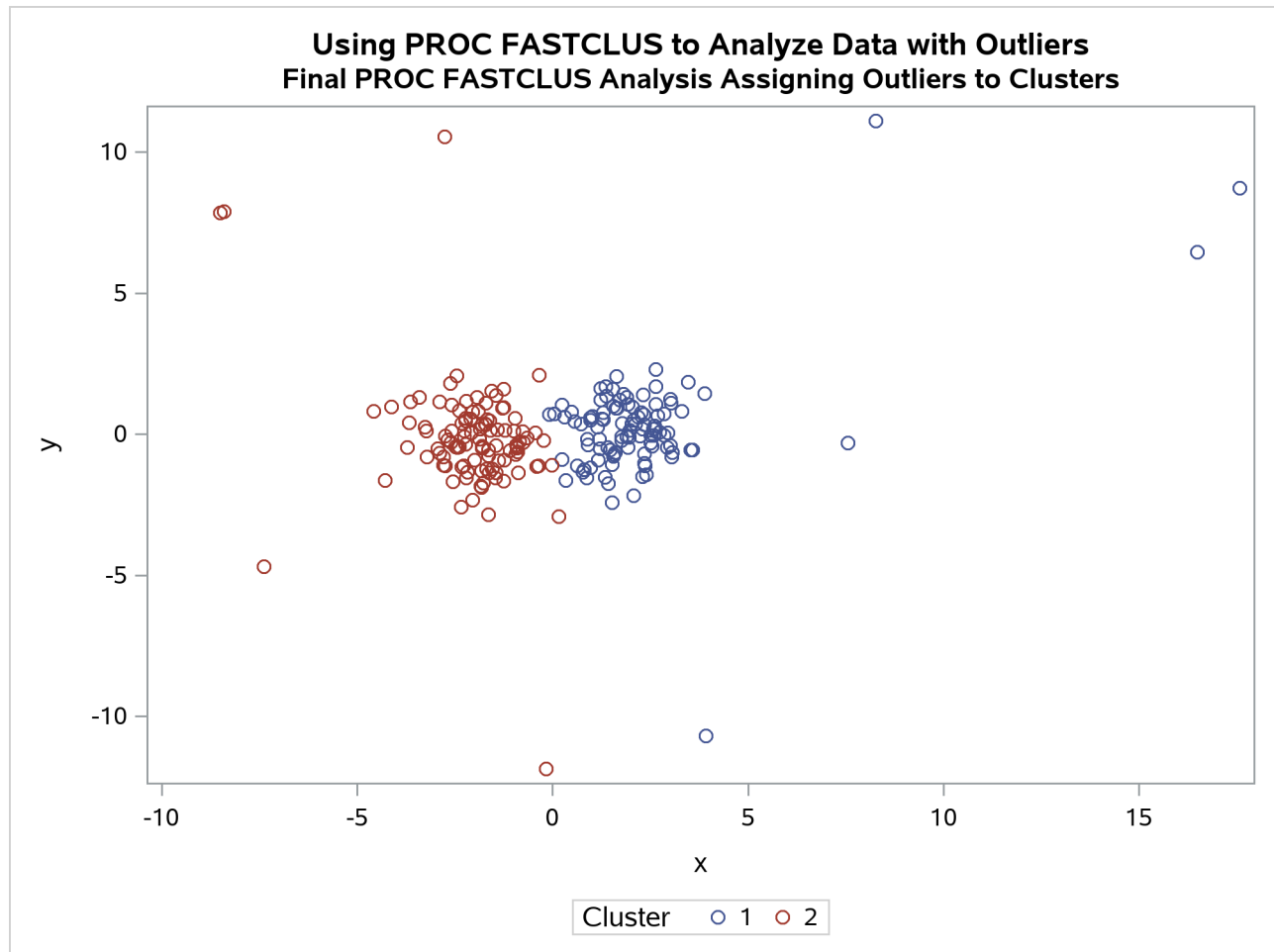
---



---

Cluster Standard Deviations		
Cluster	x	y
1	2.412264861	2.089922815
2	1.379355878	2.201567557

---

**Output 45.2.8** Cluster Analysis with Outliers Omitted: Plot Using PROC SGPLOT

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