

PRINCIPAL COMPONENTS ANALYSIS (PCA)*

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Abstract—Principal Components Analysis (PCA) as a method of multivariate statistics was created before the Second World War. However, the wider application of this method only occurred in the 1960s, during the "Quantitative Revolution" in the Natural and Social Sciences.

The main reason for this time-lag was the huge difficulty posed by calculations involving this method. Only with the advent and development of computers did the almost unlimited application of multivariate statistical methods, including principal components, become possible.

At the same time, requirements arose for precise numerical methods concerning, among other things, the calculation of eigenvalues and eigenvectors, because the application of principal components to technical problems required absolute accuracy.

On the other hand, numerous applications in Social Sciences gave rise to a significant increase in the ability to interpret these nonobservable variables, which is just what the principal components are. In the application of principal components, the problem is not only to do with their formal properties but above all, their empirical origins.

The authors considered these two tendencies during the creation of the program for principal components. This program—entitled PCA—accompanies this paper. It analyzes consecutively, matrices of variance-covariance and correlations, and performs the following functions:

- the determination of eigenvalues and eigenvectors of these matrices,
- the testing of principal components,
- the calculation of coefficients of determination between selected components and the initial variables, and the testing of these coefficients,
- the determination of the share of variation of all the initial variables in the variation of particular components,
- construction of a dendrite for the initial set of variables,
- the construction of a dendrite for a selected pattern of the principal components,
- the scatter of the objects studied in a selected coordinate system.

Thus, the PCA program performs many more functions especially in testing and graphics, than PCA programs in conventional statistical packages. Included in this paper are a theoretical description of principal components, the basic rules for their interpretation and also statistical testing.

Key Words: Principal Components Analysis, Variance-covariance matrix, Coefficients of determination, Eigenvalues, Eigenvectors, Correlation matrix, Bartlett's statistics, FORTRAN 77.

DESCRIPTION OF THE PRINCIPAL COMPONENTS METHOD

The basic aim of the analysis utilizing principal components is a reduction of the dimensions of the observation space in which given objects are studied (Kendall, 1983; Jackson and Hearne, 1973). The reduction is obtained by creating new linear combinations of variables characterizing the objects studied. These combinations, termed principal components, must satisfy certain mathematical and statistical conditions. They will be discussed in detail in subsequent sections.

The starting point in the principal components method is an observation matrix \mathbf{X} in which column

vectors list observations characterizing an object with respect to random variables X_1, X_2, \dots, X_p .

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{1n} \\ x_{21} & x_{12} & \cdots & x_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ x_{p1} & x_{p2} & \cdots & x_{pn} \end{bmatrix}.$$

Each column vector represents a point in a p -dimensional space. Because the observation matrix \mathbf{X} is compiled for a sample of the entire population (numbers p and n are finite), the variance-covariance matrix \mathbf{S} derived from observations of random variables is an estimator of general variance-covariance matrix Σ , whereas the vector of mean values $\bar{\mathbf{x}}$ is an estimator of the general vector \mathbf{U} . Thus as mentioned the task of the principal components method is to determine linear combinations with a maximum

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variance. Thus, the problem essentially is replacing the set of initial variables with their linear combinations, that is new variables with special properties. These new variables are termed principal components and are written in the form:

$$\mathbf{V} = \mathbf{A}'\mathbf{X} \quad (1)$$

where

\mathbf{V} is a matrix of the new variables,

\mathbf{A} is a matrix of orthonormal eigenvectors of matrix \mathbf{S} , and

\mathbf{X} is the observation matrix.

Transformation (1) is possible after determinantal Equation (2) has been solved.*

$$|\mathbf{S} - l\mathbf{I}| = 0 \quad (2)$$

where

\mathbf{S} is a variance-covariance matrix of order $(p \times p)$,

l is the characteristic root of the determinantal equation, and

\mathbf{I} is a unit matrix of order $(p \times p)$.

Equation (2) is a polynomial of degree p with respect to unknown l , hence it has p roots which can be ordered in such a way that

$$l_1 \geq l_2 \geq l_3 \geq \cdots \geq l_p \geq 0.$$

Because there is an orthonormal column eigenvector \mathbf{A}_i corresponding to each root l_i , the variable V_i derived from Equation (2) has the maximum value l_1 (maximum variance) and is termed the first principal component.

Because the sum $l_1 + l_2 + \cdots + l_p = \text{tr } \mathbf{S}$ and is equal to the sum of the variances of matrix \mathbf{S} (i.e. $\sigma_{11} + \sigma_{22} + \cdots + \sigma_{pp}$), l_1, l_2, \dots, l_p defines the share of variability of particular principal components in the total variance of matrix \mathbf{S} . If we consider the quotients

$$\frac{l_1}{\text{tr } \mathbf{S}} 100, \quad \frac{l_2}{\text{tr } \mathbf{S}} 100, \quad \dots, \quad \frac{l_p}{\text{tr } \mathbf{S}} 100, \quad (3)$$

we get the percent share of each component in the variance of matrix \mathbf{S} . The algorithm for the calculation of principal components is such that this is a decreasing sequence, which indicates that $l_1/\text{tr } \mathbf{S} 100$ is the largest quantity. Quantity l_2 corresponds to variable V_2 , which therefore is termed the second principal component. It is clear that there are as many principal components as initial variables.

Each root l_i has its corresponding column vector A_i , such that

$$(\mathbf{S} - l\mathbf{I})\mathbf{A}_i = 0 \quad \text{or} \quad \mathbf{S}\mathbf{A}_i = l_i\mathbf{A}_i. \quad (4)$$

*It also is possible to derive principal components by substituting the variance-covariance matrix \mathbf{S} with correlation matrix \mathbf{R} , that is by solving the equation $|\mathbf{R} - l\mathbf{I}| = 0$.

Because vectors $\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_p$ are orthonormal, that is

$$\mathbf{A}'_i \mathbf{A}_i = 1, \quad \mathbf{A}'_j \mathbf{A}_i = 0 \quad \text{for } i \neq j, \quad (5)$$

and they satisfy (2) and (4), we have

$$\mathbf{A}'_i \mathbf{S} \mathbf{A}_i = l_i, \quad \mathbf{A}'_i \mathbf{S} \mathbf{A}_j = 0 \quad \text{for } i \neq j, \quad (6)$$

$$\mathbf{I} = \mathbf{A}_1 \mathbf{A}'_1 + \cdots + \mathbf{A}_p \mathbf{A}'_p \quad (7)$$

and

$$\mathbf{S} = l_1 \mathbf{A}_1 \mathbf{A}'_1 + l_2 \mathbf{A}_2 \mathbf{A}'_2 + \cdots + l_p \mathbf{A}_p \mathbf{A}'_p. \quad (8)$$

Expression (8) is termed a spectral decomposition of a matrix \mathbf{S} .

The basic property of the new variables is the lack of correlation among them (in contrast to the initial variables). The variance of the i th component is l_i , or

$$\text{Var}(\mathbf{A}_i \mathbf{X}) = l_i, \quad (9)$$

whereas

$$\text{Cov}(\mathbf{A}_i \mathbf{X}, \mathbf{A}_j \mathbf{X}) = 0 \quad \text{for } i \neq j.$$

Because the primary aim of principal components analysis is the reduction of the dimensions of the observation space, it is necessary at some stage to decide on how many new variables should be taken into account further study. To help with the decision, the ratio of characteristic roots to the trace of the matrix is considered. For example, if the expression $l_1/\text{tr } \mathbf{S} 100$ has a great value (e.g. 90%), the set of initial variables is replaced with the first component V_1 . When the ratio is not so high, the next components are taken into account. Naturally, the elimination of some components from further analysis cannot follow solely from the researcher's subjective evaluation of the $l_i/\text{tr } \mathbf{S} 100$ quotient, but must result from the testing of the components. This problem is discussed in detail in the next section.

An important issue in Principal Components Analysis is the interpretation of the components, to help determine, after the reduction of the observation space, which initial variables have the greatest shares in the variance of particular principal components. This information can be obtained using coefficients of determination established between the components and the initial variables. It should be added that interpretation of the components differs slightly depending on whether \mathbf{S} or \mathbf{R} is used.

Interpretation of principal components derived from variance-covariance matrix \mathbf{S}

The coefficient of correlation between the i th component and the j th initial variable is defined by the equation:

$$r_{ij} = \frac{a_{ij} \sqrt{l_i}}{S_j}. \quad (10)$$

Hence the coefficient of determination has the form:

$$r_{ij}^2 = \frac{a_{ij}^2 l_i}{S_j^2}, \quad (11)$$

where a_{ij}^2 is the square of the element of the eigenvector A_i corresponding to the i th component and j th initial variable, l_i is the variance of the i th component, and S_j^2 is the variance of variable j .

On the basis of (8) and (9), making use of the variances and eigenvectors of all the principal components, it is possible to reconstruct the variance-covariance matrix \mathbf{S} . Naturally, the product $l_i \mathbf{A}_i \mathbf{A}'_i$ has the greatest share in this reconstruction. Moreover, in for example matrix $l_i \mathbf{A}_i \mathbf{A}'_i$ the elements on the main diagonal are estimates (supplied with the help of the first component) of the variance of the j th initial variable, which can be computed from a general expression:

$$\text{Var } X_j = l_i a_{ij}^2, \quad (12)$$

whereas the remaining elements are estimates of covariance, with the final element (matrix) of spectral decomposition $l_p \mathbf{A}_p \mathbf{A}'_p$ bringing the estimated variance and covariance up to real values. Given (12), (11) can be written in the form:

$$r_{ij}^2 = \frac{\text{Var } X_j}{\text{Var } X_j} = \frac{\hat{S}_j^2}{S_j^2}. \quad (13)$$

It is clear that the coefficient of determination between component i and variable j is a ratio of the estimated variance of variable j to its real variance. If we consider any (i th) matrix from the spectral decomposition, then, by summing up the elements on the main diagonal

$$\sum_{j=1}^p \hat{S}_j^2 = \sum_{j=1}^p l_i a_{ij}^2$$

$$\sum_{j=1}^p \hat{S}_j^2 = l_i \sum_{j=1}^p a_{ij}^2$$

we get

$$\sum_{j=1}^p \hat{S}_j^2 = l_i. \quad (14)$$

Thus, by adding together the estimated variances of particular variables we arrive at the variance of the i th component. This relationship can be the theoretical basis for the interpretation of the components. Using (14), we can write (3) alternatively as

$$\frac{\sum_{j=1}^p \hat{S}_j^2}{\text{tr } \mathbf{S}} 100. \quad (15)$$

Expression (15) assumes the greatest value for the first component; however, this measure should be used carefully. It follows from (14) that almost the entire variance of the i th component is made up of the estimated variance of a single variable, for example one that has a high absolute value in comparison with the remaining ones, that is one with high variance. Hence the necessity of a skillful formulation of the observation matrix, variables of which should be of a similar order of measure (15), the following dependence is proposed for use in the interpretation

of the components:

$$w = \frac{\sum_{i,j} r_{ij}^2}{p} 100 \quad (16)$$

where p is the number of variables of the observation matrix, and r_{ij}^2 is the coefficient of the determination between the i th component and j th initial variable.

Equation (16) shows the percent of the variance of all the variables accounted for by the i th component. The results of measure (16) applied to components derived from the covariance matrix are as a rule lower than those of measure (15), because in reality one (e.g. the first) component seldom accounts for more than 50% of the variance of all the variables included in the observation matrix. When a variable in the observation matrix exceeds all others markedly in value, expression (15) gives a high value of the first component, and expression (16) a low one. It is so because the variance of the component depends in this situation on a single variable only, and may not be the most important one either (its significance depends solely on the adopted units of measurement). As can be seen, expression (16) shows the actual share of the i th component in the variance of all the variables. It is worth noting that the numerator of (16) is easy to calculate because the following equation holds:

$$\sum_{i,j} r_{ij}^2 = l_i \sum_{j=1}^p \frac{a_{ij}^2}{S_j^2}. \quad (17)$$

The variance of all the initial variables is accounted for by the component if:

$$\sum_{i,j} r_{ij}^2 = l_i \sum_{j=1}^p \frac{a_{ij}^2}{S_j^2} = p.$$

Interpretation of principal components derived from the correlation matrix \mathbf{R}

The discrepancies between evaluations of principal components obtained on the basis of formulae (15) and (16) do not occur if we derive them from a correlation matrix (i.e. if use is made of normalized initial variables). This is so because the following dependencies hold by virtue of an appropriate transformation of the covariance matrix (Anderson, 1958):

$$r_{ij} = a_{ij} \sqrt{l_i}, \quad (18)$$

$$r_{ij}^2 = a_{ij}^2 l_i, \quad (19)$$

$$\sum_{i,j} r_{ij}^2 = \sum_{i,j} a_{ij}^2 l_i,$$

$$\sum_{i,j} r_{ij}^2 = l_i. \quad (20)$$

Or,

$$\frac{l_i}{\text{tr } \mathbf{S}} 100 = \frac{\sum_{i,j} r_{ij}^2}{p} 100.$$

Thus, when the correlation matrix is used, in order to determine what part of the variance of all the initial

variables is accounted for (in percent) by the i th component, it is possible to employ either measure (15) or (16). There is no such optionality in the situation of the variance-covariance matrix.

TESTING PRINCIPAL COMPONENTS

Because matrices \mathbf{S} and \mathbf{R} are only estimators of matrices Σ and \mathbf{P} (covering the entire population), the results obtained must be subjected to a verification procedure. There are several approaches to the testing of principal components (cf. Mardia, Kent, and Bibby, 1979; Anderson, 1984). They are discussed next and then used in the program. It must be emphasized that the tests used in this program are based on the asymptotic distributions of the roots and vectors of variance-covariance and correlation matrices. Thus, the size of the sample used in the calculation process may have considerable influence on the results of the testing (see Anderson, 1984, p. 468).

Testing principal components derived from variance-covariance matrix \mathbf{S}

Testing the hypothesis about the ratio of the sum of the least characteristic roots to the sum of all roots. If the sum of the characteristic roots of a few final components with relation to the trace of matrix \mathbf{S} is relatively small, then there is a justifiable temptation to eliminate these components from further analysis. They can be rejected after the following hypothesis has been verified:

$$H_0: f(\lambda) = \frac{\lambda_{k+1} + \dots + \lambda_p}{\lambda_1 + \dots + \lambda_p} \geq \delta \quad (21)$$

against an alternative hypothesis:

$$H_1: f(\lambda) < \delta,$$

where δ is assumed known.

The asymptotic variance $f(\mathbf{l})$ is determined from the equation:

$$2 \left(\frac{\delta}{\text{tr } \Sigma} \right)^2 (\lambda_1^2 + \dots + \lambda_k^2) + 2 \left(\frac{1-\delta}{\text{tr } \Sigma} \right)^2 (\lambda_{k+1}^2 + \dots + \lambda_p^2). \quad (22)$$

Hypothesis H_0 is rejected if $\sqrt{n} [f(\mathbf{l}) - \delta]$ is smaller than the corresponding point of the standardized normal distribution multiplied by the root from (22) in which estimators are substituted for real values, that is:

$$2 \left(\frac{\delta}{\text{tr } \mathbf{S}} \right)^2 (l_1^2 + \dots + l_k^2) + 2 \left(\frac{1-\delta}{\text{tr } \mathbf{S}} \right)^2 (l_{k+1}^2 + \dots + l_p^2) \quad (23)$$

whereas

$$f(\mathbf{l}) = \frac{l_{k+1} + \dots + l_p}{l_1 + \dots + l_p}.$$

Determination of the confidence interval for the proportion of variance accounted for the successive principal components. The point value of the proportion of variance accounted for by successive principal components is determined from the equation:

$$\hat{\psi} = \frac{l_1 + \dots + l_k}{l_1 + \dots + l_p}. \quad (24)$$

However, the determination of the confidence interval for quantity $\hat{\psi}$ may supply further significant information about the boundary values of the interval in which the true value of ψ may be contained.

Assuming that

$$\hat{\alpha} = \frac{l_1^2 + \dots + l_k^2}{l_1^2 + \dots + l_p^2},$$

the variance of estimator $\hat{\psi}$ is calculated from the equation:

$$\hat{\tau}^2 = \frac{2 \text{tr } \mathbf{S}^2}{(n-1)(\text{tr } \mathbf{S})^2} (\hat{\psi}^2 - 2\hat{\alpha}\hat{\psi} + \hat{\alpha}^2). \quad (25)$$

In turn, the confidence interval of $\hat{\psi}$ (for $\alpha = 0.05$) has the form:

$$\hat{\psi} \pm 1.96(\hat{\tau}^2)^{1/2}. \quad (26)$$

Testing the hypothesis that $(p-k)$ eigenvalues of matrix Σ are equal. After p principal components have been determined, it is advisable to verify the hypothesis that $(p-k)$ eigenvalues are equal. Such a situation is termed isotropy and may suggest that variance is equal in all the directions of $(p-k)$ -dimensional space spanned by the last $(p-k)$ eigenvectors. The test helps determine the number of principal components used to describe objects under study.

In the testing procedure use is made of Bartlett's asymptotic approximation:

$$\left(n - \frac{2p+11}{6} \right) (p-k) \log \left(\frac{a_0}{g_0} \right) \sim \chi^2(p-k+2)(p-k-1)/2 \quad (27)$$

where

$$a_0 = \frac{l_{k+1} + \dots + l_p}{p-k}, \quad g_0 = (l_{k+1} \times \dots \times l_p)^{1/(p-k)},$$

n is the number of observations, and the number of degrees of freedom is calculated from the equation: $df = \frac{1}{2}(p-k+2)(p-k+1)$.

With the help of statistics (27) the zero hypothesis about the equality of eigenvalues of matrix Σ is tested:

$$H_0: \lambda_p = \lambda_{p-1} = \dots = \lambda_{k+1}.$$

Hypothesis H_0 usually is tested sequentially, taking $k=0, k=1$, etc. If $\chi^2_{\text{obs}} \geq \chi^2_{\text{tab}}$, then H_0 is rejected.

Testing principal components derived from correlation matrix \mathbf{R}

Testing the hypothesis that $(p-k)$ least eigenvalues of matrix \mathbf{P} are equal. When principal components are derived from correlation matrix \mathbf{R} (which is the

estimator of the general correlation matrix \mathbf{P}), to test the hypothesis that $(p - k)$ of its eigenvalues are equal use is made of Bartlett's statistics having the form:

$$(n - 1)(p - k) \log\left(\frac{a_0}{g_0}\right), \quad (28)$$

where

$$a_0 = \frac{l_{k+1} + \cdots + l_p}{p - k},$$

$$g_0 = (l_{k+1} \times \cdots \times l_p)^{1/(p-k)}, \quad 0 < k < p - 1.$$

This expression can be treated as chi-square with $\frac{1}{2}(p - k + 2)(p - k - 1)$ degrees only if the first k components account for a relatively large portion of variance. This statistic is used to test the hypothesis:

$$H_0: \lambda_p = \lambda_{p-1} = \cdots = \lambda_{k+1}.$$

If $\chi^2_{\text{obs}} \geq \chi^2_{\alpha, df}$, then hypothesis H_0 is rejected.

INSTRUCTIONS FOR THE PCA SYSTEM

The Principal Components Analysis program (henceforth termed PCA) has been written in the FORTRAN-77 programming language. Being fully compatible with the FORTRAN-77 standard it can be used without further modifications on any computer equipped with a compiler of this language.

The high quality of the compilers used and the carefully selected (and tested) numerical procedures performing the main part of the calculations should guarantee a reliable and efficient performance of the program.

In this paper the PCA program is presented in the Appendix together with some comments relative to the Operating System DOS (for the IBM PC).

System requirements

The basis for a successful run of the PCA on IBM PC type machines is compliance with the system requirements and the constraints of the operating system DOS 3.30 (or later).

The PCA system is designed to be used in machines with at least 640 kbyte of random access memory (RAM). It does not use extended memory (provided that the user has not changed parameter settings in the beginning of the source code). If it is to be run in a given PC system, it is necessary to modify (once) the CONFIG.SYS file stored in this system by introducing into it the sentences

FILES = 20

BUFFERS = 10.

This is an indispensable modification, because the operation of the PCA program utilizes many more files simultaneously than the DOS standard allows.

Each time the PCA system is initiated, all programs residing in the RAM (e.g. Side-Kick, Norton Commander, etc.) should be removed.

Data preparation

In order to simplify as much as possible the process of data input and the derivation of results in the PCA system, a "file-to-file" method of information transmission has been introduced. Thus data can be prepared earlier, independently of the system in question, using an appropriate wordprocessor and stored in a file with a specified name facilitating its identification. The results, in turn (also made into a file), also can be inspected, analyzed, or printed independently of the PCA system (with reservations as discussed). Further on, we present a sample data file 'd1-pca' which will serve to demonstrate how to operate the PCA program and how it runs. This file has been prepared according to a pattern which must be followed in any other data file.

6						
29						
1.08	7.43	0.60	1.27	8.00	0.36	
1.00	9.01	0.71	1.08	9.01	0.36	
1.13	7.19	0.49	1.24	8.14	0.40	
1.03	6.24	0.55	1.82	6.63	0.47	
1.04	7.07	0.57	1.50	7.35	0.38	
1.17	7.63	0.59	0.88	8.90	0.42	
0.89	7.16	0.67	1.38	6.37	0.33	
1.04	9.05	0.65	1.60	9.40	0.38	
1.04	10.23	0.81	1.80	10.60	0.37	
1.15	6.49	0.51	0.95	7.49	0.41	
1.13	6.24	0.43	1.11	7.06	0.40	
1.14	6.38	0.53	1.23	7.26	0.41	
1.05	7.21	0.63	1.20	7.54	0.38	
1.15	6.97	0.54	0.95	7.99	0.40	
1.06	7.07	0.53	1.13	7.49	0.38	
1.03	7.31	0.67	1.17	7.49	0.36	
1.05	8.63	0.62	1.38	9.09	0.39	
1.06	6.05	0.46	1.29	6.42	0.38	
1.05	7.86	0.45	2.09	8.28	0.37	
1.19	5.34	0.42	0.93	6.33	0.43	
0.95	6.76	0.49	1.63	6.44	0.35	
1.12	6.37	0.53	1.0	7.13	0.39	
0.95	5.63	0.53	1.60	5.34	0.33	
0.94	7.46	0.55	1.82	6.92	0.33	
1.04	6.76	0.53	1.08	7.26	0.39	
1.04	8.27	0.67	1.27	8.62	0.38	
1.07	9.12	0.51	1.07	9.75	0.38	
1.05	9.01	0.74	1.38	9.49	0.39	
1.04	6.95	0.51	1.50	7.22	0.35	

There is a single figure in the first row of the 'd1-pca' file (further on interpreted as P —the number of variables) satisfying the condition $1 \leq P \leq 50$.

The second row contains one integer (N —the number of objects) which satisfies the condition $3 \leq N \leq 200$.

Next come elements of the observation matrix (in lexicographic order) in such a way that the figure placed in the i th row in the j th position represents the value of the j th variable of the i th object.

The PCA system does not destroy the input data file.

The operation of the system and its control

Let us assume, for the sake of simplicity, that the PCA system to be operated appears, together with a suitable data file, on a selected path of a hard disc, and that the output file will be put on this path, too. To start the system, the user should write the name

PCA

and press the ENTER key. The course which the computation process will take depends crucially on the user's answers to questions asked by the system. The final part of this documentation contains an example of a dialog with the system and the results for which it provided a basic (for the d1-pca data file). Next we describe the principal elements of this dialog.

After the display of introductory information, the system asks the user for the name of the file. It should be noted that the name should be given in single quotation marks. With the assumptions mentioned previously and in the example now discussed, the correct answer to the question about the file name is

d1-pca.

The answer should be followed by pressing the ENTER key, and this holds for each next answer.

Then follows the question about the name of the output file. In our example the answer may be

wyn.1st.

It is assumed in the PCA system that the full name of the data file and an output file may be arbitrary, but its length should not exceed 60 characters.

When the names of the two files have been given, the processing and physical formulation of the output file takes place. At the same time the first few eigenvalues of the variance-covariance matrix are displayed.

Calculations are suspended temporarily when the following message appears.

EXAMINE YOUR OUTPUT FILE IN ORDER
TO CHOOSE A NEW COORDINATE
SYSTEM THEN PRESS <ENTER>
IT IS USUALLY POSSIBLE TO EXECUTE
ANY OS COMMAND NOW
Execution suspended:

This is connected with the need for the user to evaluate the results obtained thus far and to make a decision about further calculations. If the information displayed on the screen so far is not sufficient to make such a decision, it is recommended to follow the DOS command:

type wyn.1st | more

(or its equivalent, depending on the name selected for the output file). This command will result in the part of the output file so far being displayed in page order on the screen.

Having completed the PCA analysis with the use of the variance-covariance matrix, the system proceeds automatically to the second stage, namely a PCA analysis making use of the correlation matrix. The questions that follow and the form of dialog are similar to those in the first stage of calculations.

The PCA program makes possible an analysis of the objects under study in new systems of coordinates (principal components) selected by the user. In the figure, the position of an object is denoted by a number from 1 to 9, depending on how many objects have identical coordinates in a new system. If there are more than nine objects sharing the same coordinates, a special graphic sign appears. On the right-hand side of the figure identification numbers of the objects are printed.

Running the PCA system for the exemplary data series D1-PCA—Results (file WYN.LST)

```

***** VAR.-COVARIANCE MATRIX *****
    COL( 1)      COL( 2)      COL( 3)      COL( 4)      COL( 5)
 1  0.486468D-02 -0.158013D-01 -0.229941D-02 -0.128019D-01  0.160151D-01
 2 -0.158013D-01  0.130006D+01  0.777635D-01  0.779941D-01  0.124907D+01
 3 -0.229941D-02  0.777635D-01  0.868086D-02  0.365850D-02  0.652537D-01
 4 -0.128019D-01  0.779941D-01  0.365850D-02  0.927149D-01 -0.205957D-02
 5  0.160151D-01  0.124907D+01  0.652537D-01 -0.205957D-02  0.141626D+01
 6  0.151046D-02 -0.728109D-02 -0.670036D-03 -0.289727D-02  0.335006D-02
    COL( 6)
 1  0.151046D-02
 2 -0.728109D-02
 3 -0.670036D-03
 4 -0.289727D-02
 5  0.335006D-02
 6  0.903924D-03
*****
TESTING THE PRINCIPAL COMPONENTS
(FOR VARIANCE-COVARIANCE MATRIX)
--- NO._ CRITICAL DELTA_ LEFTCONFID. ---- RIGHTCONFID.
   1     100        89.20       96.00
   2      4         97.60       99.10
   3      1         99.80       99.90
   4      1        100.00      100.00
   5      0         0.00        0.00
   6      0         0.00        0.00
BARTLET'S TEST REJECTS EIGENVECTORS NO.
 5
 6
***** NON-ZERO EIGENVALUES *****
NR.          LAMBDA      PERCENTAGE OF TRACE
 1  0.261359305742508E+01  92.57
 2  0.1631374931478640E+00  5.78
 3  0.4304858866144624E-01  1.52
 4  0.3247796870052141E-02  0.12
 5  0.3270209024478446E-03  0.01
 6  0.1384170300235664E-03  0.00
SELECTED EIGENVECTORS (FROM 1 TO 2 ) OF THE VAR.-COVARIANCE MATRIX
  A( 1)      A( 2)
 1 -0.0001155169  0.1594767997
 2 -0.6902897618 -0.5309246613
 3 -0.0387275414 -0.0614179494
 4 -0.208237984 -0.6376345788
 5 -0.7221949295  0.5291913710
 6  0.0010306523  0.0478813818
***** VALUES OF THE PRINCIPAL COMPONENTS *****
    V( 1)          V( 2)
 1  -0.1095584883804461D+02  1  -0.3684137088632902D+00
 2  -0.1277621780691318D+02  2  -0.5711549374131692D+00
 3  -0.1088636639158975D+02  3  -0.1311308911584027D+00
 4  -0.9154394532615441D+01  4  -0.8119405490473295D+00
 5  -0.1024152023331932D+02  5  -0.6714900809364176D+00
 6  -0.1173532222750920D+02  6  0.2681910528735984D+00
 7  -0.9597303384400675D+01  7  -0.1193822078561360D+01
 8  -0.1309397415020718D+02  8  -0.7065554935458379D+00
 9  -0.1478552145730417D+02  9  -0.8358495501355532D+00
10  -0.9928464507290487D+01 10  0.8389599924975855D-01
11  -0.9445589847792568D+01 11  -0.1117015714194618D+00
12  -0.9693031858935081D+01 12  -0.1607771123805059D+00
13  -0.1047145550469394D+02 13  -0.4560731083644219D+00
14  -0.1062207319044477D+02 14  0.9132649503541419D-01
15  -0.1033337592670940D+02 15  -0.3558322408807868D+00
16  -0.1050531742480956D+02 16  -0.5230999872863084D+00
17  -0.1257441980887520D+02 17  -0.5034207331926865D+00
18  -0.8857152675013044D+01 18  -0.4782461294909233D+00
19  -0.1146614062732514D+02 19  -0.9664908816771722D+00
20  -0.8292967215995477D+01 20  0.1062143760071039D+00
21  -0.9369962434875720D+01 21  -0.1082235996238010D+01
22  -0.9587472449555461D+01 22  -0.8175395451033177D-01
23  -0.7796465582402760D+01 23  -0.10486886945368204D+01
24  -0.1020611846632740D+02 24  -0.1327259443636310D+01
25  -0.995227459998097D+01 25  -0.283788604528224D+00
26  -0.1198613878838233D+02 26  -0.4960124751286308D+00

```

27	-0.1337860765538985D+02	27	-0.2071740963255488D+00
28	-0.1313025519510916D+02	28	-0.5008657100114776D+00
29	-0.1006250738816002D+02	29	-0.6743253843014311D+00

COEFFICIENTS OF DETERMINATION AND CORRELATION BETWEEN COMPONENTS V(I)
AND ORIGINAL VARIABLES X(J)

BETWEEN V(1) AND ORIGINAL VARIABLES FROM X(1) TO X(6)

X(1)	R^2= 0.00000717	R= -0.00267755	SIGNIFICANT FOR ALPHA > 0.1
X(2)	R^2= 0.95793511	R= -0.97874160	SIGNIFICANT FOR ALPHA < 0.001
X(3)	R^2= 0.45155994	R= -0.67198210	SIGNIFICANT FOR ALPHA < 0.001
X(4)	R^2= 0.01222387	R= -0.11056160	SIGNIFICANT FOR ALPHA > 0.1
X(5)	R^2= 0.96250418	R= -0.98107298	SIGNIFICANT FOR ALPHA < 0.001
X(6)	R^2= 0.00307136	R= 0.05541985	SIGNIFICANT FOR ALPHA > 0.1

TOTAL PERCENTAGE OF VARIABILITY OF ALL ORIGINAL VARIABLES

ACCOUNTED FOR BY V(1) MEASURE W(1) = 39.79%

BETWEEN V(2) AND ORIGINAL VARIABLES FROM X(1) TO X(6)

X(1)	R^2= 0.85289210	R= 0.92352158	SIGNIFICANT FOR ALPHA < 0.001
X(2)	R^2= 0.03537160	R= -0.18807339	SIGNIFICANT FOR ALPHA > 0.1
X(3)	R^2= 0.07088949	R= -0.26625080	SIGNIFICANT FOR ALPHA > 0.1
X(4)	R^2= 0.71539870	R= -0.84581245	SIGNIFICANT FOR ALPHA < 0.001
X(5)	R^2= 0.03225781	R= 0.17960461	SIGNIFICANT FOR ALPHA > 0.1
X(6)	R^2= 0.41376644	R= 0.64324680	SIGNIFICANT FOR ALPHA < 0.001

TOTAL PERCENTAGE OF VARIABILITY OF ALL ORIGINAL VARIABLES

ACCOUNTED FOR BY V(2) MEASURE W(2) = 35.34%

CONSTRUCTING A DENDRITE FOR THE EUCLIDEAN DISTANCE MATRIX

ORIGINAL VARIABLES SPACE IS CONSIDERED

```
.D( 1,  3) = 0.307083
..D( 3,  6) = 0.955405
...D( 6, 26) = 0.815476
....D( 26, 17) = 0.604401
.....D( 17,  2) = 0.502295
.....D( 17, 28) = 0.564624
.....D( 28,  8) = 0.257682
.....D( 28, 27) = 0.478748
.....D( 27,  9) = 1.60577
..D( 3, 14) = 0.397367
.D( 1, 13) = 0.516817
..D( 13,  5) = 0.386523
...D( 5, 24) = 0.672532
...D( 5, 29) = 0.189209
..D( 13, 15) = 0.192614
..D( 15, 25) = 0.389871
....D( 25, 10) = 0.394462
.....D( 10, 12) = 0.379341
.....D( 12, 22) = 0.265895
.....D( 22, 11) = 0.210000
.....D( 11, 18) = 0.695916
.....D( 18,  4) = 0.614980
.....D( 4, 21) = 0.605806
.....D( 21,  7) = 0.513614
.....D( 18, 20) = 0.814125
.....D( 18, 23) = 1.20764
..D( 13, 16) = 0.125698
.D( 1, 19) = 0.979388
```

```
MEAN = 0.55868870
STD. DEV= 0.32723257
MEAN + 2*(STD.DEV) = 1.21315384
```

CONSTRUCTING A DENDRITE FOR THE EUCLIDEAN DISTANCE MATRIX

DISTANCE MATRIX IN A COORDINATE SYSTEM WITH AXES V(1)-V(2) IS CONSIDERED

```
.D( 1,  3) = 0.247247
..D( 3, 14) = 0.345454
.D( 1, 16) = 0.476347
..D( 16,  5) = 0.302669
...D( 5, 24) = 0.656724
....D( 24,  7) = 0.623267
.....D( 7, 21) = 0.253249
.....D( 21,  4) = 0.345730
.....D( 4, 18) = 0.446883
.....D( 18, 20) = 0.812342
.....D( 18, 23) = 1.20435
...D( 5, 29) = 0.179036
..D( 16, 13) = 0.750947E-1
```


POINTS WERE PLOTTED IN THE FOLLOWING ORDER :

NO.	X(I)	Y(I)	* OBJECT NO.
1	-0.1174E+02	0.2682E+00	6
2	-0.8293E+01	0.1062E+00	20
3	-0.1062E+02	0.9133E-01	14
4	-0.9928E+01	0.8390E-01	10
5	-0.9587E+01	-0.8175E-01	22
6	-0.1089E+02	-0.1311E+00	3
7	-0.9446E+01	-0.1117E+00	11
8	-0.9693E+01	-0.1608E+00	12
9	-0.1338E+02	-0.2072E+00	27
10	-0.9952E+01	-0.2838E+00	25
11	-0.1096E+02	-0.3684E+00	1
12	-0.1033E+02	-0.3558E+00	15
13	-0.1047E+02	-0.4561E+00	13
14	-0.1199E+02	-0.4960E+00	26
15	-0.8857E+01	-0.4782E+00	18
16	-0.1313E+02	-0.5009E+00	28
17	-0.1257E+02	-0.5034E+00	17
18	-0.1051E+02	-0.5231E+00	16
19	-0.1278E+02	-0.5712E+00	2
20	-0.1024E+02	-0.6715E+00	5
21	-0.1006E+02	-0.6743E+00	29
22	-0.1309E+02	-0.7066E+00	8
23	-0.9154E+01	-0.8119E+00	4
24	-0.1479E+02	-0.8358E+00	9
25	-0.1147E+02	-0.9665E+00	19
26	-0.7796E+01	-0.1049E+01	23
27	-0.9370E+01	-0.1082E+01	21
28	-0.9597E+01	-0.1194E+01	7
29	-0.1021E+02	-0.1327E+01	24

Now the same analysis as for the variance–covariance matrix will be done.

REFERENCES

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Mardia, K. V., Kent, J. T., and Bibby, J. M., 1979, Multivariate analysis: Academic Press, London, 521 p.

APPENDIX

FORTRAN Program Listing

PROGRAM PCA

* PRINCIPAL COMPONENTS ANALYSIS PROGRAM *
* LANGUAGE: FORTRAN77 *
* BY *
* ANDRZEJ MACKIEWICZ WALDEMAR RATAJCZAK *
* TECHNICAL UNIVERSITY ADAM MICKIEWICZ UNIVERSITY *
* POZNAN, POLAND *
*FLOPPY DISK DELIVERED BY REQUEST..... *

* MAXIMUM NUMBER OF VARIABLES IS SET AT 50; *
* MAXIMUM NUMBER OF CASES IS SET AT 200; *

```

* FOR CHANGING SIZES REPLACE 50 AND 200 IN THE PARAMETER *
* STATEMENT THREE LINES BELOW. *
INTEGER I,J,J1,K,L,LA,LB,N,M,NM,NM,LL,IERR,PRMODE
PARAMETER (NM=50,MM=200)
* ----- ^ ----- CHANGED ?.
PARAMETER (PRMODE=1)
* ----- ^ ----- CONVERT THIS PARAMETER TO 0 IF YOUR
* PRINTER CAN PLOT ONLY 133 CHARACTERS PER LINE
* (STANDARD PRMODE VALUE IS 1)
REAL RINFM,RXXXM,RINF
DOUBLE PRECISION XINF,XMIN,XXXF,XXN
PARAMETER (RXXXM= 3.35E+38, XXXF= 1.7D+308, XXN= 2.3D-308)
* ----- ^ ----- ^ ----- ^ ----- -CHANGED ?.
* VAX CONSTANTS: 1.7E+38 1.7D+38 5.9D-39
*
* THESE PARAMETERS ARE MACHINE-DEPENDENT (HERE THEY HAVE BEEN
* SET FOR THE IBM PC OR ANY OTHER MACHINE EQUIPPED WITH THE
* INTEL 8087, 80287, 80387 OR COMPATIBLE. SUGGESTIONS FOR THE VAX
* ARE PRESENTED TWO LINES BELOW THE LAST PARAMETER STATEMENT).
* RXXXM - IS THE LARGEST VALUE POSITIVE (NORMALIZED) REAL DATA,
* XXXF - IS THE LARGEST VALUE POSITIVE (NORMALIZED) DOUBLE
* PRECISION DATA,
* XXN - IS THE SMALLEST VALUE POSITIVE (NORMALIZED) DOUBLE
* PRECISION DATA,
* TO ALTER THESE PARAMETERS FOR A PARTICULAR ENVIRONMENT
* CHECK THE MANUAL OF IT OR SEE THE FOLLOWING PAPER:
* FOX P.A., HALL A.D., SCHRYER N.L., *FRAMEWORK FOR A
* PORTABLE LIBRARY*, ACM TRANSACTIONS ON MATHEMATICAL
* SOFTWARE, VOL. 4, NO. 2, JUNE 1978, PP. 177-188.
*
INTEGER BB(MM),PROC(NM),H1(MM),R1(MM),ISORT(MM),NSTEPY
DOUBLE PRECISION A(NM,NM),D(NM),E(NM),X(NM),S(NM),AC(NM)
DOUBLE PRECISION AS1,TRACE,BX,DX,R,SX1,LCO(NM)
DOUBLE PRECISION U(MM),V(MM),RCO(NM)
REAL TQUANT,Y(MM,MM),WDIS(MM*(MM-1)/2),DD(MM),P(4)
LOGICAL ST
CHARACTER INSET*60,OUTSET*60,STR*9,YON*1
EQUIVALENCE (Y,WDIS),(DD,X),(E,U),(S,V)
COMMON RINFM,XINF,XMIN
RINFM= -RXXXM
XINF= XXXF
XMIN= XXN
WRITE(*,'(12X,''PRINCIPAL COMPONENTS ANALYSIS-INTERACTION PROGRAM
& ''//'))'
WRITE(*,'(12X,''*****'')'
& ',//'))'
WRITE(*,'(''***** GIVE THE PATH NAME OF THE INPUT FILE - AT
& MOST 60 CHARACTERS *****'')')
READ(*,5) INSET
WRITE(*,'(''***** GIVE THE NAME OF THE OUTPUT FILE - AT MOST
& 60 CHARACTERS *****'')')
READ(*,5) OUTSET
5 FORMAT (A)
OPEN(2,STATUS='UNKNOWN',FILE=OUTSET)
WRITE(2,'(22X,''*****'')')

```

```

      WRITE(2,'(22X, ''* PRINCIPAL COMPONENTS ANALYSIS *''))
      WRITE(2,'(22X, ''*****/******''/)')
      WRITE(2,'(/, ''* '' , '' FOR DATA FILE '',A60,''* '')') INSET
      ST=.FALSE.

10   IF (ST) THEN
        OPEN(1,STATUS='OLD',FILE=INSET)
        ELSE
        OPEN(1,STATUS='UNKNOWN',FILE=INSET)
      ENDIF
      READ(1,*) N
      IF (N.GT.MM) THEN
        WRITE(2,'(/9X,' MAXIMUM NUMBER OF VARIABLES IS EQUAL TO MM'
& //'' ARRAY SIZE IN THE CALLING PROGRAM MUST BE CHANGED FOR YOUR''/
& ,21X,'DATA BEFORE USE ''/)')
        STOP
      ENDIF
      READ(1,*) M
      IF (M.GT.MM) THEN
        WRITE(2,'(/9X,' MAXIMUM NUMBER OF CASES IS EQUAL TO MM'
& //'' ARRAYS SIZE IN THE CALLING PROGRAM MUST BE CHANGED FOR YOUR''/
& ,21X,'DATA BEFORE USE ''/)')
        STOP
      ENDIF
      IF(M.LT.3) THEN
        WRITE(2,'(/15X,' TOO FEW CASES. MINIMUM NUMBER OF CASES IS EQUA
& L TO 3''/)')
        STOP
      ENDIF
      WRITE (2,'(//)')
      WRITE(2,'(' NUMBER OF VARIABLES = ',I3,33X,'NUMBER OF CASES='',,
& I3)') N,M
      IF (M.LE.300) THEN
        NSTEPY=50
      ELSE IF (M.LE.600) THEN
        NSTEPY=100
      ELSE
        NSTEPY=200
      ENDIF
      WRITE(2,*)
      WRITE(2,*) ('<>',I=1,39)
      IF(ST) THEN
        WRITE(2,'(/19X,' CORRELATION MATRIX WAS TAKEN INTO ACCOUNT''/)')
      ELSE
        WRITE(2,'(/17X,' VAR.-COVARIANCE MATRIX WAS TAKEN INTO ACCOUNT''/
& ')')
      ENDIF
      WRITE(2,*) ('<>',I=1,39)

*-----*
*      DETERMINING THE VARIANCE-COVARIANCE MATRICES
*-----*

      CALL COVM (NM,M,N,S,A,D,E)
      WRITE(2,*)
      WRITE(2,'(17X,' DESCRIPTIVE PARAMETERS OF ORIGINAL '',
& ''VARIABLES ''/)')
      WRITE(2,'(4X,' VARIABLE'',8X,'MEAN'',13X,'VARIANCE'',7X,

```

```

&'STAND. DEV.'')')
DO 20 I=1,N
  WRITE(2,'(4X,''X('',I3,''),3X,E16.6,3X,2E16.7)') I,S(I),A(I,I),
  & DSQRT(A(I,I))
20  AC(I)=A(I,I)
*-----
*   OPTIONAL DETERMINATION OF THE CORRELATION MATRIX
*-----
IF (ST) THEN
  DO 40 I=2,N
    DO 30 J=1,I-1
      A(I,J)=A(I,J)/DSQRT(A(I,I)*A(J,J))
30    CONTINUE
40    CONTINUE
  DO 50 I=1,N
    A(I,I)=1
50    CONTINUE
  CONTINUE
  WRITE(2,'(/16X,'' #####  CORRELATION MATRIX  #####'')')
  ELSE
    WRITE(2,'(/16X,'' #####  VAR.-COVARIANCE MATRIX  #####'')')
  ENDIF
*-----
*   PRINTING THE CORRELATION MATRIX AND THE VAR.-COVAR MATRIX
*-----
DO 70 I=1,N
  DO 60 J=1,I
    A(J,I)=A(I,J)
60    CONTINUE
70    CONTINUE
K=N
DO 110 L=0,K-1,5
  WRITE(2,*)
  J1=MIN0(L+5,K)
  WRITE(2,120)(I,I=L+1,J1)
  WRITE(2,*)
  DO 100 J=1,N
    WRITE(2,130) J,(A(J,I),I=L+1,J1)
100   CONTINUE
110  CONTINUE
120  FORMAT (5X,5(3X:,COL('',I2,''),5X))
130  FORMAT (I3,5(1X:,D14.6))
*-----
*   DETERMINING EIGENVECTORS AND EIGENVALUES
*-----
CALL TRED2(NM,N,A,D,E,A)
CALL TQL2(NM,N,D,E,A,IERR)
IF (IERR.GT.0) THEN
  WRITE(2,*) ' QL ALGORITHM FAILS - FUTURE PROGRESS IMPOSSIBLE'
  STOP
ENDIF
*-----
*   TRACE OF THE MATRIX CONSIDERED IS NOW DETERMINED
*-----
TRACE=0
DO 140 I=1,N

```

```

        TRACE=TRACE+DMAX1(ODO,D(I))
140 CONTINUE
*-----
*      BARTLET'S TEST
*-----
IF (.NOT.ST) THEN
    CALL BARTLE (N,M,D,TRACE,PROC,LCO,RCO)
    ELSE
    CALL BART2(N,M,D)
ENDIF
*-----
*      PRINTING OF EIGENVALUES
*-----
WRITE(2,'(/10X,''***** NON-ZERO EIGENVALUES *****'')')
WRITE(2,'(5X,'' NR. '',15X,'' LAMBDA'',8X,
& ''PERCENTAGE OF TRACE'')')
DO 150 I=1,N
    L=N-I+1
    IF (D(L).LE.ODO) THEN
        GOTO 170
    ELSE
        WRITE(2,160) I,D(L),SNGL(100DO*D(L)/TRACE)
    ENDIF
150 CONTINUE
160 FORMAT(5X,I3,10X,E22.16,7X,F6.2)
*-----
*      PRINTING EIGENVALUES ON THE SCREEN
*-----
170 IF(ST) THEN
    WRITE(*,'(/10X,''++ CORRELATION MATRIX IS CONSIDERED +++'')')
    ELSE
    WRITE(*,'(/10X,''- VAR.-COVARIANCE MATRIX IS CONSIDERED -'')')
ENDIF
WRITE(*,'(/10X,''***** FIRST NO-ZERO EIGENVALUES *****'')')
WRITE(*,'(5X,'' NR. '',15X,'' LAMBDA'',8X,
& ''PERCENTAGE OF TRACE'')')
DO 180 I=1,AMINO(10,N)
    L=N-I+1
    IF (D(L).LE.ODO) THEN
        GOTO 190
    ELSE
        WRITE(*,160) I,D(L),SNGL(100DO*D(L)/TRACE)
    ENDIF
180 CONTINUE
190 WRITE(*,'(/1X,'' GIVE THE NUMBER OF THE PRINCIPAL COMPONENTS YOU
&WANT TO CONSIDER '')')
READ(*,*) K
*-----
*      END OF MONITORING
*-----
IF(K.GT.0) THEN
    IF(ST) THEN
        WRITE(2,*)(.,I=1,78)
        WRITE(2,'(/5X, '' SELECTED EIGENVECTORS (FROM '',I1,
& '' TO'',I3, '') OF THE CORRELATION MATRIX'')') 1,K

```

```

      ELSE
        WRITE(2,'(/5X, '' SELECTED EIGENVECTORS (FROM '',I1,
&      '' TO '',I3, '') OF THE VAR.-COVARIANCE MATRIX'')') 1,K
      ENDIF
*-----
*      PRINTING THE EIGENVECTORS
*-----
      DO 230 L=0,K-1,5
        WRITE(2,*)
        J1=MIN0(L+5,K)
        WRITE(2,240) (I,I=L+1,J1)
        WRITE(2,*)
        DO 220 J=1,N
          WRITE(2,250) J,(A(J,N-I+1),I=L+1,J1)
220      CONTINUE
230      CONTINUE
      ENDIF
240  FORMAT (5(10X:,'A('',I2,'')))
250  FORMAT (I3,5(1X:,F14.10))
      WRITE(2,'(//)')
      WRITE(2,'('' ***** VALUES OF THE PRINCIPAL COMPONENTS
& *****'')')
      DO 280 I=1,K
        CLOSE(1,STATUS='KEEP')
        OPEN(1,STATUS='OLD',FILE=INSET)
        READ(1,*) N
        READ(1,*) M
        WRITE(2,*)
        WRITE(2,'(12X,'' V('',I2,'')'')') I
        DO 270 J=1,M
          READ(1,*) (X(LL),LL=1,N)
          BX=ODO
          DO 260 LA=1,N
            BX=BX+X(LA)*A(LA,N-I+1)
260      CONTINUE
          WRITE(2,'(8X,I3,3X,D23.16)') J,BX
270      CONTINUE
280      CONTINUE
*-----
*      DETERMINATION AND CORRELATION COEFFICIENTS ARE NOW CALCULATED
*-----
      WRITE(2,*)
      WRITE(2,*) ('.',I=1,72)
      WRITE(2,*) ' COEFFICIENTS OF DETERMINATION AND CORRELATION BETWE
&EN COMPONENTS V(I) '
      WRITE(2,'(23X, '' AND ORIGINAL VARIABLES X(J)'')')
      WRITE(2,*)
      J1=M-2
      P(1)=0.1
      P(2)=0.05
      P(3)=0.01
      P(4)=0.001
      DO 320 I=1,K
      WRITE(2,*)
      WRITE(2,'('' BETWEEN V('',I3,'') AND ORIGINAL VARIABLES FROM X(1)

```

```

& TO X('',I3,''))') I,N
WRITE(2,*)
AS1=0
DO 310 J=1,N
  R=A(J,N-I+1)* A(J,N-I+1) *D(N-I+1)
  IF (.NOT.ST) R=R/AC(J)
  AS1=AS1+R
  DX=DSIGN(DSQRT(R),A(J,N-I+1))
DO 290 LA=1,4
  CALL TQ(J1,P(LA),TQUANT)
  BX=TQUANT*TQUANT
  TQUANT=SQRT(BX/(BX+J1))
  IF (DABS(DX).LE.TQUANT) THEN
    L=LA-1
    GOTO 300
  ENDIF
290  CONTINUE
L=5
300  IF (L.EQ.0) THEN
    STR=' > 0.1 '
    ELSEIF(L.EQ.1) THEN
    STR=' = .1 '
    ELSEIF(L.EQ.2) THEN
    STR=' = 0.05 '
    ELSEIF(L.EQ.3) THEN
    STR=' = 0.01 '
    ELSEIF(L.EQ.4) THEN
    STR=' = 0.001'
    ELSE
    STR=' < 0.001'
  ENDIF
  WRITE(2,'(''X('',I3,'')  R^2='',F11.8,''  R= '',F14.8, ''  S
&IGNIFICANT FOR ALPHA '',1X,A9'') J,R,DX,STR
310  CONTINUE
WRITE(2,*)
WRITE(2,'('' TOTAL PERCENTAGE OF VARIABILITY OF ALL ORIGINAL VARIA
&BLES'')')
WRITE(2,'(''      ACCOUNTED FOR BY V('',I3,'')  MEASURE W('',I3,''
&) ='',F6.2, ''%'')') I,I,AS1*100.0/DBLE(N)
320  CONTINUE
*-----
*  EUCLIDEAN DISTANCES (IN ORIGINAL VARIABLE SPACE) ARE NOW DETERMINED
*-----
WRITE(2,*)
WRITE(2,*)
  IF(.NOT.ST) THEN
    CLOSE(1,STATUS='KEEP')
    OPEN(1,STATUS='OLD',FILE=INSET)
    READ(1,*) N
    READ(1,*) M
    DO 330 J=1,M
      READ(1,*) (Y(LL,J),LL=1,N)
  330  CONTINUE
  LL=1
  DO 370 I=1,M-1

```

```

      DO 340 K=1,M
      X(K)=Y(K,I)
340   CONTINUE
      DO 360 J=I+1,M
      SX1=0.0
      DO 350 K=1,M
          SX1=SX1+(X(K)-Y(K,J))**2
350   CONTINUE
      Y(J,I)=SQRT(SX1)
360   CONTINUE
      Y(I,I)=0.0
370   CONTINUE
      DO 390 I=2,M
      DO 380 J=1,I-1
          Y(J,I)=Y(I,J)
380   CONTINUE
390   CONTINUE
      DO 410 J=2,M
      DO 400 I=1,J-1
          WDIS(LL)=Y(I,J)
          LL=LL+1
400   CONTINUE
410   CONTINUE
      CLOSE(1,STATUS='KEEP')
      WRITE(2,'(/5X,''CONSTRUCTING A DENDRITE FOR THE EUCLIDEAN DISTA
&NCE MATRIX'')')
      WRITE(2,'(/15X,''ORIGINAL VARIABLES SPACE IS CONSIDERED'',/)')
      RINF=XXXXM*1E-1
      CALL DENDRI(M,WDIS,RINF,1,1,BB,DD,H1,R1,LL,PRMODE)
      CLOSE(1,STATUS='KEEP')
      ENDIF
*-----
*     DISTANCE MATRIX IN COORDINATE SYSTEM V(1)-V(2) IS NOW COMPUTED
*-----
      CLOSE(1,STATUS='KEEP')
420   CLOSE(2,STATUS='KEEP')
      WRITE(*,*)'EXAMINE YOUR OUTPUT FILE IN ORDER TO CHOOSE A NEW COORD
&INATE SYSTEM'
      WRITE (*,*)'THEN PRESS <ENTER>'
      WRITE (*,*) 'IT IS USUALLY POSSIBLE TO EXECUTE ANY OS COMMAND NOW'
      PAUSE
415   WRITE(*,*)'TYPE CAPITAL Y IF YOU WANT TO CONSIDER A NEW PRINCIPAL
& COMPONENT '
      WRITE(*,*) 'COORDINATE SYSTEM OR TYPE CAPITAL N
      READ(*,425) YON
      IF(YON.NE.'Y' .AND. YON.NE.'N') GOTO 415
425   FORMAT(A1)
      OPEN(2,STATUS='OLD',ACCESS='APPEND',FILE=OUTSET)
      IF(YON.EQ.'N') GOTO 490
430   WRITE(*,*) 'GIVE THE NUMBER OF THE FIRST COORDINATE AXIS '
      READ(*,*) LA
      WRITE(*,*) 'GIVE THE NUMBER OF THE SECOND COORDINATE AXIS '
      READ(*,*) LB
      IF(LA.GT.N.OR.LB.GT.N) THEN
          WRITE (*,*) 'DATA ERROR - TRY AGAIN'

```

```

        GO TO 430
      ENDIF
      OPEN(1,STATUS='OLD',FILE=INSET)
      READ(1,*) N
      READ(1,*) M
      DO 440 J=1,M
        READ(1,*) (Y(J,LL),LL=1,N)
  440  CONTINUE
      CLOSE(1,STATUS='KEEP')
*-----
*     DATA FOR PLOTTING
*-----
      LA=N+1-LA
      LB=N+1-LB
      DO 460 J=1,M
        BX=ODO
        DX=ODO
        DO 450 K=1,N
          BX=BX+DBLE(Y(J,K))*A(K,LA)
          DX=DX+DBLE(Y(J,K))*A(K,LB)
  450  CONTINUE
      V(J)=DX
      U(J)=BX
  460  CONTINUE
      LL=1
      DO 480 I=2,M
        DO 470 J=1,I-1
          WDIS(LL)=SNGL(DSQRT((U(J)-U(I))**2+(V(J)-V(I))**2))
          LL=LL+1
  470  CONTINUE
  480  CONTINUE
      WRITE(2,'(/5X,''CONSTRUCTING A DENDRITE FOR THE EUCLIDEAN DISTANCE
      & MATRIX''))'
      WRITE(2,'(/5X,''DISTANCE MATRIX IN A COORDINATE SYSTEM WITH AXES
      & V('',I2,'')-V('',I2,'') IS CONSIDERED'',/)'') N+1-LA,N+1-LB
      RINF=XXXM*1E-1
      CALL DENDRI(M,WDIS,RINF,1,1,BB,DD,H1,R1,LL,PRMODE)
      WRITE(2,*)
      WRITE(2,'(/17X,'' SCATTERED PLOT IN V('',I2,'')-V('',I2,'') COORDI
      & NATE SYSTEM'/'') N+1-LA,N+1-LB
      CALL PLOTDR (U,V,M,ISORT,60,NSTEPY,PRMODE)
      WRITE(2,'(//)')
      WRITE(2,'(14X,''POINTS WERE PLOTTED IN THE FOLLOWING ORDER :''')
      WRITE(2,'(12X,60A1)') ('-',I=1,47)
      WRITE(2,'(12X,'' NO. * X(I) * Y(I) * OBJECT NO.''))
      WRITE(2,'(12X,60A1)') ('-',I=1,47)
      DO 485 I=1,M
        WRITE(2,'(12X,I3,2X,E11.4,3X,E11.4,6X,I3)')
        & I,U(ISORT(I)),V(I),ISORT(I)
  485  CONTINUE
      WRITE(2,*)
      GOTO 420
*-----
*     PRINCIPAL COMPONENTS ANALYSIS FOR THE CORRELATION MATRIX OR STOP
*-----

```



```

        ENDIF
20    CONTINUE
      S1=H(K1)
      H(K1)=H(I)

30 CONTINUE
DO 40 I=1,N
  IF (B(I).EQ.0) GOTO 40
  IF (C(I).LT.INF-1EO) THEN
    SEL=SEL+C(I)
    ELSE
    SEL=INF-1EO
    ST=1
  ENDIF
40 CONTINUE
  IF (PR.EQ.0.OR.S.NE.1) RETURN
  DO 50 I=1,N
    H(I)=0
50 CONTINUE
  DO 60 I=2,N
    J=B(I)
    H(J)=H(J)+1
60 CONTINUE
  R(1)=1
  J=1
  K=1
  DO 100 I=2,N
70    IF (H(K).EQ.0) THEN
      J=J-1
      K=R(J)
      GOTO 70
    ELSE
      H(K)=H(K)-1
      DO 80 M1=2,N
        IF (K.EQ.B(M1)) GOTO 90
80    CONTINUE
90    IF (PRMODE.EQ.1) THEN
      WRITE(LINOUT(1:),'(200A)') ('.',II=1,200)
      IF (J.LE.JJ-25) THEN
        WRITE(LINOUT(J+1:),('D(,,I4,,,,'',I4,,) = ',,
     *          G12.6E1')) K,M1,C(M1)
      ELSE
        WRITE(LINOUT((JJ-25):),'(A)') ' SORRY, LINE TOO LONG '
      ENDIF
      WRITE(2,'(200A)') LINOUT
    ELSE
      WRITE(SHORT(1:),'(133A)') ('.',II=1,133)
      IF (J.LE.JJ-25 ) THEN
        WRITE(SHORT(J+1:),('D(,,I4,,,,'',I4,,) = ',,
     *          G12.6E1')) K,M1,C(M1)
      ELSE
        WRITE(SHORT((JJ-25):),'(A)') ' SORRY, LINE TOO LONG '
      ENDIF
      WRITE(2,'(133A)') SHORT
    ENDIF
    MEAN=MEAN+C(M1)

```



```

INTEGER           N,M,K,I,IER,J,L,K1,PROC(N)
REAL              CHIPRO
DOUBLE PRECISION A0,A00,DELTA,TR1,TR2,TR3,TRACE,D(N),LCO(N),RCO(N)
LOGICAL LOGI
LOGI=.FALSE.
DO 20 K1=0,N-2
    A0=ODO
    A00=1DO
    DO 10 I=K1+1,N
        A0=A0+DABS(D(N-I+1))
        A00=A00*DABS(D(N-I+1))
10     CONTINUE
        A0=A0/(N-K1)
        A00=A00**(.DO/(N-K1))
        IF(A0/A00.GE.1D30) THEN
            LOGI=.TRUE.
            GOTO 30
        ENDIF
        CALL CDTR(SNGL((M-(2*N+11)/6D0)*(N-K1)*DLOG(A0/A00)),
&             REAL((N-K1+2)*(N-K1-1)*0.5),CHIPRO,IER)
        IF (IER.NE.0) GOTO 30
        IF(1.0-CHIPRO.GT.0.05) GOTO 30
20     CONTINUE
30     IF(LOGI.OR.IER.NE.0) THEN
        K1=N
    ENDIF
*
*      TESTING PRINCIPAL COMPONENTS
*
        DO 40 I=K1+1,N
            PROC(N-I+1)=0
            LCO(N-I+1)=ODO
            RCO(N-I+1)=ODO
40     CONTINUE
        DO 80 K=0,K1-1
            TR1=0
            TR2=0
            TR3=0
            DO 50 I=1,K
                TR1=TR1+D(N-I+1)**2
50     CONTINUE
        DO 60 I=K+1,N
            TR2=TR2+D(N-I+1)**2
            TR3=TR3+D(N-I+1)
60     CONTINUE
        DO 70 L=0,100
            DELTA=0.01*DBLE(L)
            IF(DSQRT(DBLE(M))*(TR3/TRACE-DELTA)-1.96*DSQRT(DABS(2*(DELTA
&                 /TRACE))**2*TR1+2*((1-DELTA)/TRACE)**2*TR2).LT.0) THEN
                PROC(N-K)=L
                GOTO 80
            ENDIF
70     CONTINUE
            PROC(N-K)=100
80     CONTINUE

```



```

DOUBLE PRECISION C,C2,C3,DL1,EL1,F,G,H,P,R,S,S2,TST1,TST2,PYTHAG
IERR = 0
IF (N .EQ. 1) GO TO 1001
DO 100 I = 2, N
100 E(I-1) = E(I)
F = 0.0D0
TST1 = 0.0D0
E(N) = 0.0D0
DO 240 L = 1, N
   J = 0
   H = DABS(D(L)) + DABS(E(L))
   IF (TST1 .LT. H) TST1 = H
   DO 110 M = L, N
      TST2 = TST1 + DABS(E(M))
      IF (TST2 .EQ. TST1) GO TO 120
110   CONTINUE
120   IF (M .EQ. L) GO TO 220
130   IF (J .EQ. 30) GO TO 1000
      J = J + 1
      L1 = L + 1
      L2 = L1 + 1
      G = D(L)
      P = (D(L1) - G) / (2.0D0 * E(L))
      R = PYTHAG(P,1.0D0)
      D(L) = E(L) / (P + DSIGN(R,P))
      D(L1) = E(L) * (P + DSIGN(R,P))
      DL1 = D(L1)
      H = G - D(L)
      IF (L2 .GT. N) GO TO 145
      DO 140 I = L2, N
         D(I) = D(I) - H
140   F = F + H
      P = D(N)
      C = 1.0D0
      C2 = C
      EL1 = E(L1)
      S = 0.0D0
      MML = N - L
      DO 200 II = 1, MML
         C3 = C2
         C2 = C
         S2 = S
         I = N - II
         G = C * E(I)
         H = C * P
         R = PYTHAG(P,E(I))
         E(I+1) = S * R
         S = E(I) / R
         C = P / R
         P = C * D(I) - S * G
         D(I+1) = H + S * (C * G + S * D(I))
         DO 180 K = 1, N
            H = Z(K,I+1)
            Z(K,I+1) = S * Z(K,I) + C * H
            Z(K,I) = C * Z(K,I) - S * H
180   CONTINUE
200   CONTINUE
220   IF (F .EQ. 0.0D0) GO TO 240
240   IF (TST1 .LT. 1.0D-10) GO TO 260
      TST1 = 1.0D-10
260   IF (TST1 .LT. 1.0D-10) GO TO 280
      TST1 = 1.0D-10
280   IF (TST1 .LT. 1.0D-10) GO TO 300
      TST1 = 1.0D-10
300   IF (TST1 .LT. 1.0D-10) GO TO 320
      TST1 = 1.0D-10
320   IF (TST1 .LT. 1.0D-10) GO TO 340
      TST1 = 1.0D-10
340   IF (TST1 .LT. 1.0D-10) GO TO 360
      TST1 = 1.0D-10
360   IF (TST1 .LT. 1.0D-10) GO TO 380
      TST1 = 1.0D-10
380   IF (TST1 .LT. 1.0D-10) GO TO 400
      TST1 = 1.0D-10
400   IF (TST1 .LT. 1.0D-10) GO TO 420
      TST1 = 1.0D-10
420   IF (TST1 .LT. 1.0D-10) GO TO 440
      TST1 = 1.0D-10
440   IF (TST1 .LT. 1.0D-10) GO TO 460
      TST1 = 1.0D-10
460   IF (TST1 .LT. 1.0D-10) GO TO 480
      TST1 = 1.0D-10
480   IF (TST1 .LT. 1.0D-10) GO TO 500
      TST1 = 1.0D-10
500   IF (TST1 .LT. 1.0D-10) GO TO 520
      TST1 = 1.0D-10
520   IF (TST1 .LT. 1.0D-10) GO TO 540
      TST1 = 1.0D-10
540   IF (TST1 .LT. 1.0D-10) GO TO 560
      TST1 = 1.0D-10
560   IF (TST1 .LT. 1.0D-10) GO TO 580
      TST1 = 1.0D-10
580   IF (TST1 .LT. 1.0D-10) GO TO 600
      TST1 = 1.0D-10
600   IF (TST1 .LT. 1.0D-10) GO TO 620
      TST1 = 1.0D-10
620   IF (TST1 .LT. 1.0D-10) GO TO 640
      TST1 = 1.0D-10
640   IF (TST1 .LT. 1.0D-10) GO TO 660
      TST1 = 1.0D-10
660   IF (TST1 .LT. 1.0D-10) GO TO 680
      TST1 = 1.0D-10
680   IF (TST1 .LT. 1.0D-10) GO TO 700
      TST1 = 1.0D-10
700   IF (TST1 .LT. 1.0D-10) GO TO 720
      TST1 = 1.0D-10
720   IF (TST1 .LT. 1.0D-10) GO TO 740
      TST1 = 1.0D-10
740   IF (TST1 .LT. 1.0D-10) GO TO 760
      TST1 = 1.0D-10
760   IF (TST1 .LT. 1.0D-10) GO TO 780
      TST1 = 1.0D-10
780   IF (TST1 .LT. 1.0D-10) GO TO 800
      TST1 = 1.0D-10
800   IF (TST1 .LT. 1.0D-10) GO TO 820
      TST1 = 1.0D-10
820   IF (TST1 .LT. 1.0D-10) GO TO 840
      TST1 = 1.0D-10
840   IF (TST1 .LT. 1.0D-10) GO TO 860
      TST1 = 1.0D-10
860   IF (TST1 .LT. 1.0D-10) GO TO 880
      TST1 = 1.0D-10
880   IF (TST1 .LT. 1.0D-10) GO TO 900
      TST1 = 1.0D-10
900   IF (TST1 .LT. 1.0D-10) GO TO 920
      TST1 = 1.0D-10
920   IF (TST1 .LT. 1.0D-10) GO TO 940
      TST1 = 1.0D-10
940   IF (TST1 .LT. 1.0D-10) GO TO 960
      TST1 = 1.0D-10
960   IF (TST1 .LT. 1.0D-10) GO TO 980
      TST1 = 1.0D-10
980   IF (TST1 .LT. 1.0D-10) GO TO 1000
      TST1 = 1.0D-10
1000  CONTINUE

```



```

120      SCALE = SCALE + DABS(D(K))
         IF (SCALE .NE. 0.0D0) GO TO 140
130      E(I) = D(L)
         DO 135 J = 1, L
            D(J) = Z(L,J)
            Z(I,J) = 0.0D0
            Z(J,I) = 0.0D0
135      CONTINUE
         GO TO 290
140      DO 150 K = 1, L
            D(K) = D(K) / SCALE
            H = H + D(K) * D(K)
150      CONTINUE
         F = D(L)
         G = -DSIGN(DSQRT(H),F)
         E(I) = SCALE * G
         H = H - F * G
         D(L) = F - G
         DO 170 J = 1, L
            E(J) = 0.0D0
            DO 240 J = 1, L
               F = D(J)
               Z(J,I) = F
               G = E(J) + Z(J,J) * F
               JP1 = J + 1
               IF (L .LT. JP1) GO TO 220
               DO 200 K = JP1, L
                  G = G + Z(K,J) * D(K)
                  E(K) = E(K) + Z(K,J) * F
200      CONTINUE
220      E(J) = G
240      CONTINUE
         F = 0.0D0
         DO 245 J = 1, L
            E(J) = E(J) / H
            F = F + E(J) * D(J)
245      CONTINUE
         HH = F / (H + H)
         DO 250 J = 1, L
            E(J) = E(J) - HH * D(J)
            DO 280 J = 1, L
               F = D(J)
               G = E(J)
               DO 260 K = J, L
                  Z(K,J) = Z(K,J) - F * E(K) - G * D(K)
                  D(J) = Z(L,J)
                  Z(I,J) = 0.0D0
260      CONTINUE
280      CONTINUE
290      D(I) = H
300 CONTINUE
         DO 500 I = 2, N
            L = I - 1
            Z(N,L) = Z(L,L)
            Z(L,L) = 1.0D0
            H = D(I)

```



```

      KEY(I)=I
10   CONTINUE
      M=NOBS
      DO 40 MM=1,LOGNB2
         M=M/2
         K=NOBS-M
         DO 30 J=1,K
            I=J
20   CONTINUE
      L=I+M
      IF(Y(L).GT.Y(I)) THEN
         T=Y(I)
         POM=KEY(I)
         Y(I)=Y(L)
         KEY(I)=KEY(L)
         Y(L)=T
         KEY(L)=POM
         I=I-M
         IF(I.GE.1)GO TO 20
      ENDIF
30   CONTINUE
40   CONTINUE
      YMN = Y(1)
      YMX = Y(NOBS)
      XMN = X(1)
      XMX = XMX
      DO 50 J=2,NOBS
         XMN = DMIN1(X(J),XMN)
         XMX = DMAX1(X(J),XMX)
50   CONTINUE
      IF (YMN.EQ.YMX) THEN
         YMN = YMN - 1.0D0
         YMX = YMX + 1.0D0
      ENDIF
      IF (XMN.EQ.XMX) THEN
         XMN = XMN - 1.0D0
         XMX = XMX + 1.0D0
      ENDIF
      NSX1 = NSX
      NSY1 = NSY
      CALL PLOTAX(XMN,XMX,NSX1,XMIN,XSTEP,MAXA,MAXB)
      IF (XMIN.EQ.XMN) THEN
         XMIN = XMIN - XSTEP
         NSX1 = NSX1 + 1
      ENDIF
      CALL PLOTAX(YMN,YMX,NSY1,YMIN,YSTEP,MAXYA,MAXYB)
      IF (YMIN.EQ.YMN) THEN
         YMIN = YMIN - YSTEP
         NSY1 = NSY1 + 1
      ENDIF
      CALL PLOTMN(X,Y,XMIN,XSTEP,NSX1,YMIN,YSTEP,NSY1,NOBS,MAXA,
     &MAXB,KEY,MAXYA,MAXYB,IA,IXLINE,XAXIS,PRMODE)
      RETURN
END

```



```

        ENDIF
    ENDIF
    IF (YMIN.NE.0.0D0)
&      IYZERO = -IDINT(YMIN/YSTEP+DSIGN(0.5D0,YMIN))
    NSTPX2 = NSTEPX + 2
    DO 10 I=1,NSTPX2
        IXLINE(I) = ICODE(1)
        IF (MOD(IABS(IXZERO-I+1),5).EQ.0) THEN
            IXLINE(I) = ICODE(2)
            NEND = (I-1)/5 + 1
            XAXIS(NEND) = XMIN + XSTEP*DBLE(I-1)
        ENDIF
10   CONTINUE
    IFOR = MOD(IXZERO,5)
    MAXYF = MAXYA + MAXYB + 2
    IF (MAXYF.LE.11) THEN
        IFMA(9) = NUMB(MAXYB+1)
        LYE = .FALSE.
    ELSE
        IFMA(5) = ICODE(17)
        IFMA(9) = NUMB(4)
        LYE = .TRUE.
    ENDIF
    J1 = NSTPX2/100
    J = J1 + 1
    IFMA(11) = NUMB(J)
    IFMB(6) = NUMB(J)
    J = NSTPX2/10 + 1 - J1*10
    IFMA(12) = NUMB(J)
    IFMB(7) = NUMB(J)
    J = MOD(NSTPX2,10) + 1
    IFMA(13) = NUMB(J)
    IFMB(8) = NUMB(J)
    IF (MOD(IABS(IYZERO-(NSTEPY+1)),5).NE.0) THEN
        DO 20 I=1,22
            MB(I)=CHAR(IFMB(I))
20   CONTINUE
        WRITE (2,MB) (IXLINE(I),I=1,NSTPX2)
    ELSE
        YAXIS = YMIN + YSTEP*DBLE(NSTEPY+1)
        DO 30 I=1,27
            MA(I)=CHAR(IFMA(I))
30   CONTINUE
        WRITE (2,MA) YAXIS,(IXLINE(I),I=1,NSTPX2)
    ENDIF
    NCOUNT = 1
    DO 110 J=1,NSTEPY
        K = NSTEPY - J + 1
        DO 40 I=1,NSTEPX
            IA(I) = 3
40   CONTINUE
        K1=NCOUNT
50   IF (NCOUNT.GT.NOBS) GO TO 70
        IAY = (Y(NCOUNT)-YMIN)/YSTEP + 0.5D0
        IF (IAY.EQ.0) IAY = 1

```

```

IF (IAY.LT.K) GO TO 70
II = KEY(NCOUNT)
IXAX = (X(II)-XMIN)/XSTEP + 0.5D0
IF (IXAX.EQ.0) IXAX = 1
IF (IA(IXAX).GT.3) THEN
  IA(IXAX) = IA(IXAX) + 1
ELSE
  IA(IXAX) = 4
IF (NCOUNT.GT.K1) THEN
  L1=NCOUNT-1
  Z=Y(NCOUNT)
  Q=X(KEY(NCOUNT))
  P=KEY(NCOUNT)
60   IF (L1.GE.K1) THEN
      IF(Q.LT.X(KEY(L1))) THEN
        Y(L1+1)=Y(L1)
        KEY(L1+1)=KEY(L1)
        L1=L1-1
        GOTO 60
      ENDIF
    ENDIF
    Y(L1+1)=Z
    KEY(L1+1)=P
  ENDIF
ENDIF
NCOUNT = NCOUNT + 1
GO TO 50
70   DO 80 I=1,NSTEPX
      IF (IA(I).EQ.3) THEN
        IF (K.EQ.IYZERO) THEN
          IA(I) = 1
          IF (MOD(IABS(IYZERO-I),5).EQ.0) IA(I) = 2
        ELSE
          IF (I.EQ.IYZERO) THEN
            IA(I) = 1
            IF (MOD(IABS(IYZERO-K),5).EQ.0) IA(I) = 2
          ENDIF
        ENDIF
      ENDIF
      II = MINO(IA(I),39)
      IA(I) = ICODE(II)
80     CONTINUE
      IF (PRMODE.EQ.1) THEN
        NN=30
      ELSE
        NN=10
      ENDIF
      IF (MOD(IABS(IYZERO-K),5).NE.0) THEN
        DO 90 I=1,22
          MB(I)=CHAR(IFMB(I))
90     CONTINUE
        WRITE (2,MB) ICODE(1),(IA(I),I=1,NSTEPX),ICODE(1),
                     (KEY(I),I=K1,MINO(K1+NN,NCOUNT-1))
      ELSE
        YAXIS = YMIN + YSTEP*DBLE(K)

```

```

      DO 100 I=1,27
         MA(I)=CHAR(IFMA(I))
100   CONTINUE
         WRITE (2,MA) YAXIS,ICODE(2),(IA(I),I=1,NSTEPX),ICODE(2),
&           (KEY(I),I=K1,MIN0(K1+NN,NCOUNT-1))
      ENDIF
110 CONTINUE
      IF (MOD(IABS(IYZERO),5).NE.0) THEN
         DO 120 I=1,22
            MB(I)=CHAR(IFMB(I))
120   CONTINUE
         WRITE (2,MB) (IXLINE(I),I=1,NSTPX2)
      ELSE
         YAXIS = YMIN
         DO 130 I=1,27
            MA(I)=CHAR(IFMA(I))
130   CONTINUE
         WRITE (2,MA) YAXIS,(IXLINE(I),I=1,NSTPX2)
      ENDIF
      IFOR = MOD(IXZERO,5)
      IF (IFOR.LT.0) IFOR = IFOR + 5
      ISP1 = 11 + IFOR
      IF (MAXA+MAXB+2.LE.9) ISP1 = ISP1 - MAXA
      I = ISP1/10 + 1
      IFMO(2) = NUMB(I)
      I = MOD(ISP1,10) + 1
      IFMO(3) = NUMB(I)
      MAXF = MAXA + MAXB + 2
      IF (MAXF.LE.9) THEN
         ISPACE = 10 - MAXF
         LXE = .FALSE.
         IFMO(10) = NUMB(MAXF+1)
         IFMO(12) = NUMB(MAXB+1)
         IFMO(14) = NUMB(ISPACE+1)
      ELSE
         IFMO(9) = ICODE(17)
         IFMO(10) = NUMB(10)
         IFMO(12) = NUMB(3)
         IFMO(14) = NUMB(2)
         LXE = .TRUE.
      ENDIF
      DO 140 I=1,17
         MO(I)=CHAR(IFMO(I))
140 CONTINUE
         WRITE (2,MO) (XAXIS(II),II=1,NEND,2)
         ISP2 = ISP1 + 5
         I = ISP2/10 + 1
         IFMO(2) = NUMB(I)
         I = MOD(ISP2,10) + 1
         IFMO(3) = NUMB(I)
         DO 150 I=1,17
            MO(I)=CHAR(IFMO(I))
150 CONTINUE
         WRITE (2,MO) (XAXIS(II),II=2,NEND,2)
         IF (LXE) IFMO(9) = ICODE(18)

```



```

&           -1.7816839846D-03/
DATA      PI/3.141592653589793D0/,BIG1/34.844D0/
MFLAG = .FALSE.
T = X
IF (DABS(T).GT.XMIN) THEN
  IF (DABS(T).GE.BIG1) THEN
    DGAMMA = XINF
    RETURN
  ELSE
    DGAMMA = XINF
  IF (T.LE.0.ODO) THEN
    DGAMMA = -XINF
    RETURN
  ENDIF
  ENDIF
ENDIF
IF (T.LE.0.ODO) THEN
  MFLAG = .TRUE.
  T = -T
  R = DINT(T)
  SIGN = 1.ODO
  IF (DMOD(T,2.ODO).EQ.0.ODO) SIGN = -1.ODO
  R = T-R
  IF (R.NE.0.ODO) THEN
    R = PI/DSIN(R*PI)*SIGN
  T = T+1.ODO
  ELSE
    DGAMMA = XINF
  IF (SIGN.EQ.-1.ODO) THEN
    DGAMMA = -XINF
    RETURN
  ENDIF
  ENDIF
ENDIF
IF (T.GT.12.ODO) THEN
  TOP = DLOG(T)
  TOP = T*(TOP-1.ODO)-.5D0*TOP
  T = 1.ODO/T
  B = T*T
  A = Z(7)
  DO 10 J = 1,5
10    A = A*B+Z(J)
  Y = A*T+Z(6)+TOP
  Y = DEXP(Y)
  IF (MFLAG) Y = R/Y
  DGAMMA = Y
ELSE
  I = T
  A = 1.ODO
  IF (I.GT.2) THEN
    DO 20 J=3,I
    T = T-1.ODO
    A = A*T
20    CONTINUE
  ELSE

```



```
IF(X.GT.0) THEN
  NORMAL=REAL((Z+1D0)*0.5D0)
ELSE
  NORMAL=REAL((1D0-Z)*0.5D0)
ENDIF
END
```