Chapter 27 The FASTCLUS Procedure

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Chapter 27 The FASTCLUS Procedure

Overview

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, 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 over 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 so 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 pth 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 may be highly sensitive to the order of the observations in the data set.

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 Hartigan's (1975) leader algorithm and MacQueen's (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 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 ≥ 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 may 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) using the MAXCLUSTERS= option. You can also specify a minimum distance by which the seeds must be separated 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 may 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 Hartigan's (1975, pp. 74–78) leader algorithm and the *simple cluster seeking algorithm* described by Tou and Gonzalez (1974, pp. 90–92).

Getting Started

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 fish caught off the coast of Finland; this data set is available from the Data Archive of the *Journal of Statistics Education*. The complete data set is displayed in Chapter 60, "The STEPDISC Procedure."

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';
data Fish (drop=HtPct WidthPct);
   title 'Fish Measurement Data';
   input Species Weight Length1 Length2 Length3 HtPct
         WidthPct @@;
   if Weight <= 0 or Weight = . then delete;
   Weight3=Weight**(1/3);
   Height=HtPct*Length3/(Weight3*100);
   Width=WidthPct*Length3/(Weight3*100);
   Length1=Length1/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
 ... [155 more records]
;
run;
```

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.

Variables with larger variances exert a larger influence in calculating the clusters. 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.

The STANDARD procedure is first used to standardize all the analytical variables to a mean of 0 and standard deviation of 1. The procedure creates the output data set Stand to contain the transformed variables.

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.

	Replace=FUL		CLUS Procedure usters=7 Maxiter=1	00 Converge=0.02	
		Init	ial Seeds		
		logLength			
Cluster	Length1	Ratio	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

Figure 27.1. Initial Seeds Used in the FASTCLUS Procedure

Figure 27.1 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 27.2 displays the number of observations in the cluster (frequency) and the root mean square 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.

Fish Measurement Data							
The FASTCLUS Procedure Replace=FULL Radius=0 Maxclusters=7 Maxiter=100 Converge=0.02							
			Cluster Summary				
			Maximum Distance				
		RMS Std	from Seed	Radius	Nearest	Distance Between	
Cluster	Frequency	Deviation	to Observation	Exceeded	Cluster	Cluster Centroids	
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	
	50	0.4447	2.3915		4	1.4266	

Figure 27.2. Cluster Summary Table from the FASTCLUS Procedure

Figure 27.3 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^2 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.

Fish Measurement Data					
		ASTCLUS Procedu			
Replace=FULL	Radius=0 Ma	xclusters=7 Max	iter=100 Con	verge=0.02	
	Statis	tics for Variab	oles		
Variable	Total STD		R-Square		
Length1	1.00000	0.31428			
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 = 1	.31.87		
_					
Approx	imate Expected	Over-All R-Squ	mared = 0.57	420	
	Cubia Cluator	ing Criterion =	. 37 909		
	Cubic Cluster	ing criterion =	37.000		
WARNING: The to	wo above value	s are invalid f	or correlated	variables.	

Figure 27.3. Statistics for Variables Used in the FASTCLUS Procedure

The pseudo F statistic, approximate expected overall \mathbb{R}^2 , 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 \mathbb{R}^2 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 may indicate outliers.

PROC FASTCLUS next produces the within-cluster means and standard deviations of the variables, displayed in Figure 27.4.

		Fish Mea	surement Data			
	Replace=FULL		CLUS Procedure usters=7 Maxiter=100	Converge=0.02		
		Clus	ter Means			
		logLength				
Cluster	Length1	Ratio	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						
		logLength				
Cluster	Length1	Ratio	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	

Figure 27.4. Cluster Means and Standard Deviations from the FASTCLUS Procedure

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;
```

These statements produce a frequency table of the variable Cluster versus the variable Species.

Figure 27.5 displays the marked division between clusters.

Fish Measurement Data								
The FREQ Procedure								
		Та	able of Sp	ecies by	CLUSTER			
Species	CLUSTER((Cluster)						
Frequency Percent Row Pct	 	2.1		4.1	F	cl	7.1	mata l
Col Pct	1 +					6 ++		
Bream	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.00 0.00 0.00		0.00 0.00 0.00	0.00		0.00 0.00 0.00	34 21.66
Roach	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00 0.00	0.00	19 12.10 100.00 38.00	12.10
Whitefish	0 0.00 0.00	2 1.27 33.33 10.53	0.00 0.00	1	0.00 0.00 0.00	0.00 0.00	3 1.91 50.00 6.00	6 3.82
Parkki	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00	0.00 0.00	11 7.01 100.00 100.00	0.00 0.00	0.00 0.00 0.00	11 7.01
Perch	0.00 0.00 0.00	17 10.83 30.36 89.47	0.00	12 7.64 21.43	0.00 0.00 0.00	0.00 0.00	27 17.20 48.21 54.00	56 35.67
Pike	17 10.83 100.00 100.00	0.00 0.00	0 0.00 0.00	0.00 0.00 0.00	0.00 0.00 0.00	0.00 0.00	0.00 0.00 0.00	17 10.83
Smelt	0.00 0.00 0.00	0 0.00 0.00	13 8.28 92.86 100.00	0 0.00 0.00	0 0.00 0.00 0.00	0.00 0.00	1 0.64 7.14 2.00	14 8.92
Total	17 10.83	19 12.10	13 8.28	13	11 7.01	34 21.66	50	157 100.00

Figure 27.5. Frequency Table of Cluster versus Species

For cases in which you have three or more clusters, you can use the CANDISC and GPLOT procedures to obtain a graphical check on the distribution of the clusters. In the following statements, the CANDISC and GPLOT 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;
legend1 frame cframe=ligr label=none cborder=black
        position=center value=(justify=center);
axis1 label=(angle=90 rotate=0) minor=none;
axis2 minor=none;
```

```
proc gplot data=Can;
   plot Can2*Can1=Cluster/frame cframe=ligr
                  legend=legend1 vaxis=axis1 haxis=axis2;
run;
```

First, the CANDISC procedure is invoked to perform a canonical discriminant analysis 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 GPLOT procedure plots the two canonical variables from PROC CAN-DISC, Can1 and Can2. The PLOT statement specifies the variable Cluster as the identification variable.

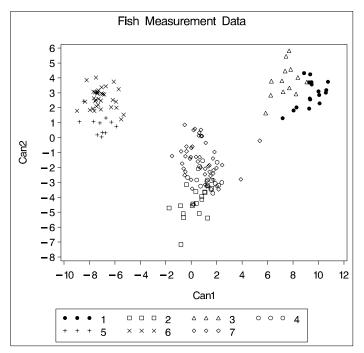


Figure 27.6. Plot of Canonical Variables and Cluster Value

The resulting plot (Figure 27.6) illustrates the spatial separation of the clusters calculated in the FASTCLUS procedure.

Syntax

The following statements are available in the FASTCLUS procedure:

```
PROC FASTCLUS MAXCLUSTERS=n | RADIUS=t < options > ;
VAR variables;
ID variable;
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 \mid RADIUS=t < options > ;
```

You must specify either the MAXCLUSTERS= or the RADIUS= argument in the PROC FASTCLUS statement.

MAXCLUSTERS=n

MAXC=n

specifies the maximum number of clusters allowed. 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 27.1 summarizes the options.

Table 27.1. Options Available in the PROC FASTCLUS Statement

Task	Options
Specify data set details	CLUSTER=
	DATA=
	MEAN=
	OUT=
	OUTITER
	OUTSEED=
	OUTSTAT=
	SEED=
Specify distance dimension	BINS=
	HC=
	HP=
	IRLS
	LEAST=
Select initial cluster seeds	RANDOM=
	REPLACE=
Compute final cluster seeds	CONVERGE=
•	DELETE=
	DRIFT
	MAXCLUSTERS=
	MAXITER=
	RADIUS=
	STRICT
Work with missing values	IMPUTE
	NOMISS
Specify variance divisor	VARDEF
Control output	DISTANCE
-	LIST
	NOPRINT
	SHORT
	SUMMARY

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 may 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.

CONVERGE=c

specifies the convergence criterion. Any nonnegative value is allowed. 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 may 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 1196. 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 . You should specify these options only if you encounter convergence problems using the default values.

For $1 , PROC FASTCLUS tries to optimize a perturbed variant of the <math>L_p$ 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 con-

vergence 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 may 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.

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 Ekblom-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 has a missing value for a variable used in the cluster analysis, the missing value is replaced by the corresponding value in the cluster seed to which the observation is assigned. If the observation is not assigned to a cluster, missing values are not replaced. 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 by the FASTCLUS procedure using the OUT-STAT= 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 Ekblom-Newton method. If you specify the IRLS option, you must also specify LEAST=p, where 1 . Use the IRLS option only if you encounter convergence problems with the default method.

LEAST= $p \mid MAX$ L= $p \mid MAX$

causes PROC FASTCLUS to optimize an L_p criterion, where $1 \le p \le \infty$ (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

allow the optimization process a chance to converge. See the MAXITER= option on page 1210.

Specifying the LEAST= option also changes the default convergence criterion from 0.02 to 0.0001. See the CONVERGE= option on page 1207.

When LEAST=2, PROC FASTCLUS tries to minimize the root mean square 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 pth root of the mean of the pth powers of the absolute differences between the data and the corresponding cluster seeds.

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	modified Merle-Spath if you specify IRLS,
	otherwise modified Ekblom-Newton
p=2	arithmetic mean
	Newton
$p = \infty$	midrange

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

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

LEAST=p	Scale Estimate
p = 1	mean absolute deviation
1	root mean pth-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 0, PROC FASTCLUS executes the third of the four steps described in the "Background" section on page 1196. 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	50
$1.5 \le p < 2$	20
p=2	10
2	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 permanent SAS data set, you must specify a two-level name. Refer to "SAS Data Files" in SAS Language Reference: Concepts for more information on permanent data sets.

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 15, "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. Refer to "SAS Data Files" in SAS Language Reference: Concepts for more information on permanent data sets.

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 may 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.

FULL requests default seed replacement as described in the section

"Background" on page 1196.

PART requests seed replacement only when the distance between the ob-

servation and the closest seed is greater than the minimum distance

between seeds.

NONE suppresses seed replacement.

RANDOM 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.

BY Statement

BY variables;

You can specify a BY statement with PROC FASTCLUS to obtain separate analyses on observations in groups 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 your input data set is not sorted in ascending order, use one of the following alternatives:

- Sort the data using the SORT procedure with a similar BY statement.
- Specify the BY statement option NOTSORTED or DESCENDING in the BY statement for 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 using the DATASETS procedure.

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, there must be exactly the same BY groups in the same order in both data sets. 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 on the BY statement, refer to the discussion in *SAS Language Reference: Concepts*. For more information on the DATASETS procedure, refer to the discussion in the *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 ≤ 0 , 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

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 than 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 than in previous releases.
- The INSTAT= option reads a SAS data set previously created by the FAST-CLUS procedure 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

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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

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 original variables
- a new variable taking values from 1 to the value specified in the MAXCLUS-TERS= option, indicating the cluster to which each observation has been assigned. 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 square standard deviation for the cluster. See Chapter 23, "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 square standard deviation but based on pth power deviations instead of squared deviations:

LEAST=1 mean absolute deviation

LEAST=p root mean pth-power absolute deviation

LEAST=MAX maximum absolute deviation

If you specify the OUTITER option, there is one set of observations in the OUT-SEED= 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 .

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.

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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 27.2 and Table 27.3)
- 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 the following table.

Table 27.2. _TYPE_ Values for all LEAST= Options

TYPE	Contents of VAR variables	Contents of OVER_ALL
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	
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 non- missing value; these values are displayed in the "Cluster Sum- mary" table

Table 27.2. (continued)

TYPE	Contents of VAR variables	Contents of OVER_ALL
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 in the following table. Least-squares clustering is obtained by omitting the LEAST= option or by specifying LEAST=2.

Table 27.3. _TYPE_ Values for Least-Squares Clustering

TYPE	Contents of VAR variables	Contents of OVER_ALL
MEAN	Mean for the total sample; this is not displayed	Missing
STD	Standard deviation for the total sample; this is labeled "Total STD" in the output	Standard deviation pooled over all the VAR variables; this is la- beled "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^2 for predicting the variable from the clusters; this is labeled "R-Squared" in the output	R^2 pooled over all the VAR variables; this is labeled "R-Squared" in the output
RSQ_RATIO	$\frac{R^2}{1-R^2}$; this is labeled "RSQ/(1-RSQ)" in the output	$\frac{R^2}{1-R^2}$; labeled "RSQ/(1-RSQ)" in the output
PSEUDO_F	Missing	Pseudo F statistic
ESRQ	Missing	Approximate expected value of \mathbb{R}^2 under the null hypothesis of a single uniform cluster
CCC	Missing	The 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 nvcp 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 may 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 may not be necessary. Otherwise, some form of standardization is strongly recommended. The STANDARD procedure can standardize all variables to mean zero and variance one. The FACTOR or PRINCOMP procedures 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 may 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 other procedures such as PRINT, PLOT, CHART, 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 FAST-CLUS repeatedly with other procedures.

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

```
proc standard mean=0 std=1 out=stan;
    var v1 v2;
run;

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

proc plot;
    plot v2*v1=cluster;
run;

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

proc plot;
    plot v2*v1=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 standard mean=0 std=1 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 plot;
    plot can2*can1=cluster;
run;
```

If the data set is not too large, it may also be helpful to use

```
proc sort;
   by cluster distance;
run;
proc print;
   by cluster;
run;
```

to list the clusters. 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 by selecting cluster seeds from this output data set 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, the subsequent PROC FASTCLUS runs should specify the STRICT option to prevent the outliers from distorting the clusters.

You can use the OUTSEED= data set with the PLOT 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 values of _GAP_ 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 may 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

- 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 , and you omit the IRLS option, an additional column is displayed in the Iteration History table. The 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 square 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

- Total STD, the total standard deviation
- Within STD, the pooled within-cluster standard deviation

- R-Squared, the R^2 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

• Pseudo F Statistic,

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

where R^2 is the observed overall R^2 , c is the number of clusters, and n is the number of observations. The pseudo F statistic was suggested by Calinski and Harabasz (1974). Refer to 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 23.2 in Chapter 23, "The CLUSTER Procedure," for a comparison of pseudo F statistics.

- Observed Overall R-Squared, if you specify the SUMMARY option
- Approximate Expected Overall R-Squared, the approximate expected value of the overall R² 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^2 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

- 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 the following table. For more information on ODS, see Chapter 15, "Using the Output Delivery System."

Table 27.4. ODS Tables Produced in PROC FASTCLUS

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

Examples

Example 27.1. 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 fifty 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. An output data set is created, and PROC FREQ is invoked to compare the clusters with the species classification. See Output 27.1.1 and Output 27.1.2 for these results. For three clusters, you can use the CANDISC procedure to compute canonical variables for plotting the clusters. See Output 27.1.3 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.';
   symbol = put(species, specname10.);
   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
64 32 45 15 2 61 28 40 13 2 48 31 16 02 1 59 30 51 18 3
55 24 38 11 2 63 25 50 19 3 64 32 53 23 3 52 34 14 02 1
49 36 14 01 1 54 30 45 15 2 79 38 64 20 3 44 32 13 02 1
67 33 57 21 3 50 35 16 06 1 58 26 40 12 2 44 30 13 02 1
77 28 67 20 3 63 27 49 18 3 47 32 16 02 1 55 26 44 12 2
50 23 33 10 2 72 32 60 18 3 48 30 14 03 1 51 38 16 02 1
61 30 49 18 3 48 34 19 02 1 50 30 16 02 1 50 32 12 02 1
61 26 56 14 3 64 28 56 21 3 43 30 11 01 1 58 40 12 02 1
51 38 19 04 1 67 31 44 14 2 62 28 48 18 3 49 30 14 02 1
51 35 14 02 1 56 30 45 15 2 58 27 41 10 2 50 34 16 04 1
46 32 14 02 1 60 29 45 15 2 57 26 35 10 2 57 44 15 04 1
50 36 14 02 1 77 30 61 23 3 63 34 56 24 3 58 27 51 19 3
```

```
57 29 42 13 2 72 30 58 16 3 54 34 15 04 1 52 41 15 01 1
71 30 59 21 3 64 31 55 18 3 60 30 48 18 3 63 29 56 18 3
49 24 33 10 2 56 27 42 13 2 57 30 42 12 2 55 42 14 02 1
49 31 15 02 1 77 26 69 23 3 60 22 50 15 3 54 39 17 04 1
66 29 46 13 2 52 27 39 14 2 60 34 45 16 2 50 34 15 02 1
44 29 14 02 1 50 20 35 10 2 55 24 37 10 2 58 27 39 12 2
47 32 13 02 1 46 31 15 02 1 69 32 57 23 3 62 29 43 13 2
74 28 61 19 3 59 30 42 15 2 51 34 15 02 1 50 35 13 03 1
56 28 49 20 3 60 22 40 10 2 73 29 63 18 3 67 25 58 18 3
49 31 15 01 1 67 31 47 15 2 63 23 44 13 2 54 37 15 02 1
56 30 41 13 2 63 25 49 15 2 61 28 47 12 2 64 29 43 13 2
51 25 30 11 2 57 28 41 13 2 65 30 58 22 3 69 31 54 21 3
54 39 13 04 1 51 35 14 03 1 72 36 61 25 3 65 32 51 20 3
61 29 47 14 2 56 29 36 13 2 69 31 49 15 2 64 27 53 19 3
68 30 55 21 3 55 25 40 13 2 48 34 16 02 1 48 30 14 01 1
45 23 13 03 1 57 25 50 20 3 57 38 17 03 1 51 38 15 03 1
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;
proc candisc anova out=can;
   class cluster;
   var SepalLength SepalWidth PetalLength PetalWidth;
   title2 'Canonical Discriminant Analysis of Iris Clusters';
legend1 frame cframe=ligr label=none cborder=black
        position=center value=(justify=center);
axis1 label=(angle=90 rotate=0) minor=none;
axis2 minor=none;
proc gplot data=Can;
   plot Can2*Can1=Cluster/frame cframe=ligr
                  legend=legend1 vaxis=axis1 haxis=axis2;
   title2 'Plot of Canonical Variables Identified by Cluster';
run:
```

Output 27.1.1. 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	30.0000000	11.00000000	1.00000000
2	77.0000000	26.00000000	69.0000000	23.00000000

Minimum Distance Between Initial Seeds = 70.85196

Fisher (1936) Iris Data

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

Iteration History

| Relative Change in Cluster Seeds | | Relative

Convergence criterion is satisfied.

Criterion Based on Final Seeds = 5.0417

Cluster Summary

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

Statistics for Variables

L STD Within	STD R-Square	e RSQ/(1-RSQ)
55298 6.80	331 0.85247	5.778291
	28066 5.49 35866 3.70 55298 6.80 52238 3.57	28066 5.49313 0.562896 25866 3.70393 0.282716 25298 6.80331 0.852476 22238 3.57200 0.781868

Pseudo F Statistic = 513.92

Approximate Expected Over-All R-Squared = 0.51539

Cubic Clustering Criterion = 14.806

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

	I	Fisher (1936) Iris	Data	
Re	place=FULL Radius	The FASTCLUS Proces		ge=0.02
		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
	Clu	ster Standard Dev	iations	
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 F	REQ Proce	dure		
2	Table of C	LUSTER by	Species		
CLUSTER(Cluster) Species					
Frequency	7]				
Percent Row Pct					
Col Pct	Setosa	•	Virginic		
	ļ	or	a		
1	- + 50	3	++ 0	•	
	33.33		0.00	35	
	94.34		0.00		
	+	÷	++		
2	0	47	50	9	
	0.00	31.33 48.45	33.33 51.55	64.6	
	0.00	94.00	100.00		
m 1	+	+	++		
Total	50 33.33	50 33.33	50 33.33	100.0	

Output 27.1.2. Fisher's Iris Data: PROC FASTCLUS with MAXC=3 and PROC FREQ

	E	isher (1936) Iris	Data				
Re	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	77.0000000	38.00000000	67.0000000	22.00000000			
3	49.00000000	25.00000000	45.00000000	17.00000000			
	Minimum Distar	ace Between Initia	l Seeds = 38.23611				

Fisher (1936) Iris Data

The FASTCLUS Procedure

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

Iteration History

		Rel	ative Cha	nge in Clus	ter Seeds
Iteration	n Crite	erion	1	2	3
1	6.	7591 0	.2652	0.3205	0.2985
2	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 from Seed to Observation	Radius Exceeded	Nearest Cluster	Distance Between Cluster Centroids
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

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

Fisher (1936) Iris Data

The FASTCLUS Procedure
Replace=FULL Radius=0 Maxclusters=3 Maxiter=10 Converge=0.02

Cluster Means

Cluster	SepalLength	SepalWidth	PetalLength	PetalWidth
1	50.06000000	34.28000000	14.62000000	2.46000000
2	68.5000000	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							
2	Table of C	LUSTER by	Species					
CLUSTER(Cluster)	Specie	s					
		_						
Frequency	7							
Percent Row Pct	!							
Col Pct	 Setosa	Versicol	Virginic	Total				
332 133			a					
	·÷	+	+					
1		0		50				
	33.33		0.00	33.33				
	100.00	0.00	0.00					
	100.00	+	0.00					
2	i o		36	38				
	0.00	•	24.00	25.33				
	0.00	5.26	94.74					
	0.00	4.00	72.00					
3	-+ 0	+ 48	+					
3	0.00	32.00	14 9.33	62 41.33				
	0.00	77.42	22.58	11.33				
	0.00	96.00	28.00					
	·÷	+	+					
Total	50	50	50	150				
	33.33	33.33	33.33	100.00				

Output 27.1.3. Fisher's Iris Data: PROC CANDISC and PROC GPLOT

		Fisher (1936) Ir			
Ca	nonical Dia	scriminant Analy	sis of Iris C	lusters	
		The CANDISC Pro	gedure		
		THE CANDIDE FIC	cedure		
Observ	ations	150 DF	Total	149	
Variab	les	4 DF	Within Class	es 147	
Classe	s	3 DF	Between Clas	ses 2	
	(Class Level Info	rmation		
	Variable	e			
CLUSTER	Name	Frequency	Weight	Proportion	
1	1	50	50.0000	0.333333	
1 2	_1 _2	38	38.0000	0.253333	
3	3	62	62.0000	0.413333	
3	_5	02	02.0000	0.110000	

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.

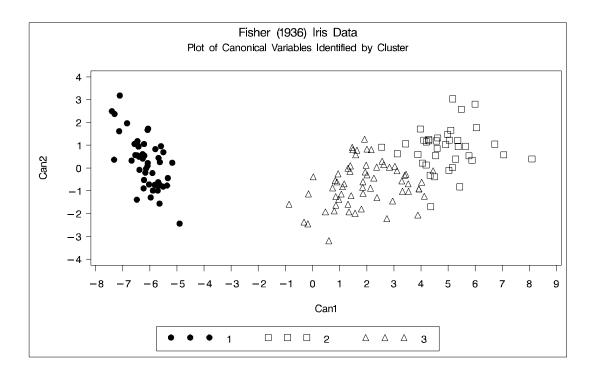
Fisher (1936) Iris Data Canonical Discriminant Analysis of Iris Clusters

The CANDISC Procedure

		C	Canonical orrelation	Adjusted Canonical Correlation	Approximate Standard Error	Canonica	1		
		1	0.976613	0.976123	0.003787	0.95377	4		
		2	0.550384	0.543354	0.057107	0.30292	:3		
		-	of Inv(E)*H /(1-CanRsq)			H0: The canor ent row and all			
					Likelihood	Approximate			
	Eigenvalue	Difference	Proportion	Cumulative	Ratio	F Value	Num DF	Den DF	Pr > F
1	20.6327	20.1981	0.9794	0.9794	0.03222337	164.55	8	288	<.0001
2	0.4346		0.0206	1.0000	0.69707749	21.00	3	145	<.0001
_	011010		0.0200		0.000.00.00				10000

The CANDISC Procedure Total Canonical Structure Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.831965 0.452137 SepalWidth Sepal Width in mm0.515092 0.810630 PetalIength Petal Length in mm. 0.995520 0.087514 PetalWidth Petal Midth in mm. 0.996325 0.087514 PetalWidth Petal Midth in mm. 0.996325 0.087514 Between Canonical Structure Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.956160 0.292846 SepalWidth Sepal Width in mm0.748136 0.663545 PetalLength Petal Length in mm. 0.998790 0.049580 PetalWidth Petal Width in mm. 0.998952 0.089883 Pooled Within Canonical Structure Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.339314 0.716082 SepalWidth Sepal Width in mm0.149614 0.914351 PetalLength Petal Length in mm. 0.000839 0.308136 PetalWidth Petal Width in mm. 0.0508123 0.404282 Fisher (1936) Iris Data Canonical Discriminant Analysis of Iris Clusters The CANDISC Procedure Total-Sample Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 0.097747341 0.900475563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Width in mm. 0.996451144 0.900475563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Width in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm4304161258 0.5442092294 PetalLength Sepal Length in mm4304161258 0.5442092294 PetalLength Petal Length in mm4304161258 0	Ca	nonical Discriminant Anal	lysis of Iris Clust	ers	
Variable Label Canl Can2		The CANDISC Pr	rocedure		
SepalLength Sepal Length in mm.		Total Canonical	Structure		
SepalWidth Sepal Width in mm.	Variable	Label	Can1	Can2	
PetalLength	SepalLength	Sepal Length in mm.	0.831965	0.452137	
Detail Width Petal Width in mm. 0.966325 0.154745	SepalWidth	Sepal Width in mm.	-0.515082	0.810630	
Detween Canonical Structure	PetalLength	Petal Length in mm.	0.993520	0.087514	
Variable Label Canl Can2	PetalWidth	Petal Width in mm.	0.966325	0.154745	
SepalLength Sepal Length in mm. 0.955160 0.292846		Between Canonical	Structure		
SepalWidth Sepal Width in mm.	Variable	Label	Can1	Can2	
SepalWidth Sepal Width in mm.					
PetalLength					
PetalWidth	=	=			
Pooled Within Canonical Structure	_				
Variable Label Can1 Can2	Petaiwidth	recal width in mm.	0.995952	0.009003	
SepalLength Sepal Length in mm. 0.339314 0.716082		Pooled Within Canoni	cal Structure		
SepalWidth Sepal Width in mm.	Variable	Label	Can1	Can2	
PetalLength	SepalLength	Sepal Length in mm.	0.339314	0.716082	
PetalLength			0 1 10 11 1		
Fisher (1936) Iris Data Canonical Discriminant Analysis of Iris Clusters The CANDISC Procedure Total-Sample Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	SepalWidth	Sepal Width in mm.	-0.149614	0.914351	
The CANDISC Procedure Total-Sample Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	_				
The CANDISC Procedure Total-Sample Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength	Petal Length in mm.	0.900839	0.308136	
The CANDISC Procedure Total-Sample Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength	Petal Length in mm.	0.900839	0.308136	
Total-Sample Standardized Canonical Coefficients Variable	PetalLength PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) 1	0.900839 0.650123	0.308136 0.404282	
Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Canl Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) 1	0.900839 0.650123	0.308136 0.404282	
SepalLength Sepal Length in mm. 0.047747341 1.021487262 SepalWidth Sepal Width in mm. -0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm. -4304161258 0.6442092294 PetalLength Petal Length in mm. 0.7976741592 -3063023132	PetalLength PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) Inonical Discriminant Anal	0.900839 0.650123 Tris Data Lysis of Iris Clust	0.308136 0.404282	
SepalWidth Sepal Width in mm. -0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563	PetalLength PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) Inonical Discriminant Anal	0.900839 0.650123 Cris Data Lysis of Iris Clust	0.308136 0.404282	
SepalWidth Sepal Width in mm. -0.577569244 0.864455153 PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563	PetalLength PetalWidth Ca	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (0.900839 0.650123 Tris Data Lysis of Iris Clust Cocedure	0.308136 0.404282	
PetalLength Petal Length in mm. 3.341309573 -1.283043758 PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm. -4304161258 0.6442092294 PetalLength Petal Length in mm. 0.7976741592 -3063023132	PetalLength PetalWidth Ca To Variable	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Canonical Coefficie	0.308136 0.404282 ers	
PetalWidth Petal Width in mm. 0.996451144 0.900476563 Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth Ca To Variable SepalLength	Petal Length in mm. Petal Width in mm. Fisher (1936) 1 nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Canonical Coefficie Can1 0.047747341	0.308136 0.404282 ers ents Can2 1.021487262	
Pooled Within-Class Standardized Canonical Coefficients Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm.	0.900839 0.650123 Tris Data Lysis of Iris Clust Cocedure Canonical Coefficie Can1 0.047747341 -0.577569244	0.308136 0.404282 eers canz 1.021487262 0.864455153	
Variable Label Can1 Can2 SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm. 4304161258 0.6442092294 PetalLength Petal Length in mm. 0.7976741592 3063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Canonical Coefficie Can1 0.047747341 -0.577569244 3.341309573	0.308136 0.404282 ers can2 1.021487262 0.864455153 -1.283043758	
SepalLength Sepal Length in mm. 0.0253414487 0.5421446856 SepalWidth Sepal Width in mm. 4304161258 0.6442092294 PetalLength Petal Length in mm. 0.7976741592 3063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Canonical Coefficie Can1 0.047747341 -0.577569244 3.341309573	0.308136 0.404282 ers can2 1.021487262 0.864455153 -1.283043758	
SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm. Petal Width in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust cocedure Canonical Coefficie Can1 0.047747341 -0.577569244 3.341309573 0.996451144	0.308136 0.404282 ers Can2 1.021487262 0.864455153 -1.283043758 0.900476563	
SepalWidth Sepal Width in mm4304161258 0.6442092294 PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength PetalWidth PetalWidth	Petal Length in mm. Petal Width in mm. Fisher (1936) Inonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm. Petal Length in mm. Petal Width in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Can1 0.047747341 -0.577569244 3.341309573 0.996451144 ed Canonical Coeffi	0.308136 0.404282 ers Can2 1.021487262 0.864455153 -1.283043758 0.900476563	
PetalLength Petal Length in mm. 0.79767415923063023132	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength PetalWidth Pooled Variable	Petal Length in mm. Petal Width in mm. Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm. Petal Width in mm. Petal Width in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Cannonical Coefficie Can1 0.047747341 -0.577569244 3.341309573 0.996451144 Ed Canonical Coefficient Can1	0.308136 0.404282 ers Can2 1.021487262 0.864455153 -1.283043758 0.900476563	
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PetalWidth Petal Width in mm. 0.3205998034 0.2897207865	PetalLength PetalWidth Ca To Variable SepalLength SepalWidth PetalLength PetalWidth Pooled Variable SepalLength SepalWidth	Fisher (1936) I nonical Discriminant Anal The CANDISC Pr tal-Sample Standardized (Label Sepal Length in mm. Sepal Width in mm. Petal Length in mm. Petal Length in mm. Within-Class Standardize Label Sepal Length in mm.	0.900839 0.650123 Cris Data Lysis of Iris Clust Cocedure Can1 0.047747341 -0.577569244 3.341309573 0.996451144 ed Canonical Coeffication	0.308136 0.404282 ers Can2 1.021487262 0.864455153 -1.283043758 0.900476563 .cients Can2 0.5421446856 0.6442092294	

Variable Label 0.0057661265 0.1233581748 -.1325106494 0.1983303556 0.1892773419 -.0726814163 0.1307270927 0.1181359305 Sepal Length in mm. 0.0057661265 Sepal Width in mm. -.1325106494 Petal Length in mm. 0.1892773419 SepalLength SepalWidth PetalLength PetalWidth Petal Width in mm. 0.1307270927 0.1181359305 Class Means on Canonical Variables CLUSTER Can1 Can2 -6.131527227 0.244761516 4.931414018 0.861972277 2 3 1.922300462 -0.725693908



Example 27.2. Outliers

The second example involves data artificially generated to contain two clusters and several severe outliers. A preliminary analysis specifies twenty 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 ten or fifty initial clusters. Examination of the plot suggests that clusters with more than five (again, the exact number is not important) observations may 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 results are displayed in Output 27.2.1 through Output 27.2.4.

```
Create artificial data set with two clusters
                                                           */
/*
     and some outliers.
                                                           */
data x;
title 'Using PROC FASTCLUS to Analyze Data with Outliers';
   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:
/* Run PROC FASTCLUS with many clusters and OUTSEED= output */
/* data set for diagnostic plot.
title2 'Preliminary PROC FASTCLUS Analysis with 20 Clusters';
proc fastclus data=x outseed=mean1 maxc=20 maxiter=0 summary;
   var x y;
run;
legend1 frame cframe=ligr label=none cborder=black
        position=center value=(justify=center);
axis1 label=(angle=90 rotate=0) minor=none order=(0 to 10 by 2);
axis2 minor=none ;
proc gplot data=mean1;
     plot _gap_*_freq_ _radius_*_freq_ /overlay frame
     cframe=ligr vaxis=axis1 haxis=axis2 legend=legend1;
run;
```

Output 27.2.1. Preliminary Analysis of Data with Outliers: PROC FASTCLUS and PROC GPLOT

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

Cluster Summary

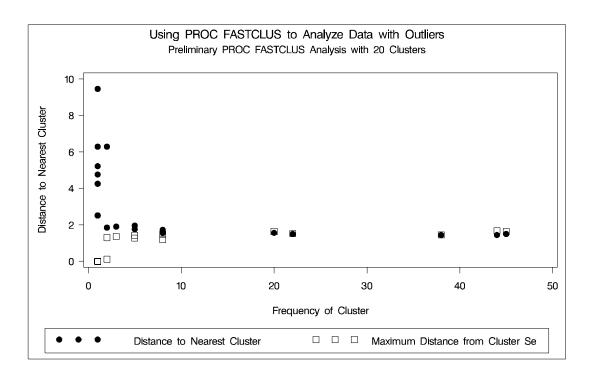
			Maximum Distance			
		RMS Std	from Seed	Radius	Nearest	Distance Between
Cluster	Frequency	Deviation	to Observation	Exceeded	Cluster	Cluster Centroids
1	 8	0.4753	1.1924		19	1.7205
2	1		0		6	6.2847
3	44	0.6252	1.6774		5	1.4386
4	1		0		20	5.2130
5	38	0.5603	1.4528		3	1.4386
6	2	0.0542	0.1085		2	6.2847
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

Approximate Expected Over-All R-Squared = 0.96103

Cubic Clustering Criterion = -2.503

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



```
/*
         Remove low frequency clusters. */
data seed;
   set mean1;
   if _freq_>5;
run;
   /*
        Run PROC FASTCLUS again, selecting seeds from the
                                                                    */
   /*
        high frequency clusters in the previous analysis
                                                                    */
                                                                    */
        using LEAST=1 Clustering Criterion
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;
legend1 frame cframe=ligr label=none cborder=black
        position=center value=(justify=center);
axis1 label=(angle=90 rotate=0) minor=none;
axis2 minor=none;
proc gplot data=out;
   plot y*x=cluster/frame cframe=ligr
                  legend=legend1 vaxis=axis1 haxis=axis2;
run;
```

Output 27.2.2. 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

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

Number of Bins = 100

Iteration History

		Maximum		ve Change ster Seeds
Iteration	Criterion	Bin Size	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.

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

Criterion Based on Final Seeds =

Cluster Summary

1.0771

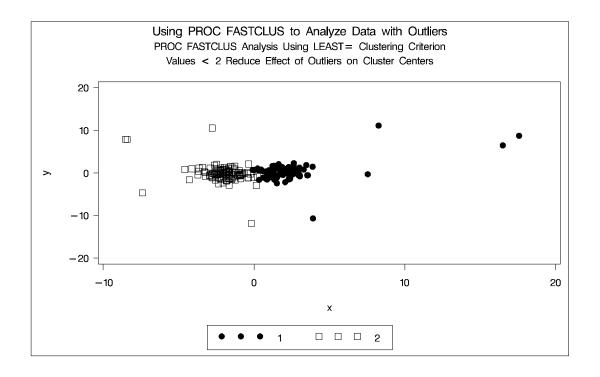
Cluster	Frequency	Mean Absolute Deviation	Maximum Distance from Seed to Observation	Radius Exceeded	Nearest Cluster	Distance Between Cluster Medians
1	102	1.1278	24.1622		2	4.2585
2	108	1.0494	14.8292		1	4.2585

Cluster Medians

Cluster	x	У
1	1.923023887	0.222482918
2	-1.826721743	-0.286253041

Mean Absolute Deviations from Final Seeds

Cluster	x	У
1	1.113465261	1.142120480
2	0.890331835	1.208370913



```
/*
        Run PROC FASTCLUS again, selecting seeds from the
                                                                  */
        high frequency clusters in the previous analysis
                                                                  */
        STRICT= prevents outliers from distorting the results.
                                                                 */
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 gplot data=out;
   plot y*x=cluster/frame cframe=ligr
                  legend=legend1 vaxis=axis1 haxis=axis2;
run;
```

Output 27.2.3. Cluster Analysis with Outliers Omitted: PROC FASTCLUS and PROC GPLOT

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	У
1	2.794174248	-0.065970836
2	-2.027300384	-2.051208579

Criterion Based on Final Seeds = 0.9515

Cluster Summary

Cluster	Frequency	RMS Std Deviation	from Seed to Observation	Radius Exceeded	Nearest Cluster	Distance Between Cluster Centroids
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
У	1.02113	1.00352	0.039093	0.040683
OVER-ALL	1.63119	0.93959	0.669891	2.029303

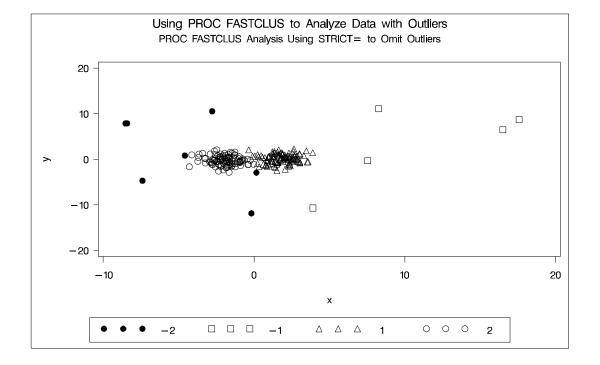
Pseudo F Statistic = 397.74

Approximate Expected Over-All R-Squared = 0.60615

Cubic Clustering Criterion = 3.197

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

```
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
                   Cluster Means
      Cluster
        1
                 1.825111432
                                 0.141211701
                 -1.919910712
                                 -0.261558725
             Cluster Standard Deviations
      Cluster
      .
                  0.889549271
                                  1.006965219
        2
                  0.852000588
                                  1.000062579
```



Output 27.2.4. Final Analysis with Outliers Assigned to Clusters: PROC FAST-CLUS and PROC GPLOT

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

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 above values are invalid for correlated variables.

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

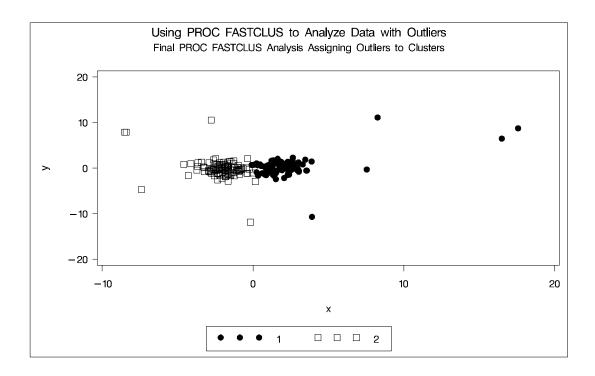
Cluster Means

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



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