

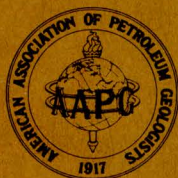
DANIEL F. MERRIAM, Editor

**FORTRAN IV PROGRAMS FOR
CANONICAL CORRELATION
AND CANONICAL TREND-
SURFACE ANALYSIS**

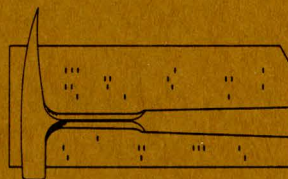
By

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in cooperation with the
American Association of Petroleum Geologists
Tulsa, Oklahoma



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The University of Kansas, Lawrence

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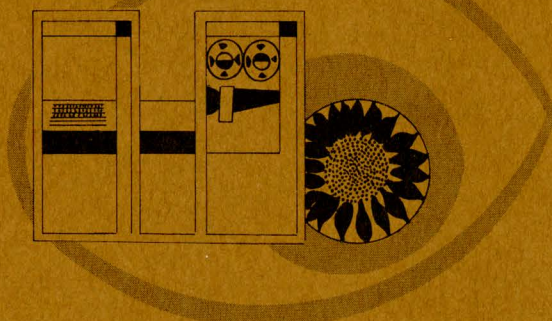
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For a limited time the Geological Survey will make available on magnetic tape the canonical correlation and canonical trend-surface programs as described here for \$20.00 (US). An extra charge of \$10.00 is made if punched cards are required.

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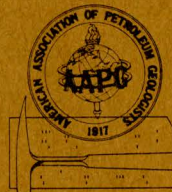


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FORTRAN IV PROGRAMS FOR CANONICAL CORRELATION AND CANONICAL TREND- SURFACE ANALYSIS

By
P.J. Lee *

INTRODUCTION

In the statistical technique of simple linear regression a dependent variable, Y , is related to an independent variable, X , by an equation of the type

$$Y = bX + e,$$

where e is a random variable. The "strength of the relationship" of Y and X may be expressed by the correlation coefficient, r .

In multiple linear regression, the dependent variable is related to several independent variables by an equation of this type

$$Y = \sum b_i X_i + e.$$

The multiple correlation coefficient serves as a measure of the "strength of the relationship". More precisely, the square of the multiple correlation coefficient gives the proportion of the total sums of squares of Y which may be attributed to variation of the X_i .

Multiple correlation techniques have been applied frequently in geology. A typical application might relate a bulk property of a rock (e.g. permeability) to a series of mineralogical or textural properties (e.g. mean grain size, sorting, skewness, etc.).

It is not unusual, however, for geologists to make two (or more) sets of measurements on a single specimen (e.g. size and compositional parameters, trace element and major elements, or chemical and modal analyses) or at a single locality (e.g. formation thickness, sand percentage, etc., and size or compositional parameters). It may be of interest to attempt to relate one set of variables to another set of variables, to discover equations of the type

$$U = \sum a_i X_i, \text{ and}$$

$$V = \sum b_i Y_i,$$

where the coefficients a_i and b_i are chosen to give the largest possible correlation between U and V . This technique is called canonical correlation.

As an extension of this technique, the X_i might be chosen to be geographical coordinates (and their polynomials) of a set of spatially distributed variables, Y_i . In this instance, the technique would be similar to that of trend analysis, except that the trend which is determined is not the trend of any particular variable, Y , but is the common trend of a set of variables, Y_i . This technique may be called canonical trend-surface analysis.

Acknowledgments. - Special thanks are due to Prof. G. Middleton for his valuable comments. The writer is indebted to Dr. George Lynts of Duke University for supplying the raw data. The Geological Survey of Canada provided funds for support of the research.

CANONICAL CORRELATION

Suppose a number of rock specimens are collected from a formation. On each specimen, the size parameters (mean sorting coefficient and skewness) and petrographic composition (percentage of quartz, feldspar, rock fragments) are determined. It may be uncertain whether or not a relationship is present between the grain-size parameters and petrographic variables. A simple correlation coefficient indicates a possible relationship between one grain-size parameter and one petrographic parameter. Nine correlation coefficients thus are required to describe all possible relationships. A further study of the relationship between the two sets of variables is, however, possible.

Canonical correlation analysis was introduced by Hotelling in 1936 (the paper was read in 1935) as a technique to understand the relationship between two sets of variables. The relationship is summarized and expressed by a simple index. For example, the grain-size and petrographic parameters may be weighted and combined into two linear combinations

$$U = a_1 (\text{median}) + a_2 (So) + a_3 (Sk), \text{ and}$$

$$V = b_1 (\text{quartz}) + b_2 (\text{feldspar}) + b_3 (\text{rock fragments}),$$

where the a_i and b_i are weights to be determined

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such that U and V have maximum simple correlation. The coefficient of correlation of U and V is called the canonical correlation coefficient, and measures the strength of the link between the two sets of variables. The nature of the link is indicated by the relative sizes of the weighting coefficients, a_i and b_i .

For standardized variables the larger coefficients indicate those variables which are correlated most closely between the two sets. In this situation, canonical correlation is used in a correlation model, where each of the two sets, U and V, is defined as subject to random error fluctuations, i.e. they are random variables or variates.

Another possible application of canonical correlation is as a tool to predict a combination of two or more dependent variates from a set of independent variates. Here, canonical correlation is used as a regression model of the type

$$U = c + kV,$$

where c and k are determined in the same way as in linear regression analysis. The canonical correlation coefficient then may be considered as the simple correlation coefficient between U and V.

Computational Procedures

The computations for canonical correlation are carried out in five major steps.

STEP 1 Transformation of variates if desired.

STEP 2 Calculation of correlation matrix

$$\begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}, \quad (1)$$

where R_{11} is correlation matrix of set Z_1 (contains p_1 variates), and R_{22} is correlation matrix of set Z_2 (contains p_2 variates). $R_{12} = R_{21}'$ is the correlation matrix between the two sets. It is assumed that $p_1 \geq p_2$.

STEP 3 Computation of the eigenvalues and eigenvectors of equation (2) by using a Jacobilike method (Eberlein, 1962).

$$\begin{vmatrix} R_{22}^{-1} & R_{21} & R_{11}^{-1} & R_{12} \\ & & & \end{vmatrix} - \Lambda^2 I = 0 \quad (2)$$

The column matrix A_i which is the eigenvector of equation (2) contains the canonical coefficients of p_2 variates of i -th canonical root. $A_i' A_i = 1$.

STEP 4 The matrix, B_i , which contains the canonical coefficients of p_1 variates of i -th canonical root is

calculated as

$$B_i = R_{11}^{-1} R_{12} A_i / \lambda_i \quad (\lambda_i \neq 0), \quad (3)$$

where $B_i' B_i = 1$. Finally, the canonical variates U and V of i -th canonical root are given by the equations

$$U_i = A_i' Z_1, \text{ and } V_i = B_i' Z_2. \quad (4)$$

The numerical approach of this program is different from the canonical correlation program given by Cooley and Lohnes (1962) which was adopted in the Scientific Subroutine Package for IBM System/360.

STEP 5 Statistical test of canonical root.

Bartlett's statistic (Bartlett, 1938)

$$X^2 = - \left[N - \frac{1}{2}(p_1 + p_2 + 1) \right] \log_e L, \quad (5)$$

where $L = \pi^2 (1 - \lambda_i^2)$, follows approximately a chi-square distribution with $(p_1 - r + 1)(p_2 - r + 1)$ degrees of freedom. The assumption is made that Z_1 and Z_2 follow a multivariate normal distribution with zero means.

Detailed discussion of canonical correlation is given by Anderson (1958, p. 288-306), Wilks (1963, p. 587-590), and Lee (1968).

Example - Recent Sediment From Buttonwood Sound

Recent sediment specimens were collected by Lynts (1966) from 19 stations located in Buttonwood Sound, Florida Bay. Three samples of size 19 were taken on August 14th, 17th, and 20th, 1962, respectively. A sample of size 16 was taken on February 9th, 1963. For each location, the environmental parameters, depth of water, temperature, salinity, pH, and Eh, of the sediment-water interface were measured. The dominant element of macroflora in the Sound was grass, in particular, turtle grass. The distribution of turtle grass was mapped as very dense, dense-moderate, and patchy. The abundance of the turtle grass was coded by the writer as follows: very dense—1, dense-moderate—0, and patchy—-1.

The problem here is to determine to what extent the environmental factors, depth, temperature, salinity, pH, and abundance of turtle grass, are related to size parameters of sediments. Four samples were grouped together and considered as a single sample of size 73, because the turtle grass map is not specific to any one of the four sampling dates.

From examination of the simple correlation coefficients of all possible pairs of the seven variates (Table 1), it may be concluded that the turtle grass is related positively to silt and related negatively to sand. The simple correlation coefficients between the sediments and depth, temperature, salinity, and pH

Table 1.- Simple correlation coefficients of sediments from Buttonwood Sound

Turtle grass	1.000					
Depth	-0.061	1.000				
Temperature	0.091	-0.059	1.000			
Salinity	-0.085	0.086	-0.976	1.000		
pH	-0.194	0.242	0.122	-0.070	1.000	
Sand	-0.665	0.073	-0.192	0.194	0.173	1.000
Silt	0.458	0.084	0.015	0.001	-0.139	-0.602

are small.

A canonical analysis was performed on this set of data. The first canonical root is equal to 0.683 which is significant at the 1 percent level. The second canonical correlation (0.242) is not significant at the 5 percent level. This would suggest that in studying the relation between these two sets, attention may be restricted to the first pair of canonical variates which is listed in equation (6) and (7)

$$U_1 = -0.98(\text{turtle grass}) - 0.00(\text{depth}) - 0.07(\text{temperature}) + 0.13(\text{salinity}) + 0.10(\text{pH}), \text{ and} \quad (6)$$

$$V_1 = 1.00(\text{sand}) - 0.09(\text{silt}). \quad (7)$$

It is interpreted from the large coefficients that the distribution of sand is correlated closely with the abundance of turtle grass. Sands are more abundant in regions of less grass in Buttonwood Sound. Lynts (1966) arrived at the same conclusion by comparing the turtle grass map with sediment-size distribution map.

Principal component analysis also was performed on the correlation matrix of the same set of data. The rotated and normalized eigenvectors of the last principal component are practically zero. The eigenvectors of the sixth and fifth eigenvalues indicate the same relationship on sand, silt and turtle grass as that of the first eigenvalues (Table 2). These two principal components imply that there is slight interaction between the variates of sand and silt.

The coefficients of the first component are loaded highly with turtle grass and sand, with coefficients of opposite sign. This indicates that the first canonical variate is similar to the first component obtained by an ordinary principal component analysis. This component is interpreted as a "sediment stabilizer" factor.

It is interesting to examine the physical meaning of the second canonical correlation even though it is not statistically significant. The corresponding canonical variates are

Table 2.- Rotated and normalized seven principal components for sediment from Buttonwood Sound

Component Variate	1	2	3	4	5	6	7
Turtle grass	0.93	0.04	-0.03	0.09	-0.21	0.27	-0.00
Temperature	0.04	0.99	-0.02	-0.07	-0.01	0.06	-0.11
Salinity	-0.03	-0.99	0.04	0.02	-0.01	-0.06	-0.10
Depth	-0.02	-0.05	0.99	-0.12	-0.05	-0.03	-0.00
Sand	-0.37	-0.13	0.09	-0.08	0.34	-0.85	0.00
pH	-0.08	0.07	0.13	-0.98	0.06	-0.06	-0.00
Silt	0.20	-0.01	0.06	0.06	-0.94	0.24	-0.00
Eigenvalues	2.362	1.902	1.208	0.705	0.518	0.283	0.022
Cumulative percent	33.74	60.91	78.17	88.24	95.64	99.69	100.00

$$U_2 = 0.55(\text{sand}) + 0.84(\text{silt}), \text{ and} \quad (8)$$

$$V_2 = 0.05(\text{turtle grass}) + 0.26(\text{depth}) + 0.56(\text{temperature}) + 0.78(\text{salinity}) - 0.12(\text{pH}) \quad (9)$$

The second canonical correlation suggests that the amount of sand and silt could be predicted by certain combinations of environmental factors. If all variates are standardized (the origin of each variate is placed at its mean, and standard deviation is used as the unit of measurement), then the larger positive V_2 values implies higher percentages of both sand and silt, whereas larger negative V_2 values imply lower percentages of sand and silt. If the percentage of sand is high and the percentage of silt is low, or vice versa, then a small V_2 value will be given by equation (9). The variance of equation (8) explained by equation (9) is equal to 6 percent. However, this interpretation is merely an illustrative example to show multivariate prediction.

Limitations To Canonical Correlation

(1) The results of canonical correlation analysis may be difficult to interpret. Linear combinations of sets of variates need not have any intrinsic meaning. If the result shows a low canonical correlation, no doubt correlations do not exist between the two sets, no matter what types of linear combinations are used. Thus, the canonical correlation is the maximum correlation between linear combinations of the two sets of variates. The coefficients of the linear combination are not stable as variates are removed from (or new variates added to) the analysis. The technique is best regarded as an exploratory tool which will

give some idea of the complicated structure of a multivariate relation.

(2) For small sample sizes the shape of a sample cluster of the sets of variates may not be well defined. In this situation there may be a large sampling error in calculating simple correlation coefficients between any two variates in one set. Consequently, the direction of the canonical variates U , V will not necessarily pass through the center of the sample cluster of one set of variates and the signs and magnitudes of the coefficients (i.e. the direction cosines of the canonical variates) may not correspond to expectations.

A better result is produced by a more clearly defined sample cluster, that is in general by a larger sample size.

(3) If there is a relationship between the variates which changes at different levels of another variate (Fig. 1), i.e. if there is strong interaction between any two variates, the results of canonical correlation will be ambiguous.

(4) If the variates within one set are highly intercorrelated (i.e. the correlation matrix R_{11} or R_{22} of equation 2 is singular or nearly singular), and if the nature of the problem studied defined its canonical roots poorly (i.e. if the limiting eigenvalues of equation 2 are poorly defined), then the results of canonical correlation will be meaningless.

(5) Variates are assumed to be distributed normally for the purposes of making a statistical test on the canonical correlation coefficients (though not for the basic computational analysis).

Comparison With Other Statistical Techniques

(1) Multiple Correlation and Regression.— If in

a special situation of canonical correlation, the number of variates of one set is equal to one, then the canonical correlation will be the same as the multiple correlation. In a regression model, canonical correlation analysis permits the estimation of two or more dependent variates, whereas only one dependent variate may be estimated in conventional multiple regression. Natural variation is multivariate and consequently there are advantages to a model which analyses the variation of several dependent variates simultaneously.

(2) Principal Component Analysis.— Both canonical correlation analysis and principal component analysis result from orthogonal rotation. In canonical correlation, the purpose of rotation is to inquire how two linear combinations should be constructed so that the simple correlation coefficient between them is as large as possible; whereas in principal component analysis, the purpose of rotation is to seek the direction of the maximum variance or variation of a sample cluster.

In order to demonstrate geometrically the differences between principal component and canonical correlation, consider an example of two variates. Suppose a set of bivariate observations is made on X_1 and X_2 , and each observation is plotted on a two-dimensional space (Fig.2A) forming a swarm of points. In principal component analysis an orthogonal rotation is carried out such that the first principal component, C_1 , passes through the cluster and accounts for or "explains" the maximum variance (or variation) of the sample; whereas the second principal component, C_2 , which is perpendicular to C_1 , "explains" the maximum variance in another direction (Fig.2B).

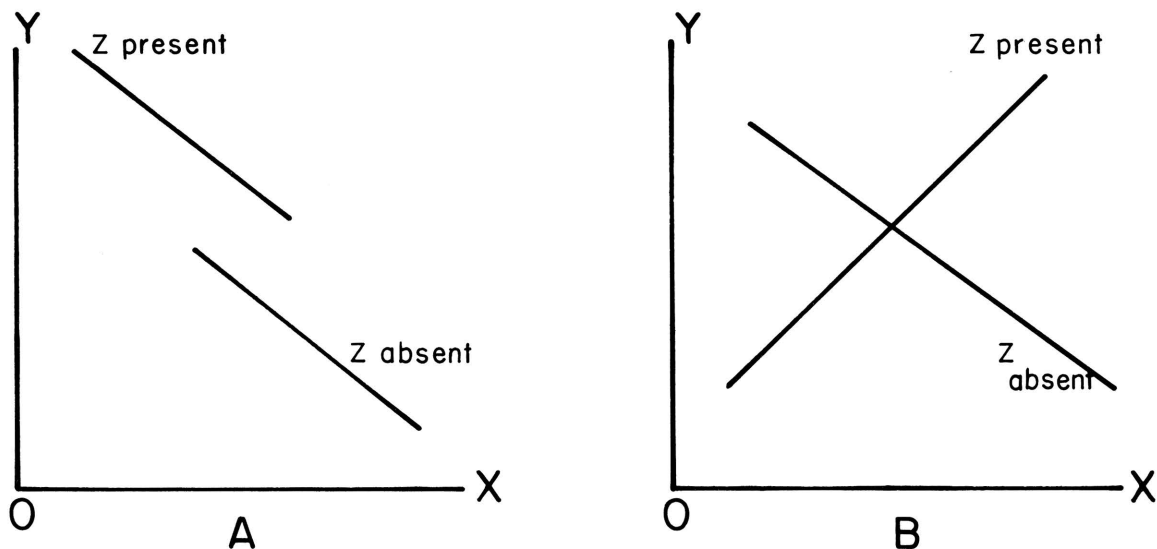


Figure 1.— A, No interactions between variates X and Y , simple correlation between them is high. B, Strong interaction occurs between variates X and Y , simple correlation between them is equal to zero.

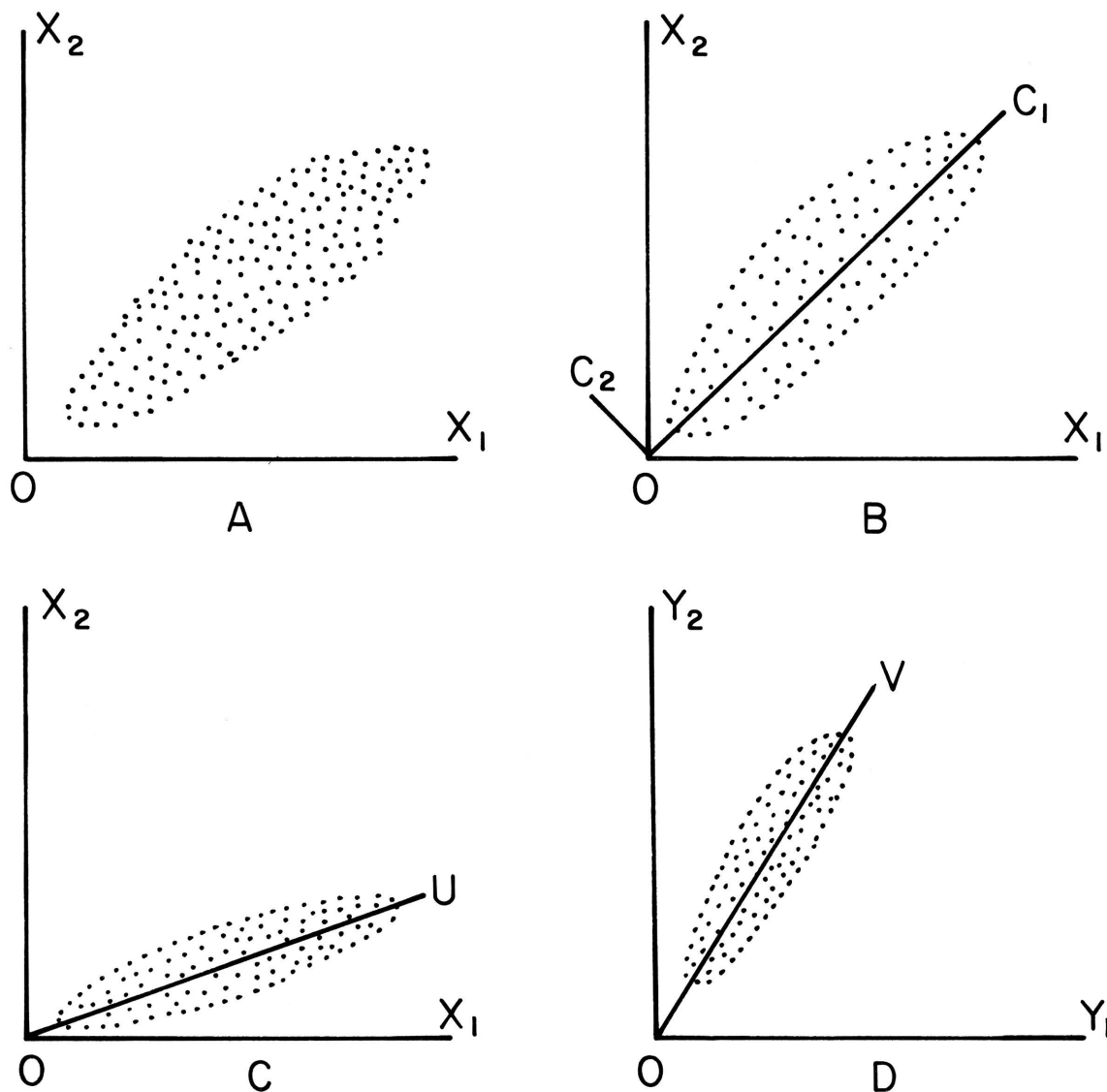


Figure 2.- A, Well-defined sample cluster of bivariate observations. B, Principal component analysis on bivariate observation. C, Canonical variate U passing through a sample cluster in $X_1 - X_2$ coordinates. D, Canonical variate V passing through a sample cluster in $Y_1 - Y_2$ coordinates.

The principal components C_1 and C_2 are linear combinations of variates X_1 and X_2 .

In canonical correlation, assume that one set consists of two variates, X_1 and X_2 , and the second set consists of variates Y_1 and Y_2 . A set of observations is made on these four variates. For the convenience of graphic representation, the observations are plotted on coordinates, X_1 - X_2 , and Y_1 - Y_2 , respectively, forming a swarm of points in each diagram (Figs. 2C and 2D), but actually the observations are considered properly as one set of points in a four-dimensional space. Then there will be a canonical variate passing through each swarm of points, respectively, in each of the two-dimensional spaces. We can imagine that the origins of these two systems

join together and that an orthogonal rotation is carried out such that the angle between U and V is the least possible. After determination of U and V in terms of the variates of each set, the U and V may be treated in a further two-dimensional space as $U = c + kV$, where c and k are constants.

Principal component analysis tends to express interactions by extra principal components correlated with the interacting components. But the way in which slight interactions can be detected from the results of canonical correlation analysis has not yet been discovered.

For solving a problem, the sample size for a canonical correlation analysis usually should be larger than that used for principal component analysis.

Principal component solution reveals more extensive information about internal relations of a set of measures than canonical correlation and is likely to

be a powerful tool for displaying these internal relations. On the other hand, where the purpose is to investigate the relations between two sets of variates, or to predict many dependent variates, the technique of canonical correlation is more appropriate.

Other Applications

(1) Matching factor patterns.— Suppose a separate factor or principal component analysis has been conducted for a rock body at different geographic localities or different stratigraphic sections. It may be that the factor patterns obtained at the various localities seem different but that canonical transformations exist such that some of the factors or principal components in one set would be found to correspond closely to factors or principal components in the other set. The technique has been generalized for m factor pattern by Horst (1961a, 1961b) to m canonical transformations which will yield new patterns having maximum similarity. A geologic example is given by Lee (1968).

(2) Q-technique canonical correlation.— Canonical correlation is used in this situation for dealing with sample space. Suppose there are two sets of samples collected from different groups (such as localities, or different formations), and the problem is to determine to what extent the two sets of samples are similar, based on observable variates. The canonical root provides an index of the maximum degree of similarity between the two groups of samples. The technique is applicable to samples of small size. A detailed discussion is given by Lee (1968).

Instructions For Using Program

Input to program

1. Title card
The project title and the investigator's name will be punched on one card.
2. Control card (all digits are right justified)

Cols. 1-5	Total number of observations.
Cols. 6-7	Number of variables of left-hand set, maximum of 30.
Cols. 8-9	Number of variables of right-hand set, maximum of 30. The number of variables of left-hand set must always be greater than or equal to that of right-hand set.
Cols. 10-11	Total number of variables subject to transformations, blank or zero for no transformation.
Col. 12	1 for correlation matrix input 2 for raw data matrix input
3. Transformation card(s) (optional)
Assume the 3-digit transformation code to be of the general form IJJ. II defines the subscript of the variables. J defines the type of transformation.

$$J=1 \quad \sin^{-1} \sqrt{x},$$

$$J=2 \quad \log_{10} x,$$

$$J=3 \quad \log_{10}(x + 1.0)$$

$$J=4 \quad \log_e x$$

$$J=5 \quad \log_e (x + 1.0)$$

$$J=6 \quad \sqrt{x}$$

Twenty-six variables are punched on one card, if there are more than twenty-six variables to be transformed, then two or more cards will be used.

4. Variable name card(s)

The output of the program is designed for self-explanation, so the variable names will be input together with data. Twelve characters are used for the names of each variable. They should be punched in a continuous sequence and also in the same order as in the data matrix or correlation matrix. Six names are punched on one card.

5. Data format card

This is used for the input data card.

6. Data cards

Each observation has its own separate data card—(s) two or more observations sharing one data card is not allowed. The data of left-hand set must be followed by the data of right-hand set. The correlation matrix must be stored row by row, each row going up to the diagonal elements.

7. Job-done card

The investigator may run more than one project at a time. Each project must contain all instruction cards mentioned above. A card with a word, DONE, punched on the first four columns is placed at the end of the deck.

Output from program

1. Project title and the investigator's name,
2. Correlation matrix,
3. Mean, variance, and standard deviation of each variable, if raw data is input,
4. Canonical roots, chi-square values, and significant level,
5. Canonical variates both of left and right-hand sets.

CANONICAL TREND SURFACES

Trend-surface analysis is now a familiar technique in geology and geography. The technique attempts to determine the "trend" of an areally distributed variate by constructing a surface from a polynomial expansion of the X, Y coordinates of the sample localities. One of the limitations of the technique is that it can be applied only to one variate

at a time. Commonly more than one variate has been measured at each locality, so that it seemed worth while to seek a multivariate trend surface which would summarize the areal variation of a set of variates simultaneously.

A multivariate trend surface was constructed by using the principle of canonical correlation analysis. This trend surface which is called canonical trend surface is a parsimonious summarization of areal variations of a set of geologic variates from a single population. By use of this type of trend it is possible to reveal the underlying pattern of geographic variations common to a set of variates. Details of the theory and computational procedures of canonical trend is given by Lee and Middleton (1967) and Lee (1968, in press).

The geographic coordinates, X and Y , and their various powers and cross-products constitute one set of p_1 variates, and the p_2 geologic variates, Z_1 , constitute the second set. The function of canonical trend analysis is to find one linear combination for the (X, Y) coordinates, and one for Z_1 such that these two linear combinations have a maximum correlation.

Example - Permian System in Western Kansas And Eastern Colorado

The stratigraphic data of upper Permian rocks in western Kansas and eastern Colorado were used as an example to illustrate the validity of the canonical trend in a practical situation. The hypothesis is that the area studied shows the characteristics of a sedimentary basin. In other words, the question is asked whether or not it is possible to evaluate a trend which is common to the thickness of sand, shale, carbonate, and evaporite. Thus, the thickness of sand, shale, carbonate, and evaporite were treated by canonical trend-surface analysis. The raw data were published by Krumbein (1962), and has been analyzed by using factor-vector method (Krumbein and Imbrie, 1963).

The data were subjected to canonical trend analysis. After three iterations, the highest canonical root that could be reached was 0.9464 which indicates that a cubic polynomial is the most predictable response surface. The canonical variate for the four sediments was

$$U = 0.516(\text{sand}) + 0.408(\text{shale}) - 0.104(\text{carbonate}) + 0.746(\text{evaporite}). \quad (10)$$

The canonical variate for the polynomial was

$$V = -0.407 X - 0.914 Y + 0.002 X^2 - 0.001 XY - 0.001 Y^2 \quad (11)$$

Equation (10) mainly indicates the variations in thickness of evaporite, shale, and sand. Equation

(11) and Figure 3 show that evaporite, shale, and sand thicken toward the southwest corner of Kansas. The variance of the linear function (10) explained by the linear function (11) is equal to 91 percent (the square of 0.9464). The canonical trend establishes the hypothesis suggested before carrying out the analysis.

The essential approach to the interpretation of a canonical trend surface is to visualize the geologic implications of the variations of all or most of the variates being displayed realistically in a single map.

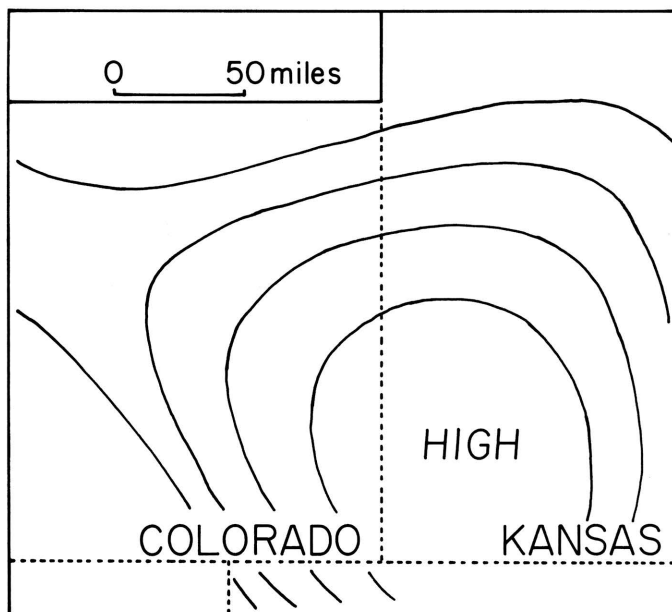


Figure 3.- Canonical trend surface for thickness of sand, shale, and evaporite of Permian unit in western Kansas and eastern Colorado.

Instructions For Using Program

Input to program

1. Title card
The project title and the investigator's name are punched on one card.
2. Control card (all digits are right justified)

Cols. 1-3	Total number of observations or sample size, maximum of 300.
Cols. 4-5	Number of dependent variables, maximum of 15.
Cols. 6-7	Total number of variables subjected to transformations.
Col. 8	Order of canonical polynomial, maximum of 6. If a number 6, was punched on column 8 the program would stop computing the higher order polynomial (≤ 6) if the difference of two successive canonical correlation was less than 0.05.
Cols. 9-16	Scale of trend map. In general we

use an arbitrary system for sample location. In order to have an actual scale for the map printed by the printer, the distance in meters which is equal to 1 unit in the arbitrary coordinate system is punched on columns 9-16. The input format is F8.0.

3. Transformation card

This instruction card enables the investigator to transform the dependent variables by using various transformations (see instructions for using canonical correlation program).

4. Variable name card

Twelve characters are used for the names of each variable. They should be punched in the same order as in the data matrix. Six names are punched on one card.

5. Data format card

This format is used for the input data cards. No more than 80 characters are allowed.

6. Data cards

The X-, Y-coordinates must be in the first two places and are followed by the data. The origin of the coordinate may be placed anywhere, but the convention for the sign of the reference coordinate is the same as the Cartesian coordinate system. The maximum length of the X-axis (horizontal axis) must be greater than or equal to that of the Y-axis (vertical axis). Each sample has its own separate data card(s). Two or more samples sharing one data card are not allowed.

Output from program

1. Project title and investigator's name,

2. Mean, and standard deviation of each geologic variable,
3. Covariance matrix for the standardized geologic variable,
4. Record of successive evaluation of the degree of the trend surface,
5. Each canonical correlation coefficient has one set of the following outputs
 - (I) Trend-surface equation and linear function of geologic variables,
 - (II) Observed, calculated, and residual values with X-, Y-coordinates,
 - (III) Contoured trend-surface map with explanation, and
 - (IV) Residual map.

CONCLUDING REMARKS

If there are two sets of variates relating to one set of samples, various statistical techniques may be adapted according to the nature of the problem discussed. We may, for example, factorize the two sets together, or we may factorize each set independently, and try to correlate factors, or we may perform a canonical correlation analysis between the two sets of variates in order to yield a maximum correlation.

There are no standard rules for discovering relationships among a set of variates. The easy availability of computer programs for statistical analysis will certainly enable a geologist to look at his own data in different ways.

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APPENDIX I. Complete FORTRAN IV source listing of canonical correlation program.

```

C      CANONICAL CORRELATION ANALYSIS PROGRAM
C      P J LEE AUGUST 1966
C      DEPARTMENT OF GEOLOGY, MCMASTER UNIVERSITY, HAMILTON, CANADA
C
C      SUBROUTINES REQUIRED: EBERVC, MATRIX, MATINV, AND ROSIE
C
C
      DIMENSION Q(1830), COR(30,30), A2(30,30), B(30,30), SUMSQ(60),
      1B1(30,30), TITLE(20), NTYPE(60), FMT(20), SUM(60), D(60), CHI(37),
      2NTRA(60)
      COMMON VEC(30,30), VARIAT(180), NUMBER(30), B2(30,30)
      DATA CHI/ 6.6349, 9.2103, 11.3449, 13.2767, 15.0863, 16.8119, 18
      1.4753, 20.0902, 21.6660, 23.2093, 24.7250, 26.2170, 27.6883, 29.14
      213, 30.5779, 31.9999, 33.4087, 34.8053, 36.1908, 37.5662, 38.9321,
      3 40.2894, 41.6384, 42.9798, 44.3141, 45.6417, 46.9630, 48.2782, 49
      4.5879, 50.8922, 63.6907, 76.1539, 88.3794, 100.4250, 112.3290, 124.11
      560, 135.8070/
      DATA HALT/4H DONE/
      DO 28 I=1,30
28  NUMBER(I)=I
90  READ(5,2) TITLE
      2 FORMAT(20A4)
      IF(TITLE(1).EQ.HALT) STOP
      READ(5,1) N,NL,NR,MTRA,I1
      1 FORMAT(I5,3I2,I1)
      WRITE(6,3) TITLE
      3 FORMAT(1H1,30X,20A4)
      WRITE(6,4)
      4 FORMAT(///)
      IF(MTRA.EQ.0) GOTO 17
      READ(5,103) (NTRA(I),NTYPE(I),I=1,MTRA)
103  FORMAT(26(I2,I1))
      17 M=NL+NR
      NV=3*M
      S=N
      M1=(M+1)*M/2
      READ(5,7) (VARIAT(I),I=1,NV)
      7 FORMAT(18A4)
      READ(5,2) FMT
      IF(I1.EQ.1) GOTO 9
      DO 10 J=1,M
      SUM(J)=0.0
10  SUMSQ(J)=0.0
      DO 11 J=1,M1
11  Q(J)=0.0
      DO 20 NSAMPL=1,N
      READ(5,FMT) (D(J),J=1,M)
      IF(MTRA.EQ.0) GOTO 13
      DO 104 ITRA=1,MTRA
      JTRA=NTRA(ITRA)
      KTYPE=NTYPE(ITRA)
      IF(KTYPE.EQ.1.OR.KTYPE.EQ.2.OR.KTYPE.EQ.3.OR.KTYPE.EQ.4.OR.KTYPE.
      1EQ.5.OR.KTYPE.EQ.6) GOTO 18
      WRITE(6,16)
16  FORMAT(1H0,37H WRONG CODE NUMBER FOR TRANSFORMATION)
      STOP
      18 GOTO(14,15,105,106,107,108), KTYPE
      14 D(JTRA)=ARSIN(SQRT(D(JTRA)))

```

```

      GOTO 104
15  D(JTRA)=ALOG10(D(JTRA))
      GOTO 104
105 D(JTRA)=ALOG10(D((JTRA)+1.0))
      GOTO 104
106 D(JTRA)=ALOG(D(JTRA))
      GOTO 104
107 D(JTRA)=ALOG(D(JTRA)+1.0)
      GOTO 104
108 D(JTRA)=SQRT(D(JTRA))
104 CONTINUE
13  DO 19 J=1,M
      SUM(J)=SUM(J)+D(J)
19  SUMSQ(J)=SUMSQ(J)+D(J)*D(J)
      M2=M-1
      DO 20 K=1,M2
      DO 20 K1=K,M
      L=K1*(K1-1)/2+K
88  IF(K1-K) 21,22,21
22  Q(L)=1.000
      GOTO 20
21  Q(L)=Q(L)+D(K)*D(K1)
20 CONTINUE
      DO 23 I=1,M2
      DO 23 J=I,M
      K=J*(J-1)/2+I
      IF(I-J) 24,25,24
25  Q(K)=1.000
      GOTO 23
24  Q(K)=(S*Q(K)-SUM(I)*SUM(J))/SQRT((S*SUMSQ(I)-SUM(I)*SUM(I))*
1  (S*SUMSQ(J)-SUM(J)*SUM(J)))
23 CONTINUE
      Q(K+1)=1.000
      WRITE(6,99)
99  FORMAT(1H1,30X,5H MEAN,11X,9H VARIANCE,7X,19H STANDARD DEVIATION/)
      IV1=0
      DO 101 I=1,M
      AMEAN=SUM(I)/S
      VAR=(S*SUMSQ(I)-SUM(I)**2)/(S*(S-1.0))
      DEV=SQRT(VAR)
      IV=IV1+1
      IV1=IV+2
101 WRITE(6,100) ((VARIAT(J),J=IV,IV1),AMEAN,VAR,DEV)
100 FORMAT(1H ,10X,3A4,5X,F8.3,9X,E12.4,9X,F8.3)
      GOTO 26
9  READ(5,FMT) (Q(I),I=1,M1)
26 DO 27 L=1,M,10
      WRITE(6,30) N
30 FORMAT(1H1,10X,50H CORRELATION MATRIX      THE SAMPLE SIZE IS EQUAL
1  TO,15///)
96 J2=(L-1)*3+1
      J3=J2+2
      DO 27 J=L,M
      K=0
      DO 29 I=L,J
      LIMIT=L+9
      IF(I.GT.LIMIT) GOTO 86
      KK=J*(J-1)/2+I
      K=K+1
29  D(K)=Q(KK)

```

```

86 WRITE(6,84) ((VARIAT(J1),J1=J2,J3),(D(K1),K1=1,K))
84 FORMAT(1H0,5X,3A4,10F8.3)
  J2=J3+1
  J3=J2+2
27 CONTINUE
  DO 32 I=1,NL
  DO 32 J=I,NL
  L=J*(J-1)/2+I
  A2(I,J)=Q(L)
32 A2(J,I)=A2(I,J)
  CALL MATINV(A2,NL,0,IERR)
  IF(IERR.EQ.0) GOTO 34
  WRITE(6,85)
85 FORMAT(1H0,85H CORRELATION MATRIX ON THE LEFT HAND SET CANNOT BE
1INVERTED TRANSFORMATION IS NEEDED)
  GOTO 90
34 DO 50 J=1,NR
  DO 50 I=1,NL
  K=(J+NL-1)*(J+NL)/2+I
50 COR(I,J)=Q(K)
  CALL MATRIX(NR,NL,NL,A2,COR,B)
  DO 52 K=1,NR
  DO 52 I=1,NR
  B1(K,I)=0.0
  DO 52 J=1,NL
52 B1(K,I)=B1(K,I)+COR(J,K)*B(J,I)
  DO 59 I=1,NR
  DO 59 J=I,NR
  L=(J+NL-1)*(J+NL)/2+I+NL
  A2(I,J)=Q(L)
59 A2(J,I)=A2(I,J)
  CALL MATINV(A2,NR,0,IERR)
  IF(IERR.EQ.0) GOTO 55
  WRITE(6,56)
56 FORMAT(1H1,85H CORRELATION MATRIX ON THE RIGHT HAND SET CANNONT BE
1INVERTED TRANSFORMATION IS NEEDED)
  GOTO 90
55 CALL MATRIX(NR,NR,NR,A2,B1,B2)
  DO 60 I=1,NR
  DO 60 J=1,NR
  IF(I.EQ.J) GOTO 61
  VEC(I,J)=0.0
  GOTO 60
61 VEC(I,J)=1.000
60 CONTINUE
  CALL EBERVC(NR,1,200,0.01,0.001,1000.0,30,1)
  M3=NR-1
  DO 62 I=1,M3
  IJ=I+1
  DO 62 J=IJ,NR
  IF(B2(I,I).GE.B2(J,J)) GOTO 62
  TEMP=B2(I,I)
  B2(I,I)=B2(J,J)
  B2(J,J)=TEMP
  DO 63 K=1,NR
  D(K)=VEC(K,I)
  VEC(K,I)=VEC(K,J)
63 VEC(K,J)=D(K)
62 CONTINUE
  WRITE(6,65)

```

```

65 FORMAT(1H1,10X,47H STATISTICAL TEST OF SUCCESSIVE CANONICAL ROOTS)
   WRITE(6,64)
64 FORMAT(1H0,16H CANONICAL ROOTS,8X,17H CHI SQUARE VALUE,5X,18H DEGR
   EEE OF FREEDOM,5X,18H SIGNIFICANT LEVEL)
   WL=1.000
   NROOT=0
   DO 66 I=1,NR
     JJ=NR-I+1
     IF(B2(JJ,JJ).LT.0.000) B2(JJ,JJ)=0.0
     WL=WL*(1.00-B2(JJ,JJ))
     L=(NR-JJ+1)*(NL-JJ+1)
     CHISQ=-1.00*(S-0.5*(FLOAT(M)+1.000))*ALOG(WL)
     IF(B2(JJ,JJ).NE.0.000) GOTO 67
     GOTO 68
67 NROOT=NROOT+1
   B2(JJ,JJ)=SQRT(B2(JJ,JJ))
68 IF(L.GE.30) GOTO 69
   IF(CHISQ.GE.CHI(L)) GOTO 70
71 F=-0.01
   GOTO 66
70 F=0.01
   GOTO 66
69 IF(L.GT.100) GOTO 51
   L=(L-25)/10+30
   IF(CHISQ.GE.CHI(L)) GOTO 70
   GOTO 71
51 CHI1=0.5*(2.3263+SQRT(2.0*FLOAT(L)-1.000))*2
   IF(CHISQ.GE.CHI1) GOTO 70
   GOTO 71
66 WRITE(6,72) B2(JJ,JJ),CHISQ,L,F
72 FORMAT(1H0,6X,F8.3,15X,F8.3,18X,I4,12X,F6.2)
   WRITE(6,12)
12 FORMAT(1H0,56H 0.01 SIGNIFICANT AT 1 PERCENT LEVEL,-0.01 INSIGNIFI
   ICANT)
   WRITE(6,73)
73 FORMAT(1H1,10X,41H CANONICAL VARIATE ON THE RIGHT HAND SET //)
   NLL=NL*3
   CALL ROSIE(NROOT,NR,NLL)
   CALL MATRIX(NROOT,NL,NR,B,VEC,COR)
   DO 77 I=1,NROOT
     DO 77 J=1,NL
77 COR(J,I)=COR(J,I)/B2(I,I)
     DO 78 I=1,NROOT
       D(I)=0.0
     DO 78 J=1,NL
78 D(I)=D(I)+COR(J,I)*COR(J,I)
     DO 79 I=1,NROOT
       DO 79 J=1,NL
79 VEC(J,I)=COR(J,I)/SQRT(D(I))
   WRITE(6,89)
89 FORMAT(///)
   WRITE(6,80)
80 FORMAT(1H0,10X,40H CANONICAL VARIATE ON THE LEFT HAND SET //)
   CALL ROSIE(NROOT,NL,0)
   GOTO 90
83 STOP
END

```

```

SUBROUTINE MATRIX(M,K,L,P,X,C)
DIMENSION P(30,30),X(30,30),C(30,30)
DO 201 I=1,M
DO 201 J=1,K
C(J,I)=0.0
DO 201 K1=1,L
201 C(J,I)=C(J,I)+P(J,K1)*X(K1,I)
RETURN
END

```

```

SUBROUTINE EBERVC(N,IN,NBMAX,EPS,EPS1,EF,NN,IND)
COMMON AV(30,30),VARIAT(180),NUMBER(30),A(30,30)
DO 16 II=1,IN
EPS=EPS/EF
EPS1=EPS1/EF
NB=0
18 DR=0.0
DI=0.0
DO 17 I=2,N
IJ=I-1
DO 17 J=1,IJ
C=A(I,J)+A(J,I)
D=A(I,I)-A(J,J)
IF(EPS.LE.ABS(C)) GOTO 23
21 CC=1.0
SS=0.0
GOTO 22
23 CC=D/C
SIG=SIGN(1.0,CC)
COT=CC+SIG*SQRT(1.0+CC*CC)
SS=SIG/SQRT(1.0+COT*COT)
CC=SS*COT
DR=DR+1.0
22 E=A(I,J)-A(J,I)
IF(EPS.GT.ABS(E)) GOTO 31
CO=CC*CC-SS*SS
SI=2.0*SS*CC
H=0.0
G=0.0
HJ=0.0
DO 40 K=1,N
IF(K.EQ.I) GOTO 40
IF(K.EQ.J) GOTO 40
H=H+A(I,K)*A(J,K)-A(K,I)*A(K,J)
S1=A(I,K)*A(I,K)+A(K,J)*A(K,J)
S2=A(J,K)*A(J,K)+A(K,I)*A(K,I)
G=G+S1+S2
HJ=HJ+S1-S2
40 CONTINUE
D=D*CO+C*SI
H=2.0*H*CO-HJ*SI
F=(2.0*E*D-H)/(4.0*(E*E+D*D)+2.0*G)
IF(EPS1.GT.ABS(F)) GOTO 31
CH=1.0/SQRT(1.0-F*F)
SH=F*CH
DI=DI+1.0

```

```

      GOTO 36
31  CH=1.0
    SH=0.0
36  C1=CH*CC-SH*SS
    C2=CH*CC+SH*SS
    S1=CH*SS+SH*CC
    S2=SH*CC-CH*SS
    IF((ABS(S1)+ABS(S2)).EQ.0.0) GOTO 17
    DO 52 L=1,N
      A1=A(L,I)
      A2=A(L,J)
      A(L,I)=C2*A1-S2*A2
      A(L,J)=C1*A2-S1*A1
      IF(IND.LT.0) GOTO 52
      A1=AV(L,I)
      A2=AV(L,J)
      AV(L,I)=C2*A1-S2*A2
      AV(L,J)=C1*A2-S1*A1
52  CONTINUE
    DO 53 L=1,N
      A1=A(I,L)
      A2=A(J,L)
      A(I,L)=C1*A1+S1*A2
      A(J,L)=C2*A2+S2*A1
      IF(IND.GT.0) GOTO 53
      A1=AV(I,L)
      A2=AV(J,L)
      AV(I,L)=C1*A1+S1*A2
      AV(J,L)=C2*A2+S2*A1
53  CONTINUE
17  CONTINUE
    IF((DR+DI).LT.0.5) GOTO 16
    NB=NB+1
    IF(NB.NE.NBMAX) GOTO 18
16  CONTINUE
    EPS=EPS*EF**IN
    EPS1=EPS1*EF**IN
    IF(IND.LE.0) GOTO 70
    DO 80 I=1,N
      SUM=0.0
      DO 81 J=1,N
81   SUM=SUM+AV(J,I)**2
      SUM=SQRT(SUM)
      DO 82 J=1,N
82   AV(J,I)=AV(J,I)/SUM
80  CONTINUE
    RETURN
70  DO 90 I=1,N
      SUM=0.0
      DO 91 J=1,N
91   SUM=SUM+AV(I,J)**2
      SUM=SQRT(SUM)
      DO 92 J=1,N
92   AV(I,J)=AV(I,J)/SUM
90  CONTINUE
    RETURN
  END

```

```

C      SUBROUTINE MATINV(A,N,M,IERR)
C      ADAPTED FROM MULTIVARIATE PROCEDURES FOR THE BEHAVIOURAL
C      SCIENCES BY COOLEY AND LOHNES, P.198.
C
      DIMENSION IPIVOT(30),A(30,30),INDEX(30,2),PIVOT(30)
      EQUIVALENCE (IROW,JROW),(ICOLUM,JCOLUM),(AMAX,T,SWAP)
      IERR=0
      DETERM=1.0
      DO 20 J=1,N
20    IPIVOT(J)=0
      DO 550 I=1,N
      AMAX=0.0
      DO 105 J=1,N
      IF(IPIVOT(J)-1) 60,105,60
60    DO 100 K=1,N
      IF(IPIVOT(K)-1) 80,100,740
80    IF(ABS(AMAX)-ABS(A(J,K))) 85,100,100
85    IROW=J
      ICOLUM=K
      AMAX=A(J,K)
100   CONTINUE
105   CONTINUE
      IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
      IF(IROW-ICOLUM) 140,260,140
140   DETERM=-DETERM
      DO 200 L=1,N
      SWAP=A(IROW,L)
      A(IROW,L)=A(ICOLUM,L)
200   A(ICOLUM,L)=SWAP
260   INDEX(I,1)=IROW
      INDEX(I,2)=ICOLUM
      PIVOT(I)=A(ICOLUM,ICOLUM)
      DETERM=DETERM*PIVOT(I)
      IF(PIVOT(I).GT.-0.0005.AND.PIVOT(I).LT.0.0005) GOTO 760
      A(ICOLUM,ICOLUM)=1.000
      DO 350 L=1,N
350   A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)
      DO 550 L1=1,N
      IF(L1-ICOLUM) 400,550,400
400   T=A(L1,ICOLUM)
      A(L1,ICOLUM)=0.0
      DO 450 L=1,N
450   A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
550   CONTINUE
      DO 710 I=1,N
      L=N+1-I
      IF(INDEX(L,1)-INDEX(L,2)) 630,710,630
630   JROW=INDEX(L,1)
      JCOLUM=INDEX(L,2)
      DO 705 K=1,N
      SWAP=A(K,JROW)
      A(K,JROW)=A(K,JCOLUM)
      A(K,JCOLUM)=SWAP
705   CONTINUE
710   CONTINUE
740   RETURN
760   IERR=1
      RETURN
      END

```

```

SUBROUTINE ROSIE(NROOT,NOV,IVAR)
COMMON VEC(30,30),VARIAT(180),NUMBER(30),B2(30,30)
IV1=IVAR
DO 1 L=1,NROOT,10
LIMIT=L+9
IPRINT=NROOT
IF(NROOT.GT.LIMIT) IPRINT=LIMIT
WRITE(6,2) (NUMBER(J),J=1,IPRINT)
2 FORMAT(1H0,2X,15H CANONICAL ROOT,1X,10I8//)
DO 1 K=1,NOV
IV=IV1+1
IV1=IV+2
1 WRITE(6,3) ((VARIAT(J),J=IV,IV1),(VEC(K,J),J=L,IPRINT))
3 FORMAT(1H ,5X,3A4,10F8.2)
RETURN
END

```

APPENDIX II. Input for sample problem of canonical correlation.

CANONICAL CORRELATION ANALYSIS ON BUTTONWOOD SOUND, FLORIDA BAY

73 5 2 2

TURTLE GRASSDEPTH TEMPERATURE SALINITY PH SAND
SILT

(F2.0,F3.1,3F5.1,2F5.0)

0	12	281	253	79	24	38	38
-1	20	282	265	77	66	5	29
-1	23	297	265	77	68	6	26
0	9	295	257	69	37	20	43
1	21	296	261	73	25	21	54
0	24	300	259	76	30	44	26
0	26	310	258	79	38	11	51
0	24	301	255	80	23	35	42
0	24	300	253	80	67	11	22
0	24	324	257	80	24	62	14
0	23	304	261	81	29	41	30
1	18	320	258	76	12	37	51
0	20	301	263	73	23	51	26
0	26	299	261	73	25	54	21
0	24	300	259	78	20	45	35
0	24	310	263	77	31	31	38
0	18	311	265	79	58	8	34
1	24	298	262	81	11	71	18
0	23	301	261	79	46	27	27
0	12	321	262	78	25	45	30
-1	20	311	265	79	74	13	13
-1	23	321	267	82	52	19	29
0	9	319	264	79	33	40	27
1	21	316	258	73	18	45	37
0	24	320	262	82	42	29	29
0	26	314	264	78	23	32	45
0	24	317	263	79	24	63	13
0	24	310	261	76	43	25	32
0	24	308	267	78	37	44	19
0	23	309	263	81	32	23	45
1	18	311	256	79	12	29	59
0	20	311	258	79	20	7	73
0	26	313	253	80	24	38	38
0	24	314	262	79	12	25	63
0	20	314	254	82	38	10	52
0	18	316	289	80	34	40	26
1	24	316	259	82	6	53	41
0	23	318	256	89	44	28	28
0	12	303	271	76	15	25	60
-1	20	301	266	80	88	6	6
-1	23	300	269	77	46	36	18

0	9	304	264	77	21	59	20
1	21	307	261	76	13	52	35
0	24	304	261	76	36	37	27
0	26	307	268	80	36	40	24
0	24	310	270	78	25	38	37
0	24	310	270	78	70	24	6
0	24	307	268	77	26	37	37
0	23	310	265	80	18	47	35
1	18	314	261	73	9	55	36
0	20	309	264	81	38	31	31
0	26	308	259	79	14	43	43
0	24	305	264	79	2	35	63
0	20	312	265	81	41	15	44
0	18	304	266	82	34	28	38
1	24	309	266	82	6	31	63
0	23	313	259	79	32	54	14
0	12	200	386	78	25	32	43
-1	23	195	400	79	74	11	15
-1	24	200	408	78	70	12	18
0	15	195	393	79	44	29	27
0	27	202	400	77	35	40	25
0	27	203	393	80	34	44	22
0	24	205	393	80	18	35	47
0	26	205	393	80	41	38	21
0	26	207	408	77	40	39	21
0	26	210	393	78	29	47	24
1	15	209	386	70	18	42	40
0	24	209	386	78	26	54	20
0	18	211	393	79	45	35	20
0	15	212	393	80	41	47	12
1	26	213	379	78	41	40	19
0	26	220	386	76	52	28	20

DONE

APPENDIX III. Output for sample problem of canonical correlation.

CANONICAL CORRELATION ANALYSIS ON DUTTONWOOD SOUND, FLORIDA BAY

	MEAN	VARIANCE	STANDARD DEVIATION
TURTLE GRASS	0.041	0.2622E 00	0.512
DEPTH	2.141	0.2083E 00	0.456
TEMPERATURE	28.551	0.1867E 02	4.321
SALINITY	29.104	0.3005E 02	5.481
PH	7.836	0.8711E-01	0.295
SAND	33.603	0.3280E 03	18.111
SILT	34.137	0.2290E 03	15.131

CORRELATION MATRIX THE SAMPLE SIZE IS EQUAL TO 73

TURTLE GRASS	1.000						
DEPTH	-0.061	1.000					
TEMPERATURE	0.091	-0.059	1.000				
SALINITY	-0.085	0.087	-0.976	1.000			
PH	-0.194	0.242	0.122	-0.070	1.000		
SAND	-0.701	0.070	-0.208	0.202	0.133	1.000	
SILT	0.476	0.057	-0.017	0.047	-0.124	-0.631	1.000

STATISTICAL TEST OF SUCCESSIVE CANONICAL ROOTS

CANONICAL ROOTS	CHI SQUARE VALUE	DEGREE OF FREEDOM	SIGNIFICANT LEVEL
0.294	6.242	4	-0.01
0.716	55.820	10	0.01

0.01 SIGNIFICANT AT 1 PERCENT LEVEL, -0.01 INSIGNIFICANT

CANONICAL VARIATE ON THE RIGHT HAND SET CANONICAL VARIATE ON THE LEFT HAND SET

CANONICAL ROOT	1	2	CANONICAL ROOT	1	2
SAND	1.00	0.53	TURTLE GRASS	-0.98	0.05
SILT	-0.00	0.85	DEPTH	0.02	0.12
			TEMPERATURE	-0.20	0.59
			SALINITY	0.01	0.79
			PH	0.02	-0.09

APPENDIX IV. Complete FORTRAN IV source listing of canonical trend-surface program.

```

C      CANONICAL TREND SURFACE PROGRAM
C      P J LEE JULY 1966
C      DEPARTMENT OF GEOLOGY, MCMASTER UNIVERSITY, HAMILTON, CANADA
C
C      SUBROUTINES REQUIRED: EBERVC, MATINV
C
C
      REAL IPOLY
      DOUBLE PRECISION Q(903),R11(27,27),R22(15,15),R12(27,15),
1 PRD(27,15),PRO1(15,15),SUMSQ(42),SUM(42),A(9,9)
      DIMENSION SIG(300),E(42),DOT(10),P(42),D(42),NTRA(15),NTYPE(15),
1 POLY(50,50),B(300),C(300),FMT(20),DM(300,17),TITLE(20),VARIAT(45),
2 IPOLY(50,50),RESIDU(300),TERM(27),MAPING(300,2)
      COMMON VEC(15,15),PRO2(15,15)
      EQUIVALENCE (POLY,IPOLY)
      DATA TERM/4H X,4H Y,4H X2,4H XY,4H Y2,4H X3,4H X2Y,4H XY2,
14H Y3,4H X4,4H X3Y,4HX2Y2,4H XY3,4H Y4,4H X5,4H X4Y,4HX3Y2,
24HX2Y3,4H XY4,4H Y5,4H X6,4H X5Y,4HX4Y2,4HX3Y3,4HX2Y4,4H XY5,
34H Y6/
      DATA DOT/2H 0,2H 1,2H 2,2H 3,2H 4,2H 5,2H 6,2H 7,2H 8,2H 9/
      DATA SAMPLE,BLANK/2H *,2H /
      READ(5,2) TITLE
2  FORMAT(20A4)
      READ(5,1) N,M,MTRA,NORDER,FEET
1  FORMAT(I3,2I2,I1,F8.0)
      S=N
      WRITE(6,3) TITLE
3  FORMAT(1H1,20X,20A4///)
      IF(MTRA.EQ.0) GOTO 13
      READ(5,201) (NTRA(I),NTYPE(I),I=1,MTRA)
201 FORMAT(26(I2,I1))
13 MU=M*3
      READ(5,6) (VARIAT(I),I=1,MU)
6  FORMAT(18A4)
      READ(5,2) FMT
      XMAX=-100000.0
      XMIN=100000.0
      YMAX=-100000.0
      YMIN=100000.0
      M90=M+27
      IM90=(27+M+1)*(27+M)/2
      DO 20 I=1,M90
      SUM(I)=0.0
20 SUMSQ(I)=0.0
      DO 21 I=1,IM90,1
21 Q(I)=0.0
      DO 131 ISAMPL=1,N
      READ(5,FMT) X,Y,(D(J),J=1,M)
      IF(MTRA.EQ.0) GOTO 11
      DO 15 ITRA=1,MTRA
      JTRA=NTRA(ITRA)
      KTYPE=NTYPE(ITRA)
      IF(KTYPE.EQ.1.OR.KTYPE.EQ.2.OR.KTYPE.EQ.3.OR.KTYPE.EQ.4.OR.
1KTYPE.EQ.5.OR.KTYPE.EQ.6) GOTO 202
19 WRITE(6,12)
12 FORMAT(1H0,30H WRONG CODE FOR TRANSFORMATION)
      STOP
202 GOTO(9,10,301,302,303,304),KTYPE

```

```

9 D(JTRA)=ARSIN(SQRT(D(JTRA)))
  GOTO 15
10 D(JTRA)=ALOG10(D(JTRA))
  GOTO 15
301 D(JTRA)=ALOG10(D(JTRA)+1.0)
  GOTO 15
302 D(JTRA)=ALOG(D(JTRA))
  GOTO 15
303 D(JTRA)=ALOG(D(JTRA)+1.0)
304 D(JTRA)=SQRT(D(JTRA))
  15 CONTINUE
11 DO 16 J=1,M
16 DM(ISAMPL,J)=D(J)
  DM(ISAMPL,M+1)=X
  DM(ISAMPL,M+2)=Y
  XMAX=AMAX1(X,XMAX)
  YMAX=AMAX1(Y,YMAX)
  XMIN=AMIN1(X,XMIN)
  YMIN=AMIN1(Y,YMIN)
  DO 130 I=1,M
  SUM(I)=SUM(I)+D(I)
130 SUMSQ(I)=SUMSQ(I)+D(I)*D(I)
131 CONTINUE
  DO 126 I=1,M
  SUMSQ(I)=DSQRT((S*SUMSQ(I)-(SUM(I))**2)/(S*(S-1.0)))
126 SUM(I)=SUM(I)/S
  WRITE(6,96)
  96 FORMAT(1H1,30X,5H MEAN,5X,19H STANDARD DEVIATION/)
  IV1=0
  DO 93 I=1,M
  IV=IV1+1
  IV1=IV+2
  93 WRITE(6,95) ((VARIAT(J),J=IV,IV1),SUM(I),SUMSQ(I))
  95 FORMAT(1H0,10X,3A4,5X,F10.3,7X,F12.3)
  WRITE(6,106)
106 FORMAT(///)
  DO 127 J=1,N
  DO 127 I=1,M
127 DM(J,I)=(DM(J,I)-SUM(I))/SUMSQ(I)
  DO 129 I=1,M90
129 SUM(I)=0.0
  DO 8 IS=1,N
  DO 128 J=1,M
128 D(J)=DM(IS,J)
  X=DM(IS,M+1)
  Y=DM(IS,M+2)
  L=M
  A(1,1)=1.0
  DO 17 I=1,6
  DO 18 J=1,I
  A(J,I+1)=A(J,I)*X
  L=L+1
18 D(L)=A(J,I+1)
  A(I+1,I+1)=A(I,I)*Y
  L=L+1
17 D(L)=A(I+1,I+1)
  DO 8 I=1,M90
22 SUM(I)=SUM(I)+D(I)
  DO 8 J=1,M90
  L=(J-1)*J/2+1

```

```

      Q(L)=Q(L)+D(J)*D(I)
8  CONTINUE
      DO 25 I=1,M90
      DO 25 J=I,M90
      K=(J-1)*J/2+I
25  Q(K)=(S*Q(K)-SUM(I)*SUM(J))/(S*(S-1.0))
      J3=0
      WRITE(6,102) N
102  FORMAT(1H0,10X,19H COVARIANCE  MATRIX,10X,21H THE SAMPLE SIZE IS
      1I5//)
      DO 103 J=1,M
      K=0
      DO 104 I=1,J
      KK=J*(J-1)/2+I
      K=K+1
104  E(K)=Q(KK)
      J2=J3+1
      J3=J2+2
      WRITE(6,105) ((VARIAT(J1),J1=J2,J3),(E(K1),K1=1,K))
105  FORMAT(1H0,5X,3A4,15F7.3)
103  CONTINUE
      ROOT=0.000
      ITERM=0
      WRITE(6,113)
113  FORMAT(1H1,10X,53H RECORD OF SUCCESSIVE EVALUATION TREND SURFACE D
      1EGREE///)
125  DO 27 NPOWER=1,NORDER
      IPOWER=NPOWER
      ITERM=IPOWER+ITERM+1
      IF(M.GT.ITERM) GOTO 37
      NL=ITERM
      NR=M
      DO 32 I=1,NR
      DO 32 J=1,NL
      K=(J+M-1)*(J+M)/2+I
32  R12(J,I)=Q(K)
33  DO 35 I=1,NR
      DO 35 J=I,NR
      L=J*(J-1)/2+I
      R22(I,J)=Q(L)
35  R22(J,I)=R22(I,J)
      CALL MATINV(R22,NR,15,IERR)
      IF(IERR.EQ.0) GOTO 29
39  WRITE(6,34)
34  FORMAT(1H0,45H GEOLOGICAL VARIATE MATRIX CANNOT BE INVERTED)
      STOP
29  DO 31 I=1,NL
      DO 31 J=I,NL
      K=(J+M-1)*(J+M)/2+I+M
      R11(I,J)=Q(K)
31  R11(J,I)=R11(I,J)
      CALL MATINV(R11,NL,27,IERR)
      IF(IERR.EQ.0) GOTO 36
43  WRITE(6,30)
30  FORMAT(1H0,42H X-Y COORDINATES MATRIX CANNOT BE INVERTED)
      STOP
37  NL=M
      NR=ITERM
42  DO 44 I=1,NR
      DO 44 J=I,NR

```

```

      K=(J+M-1)*(J+M)/2+I+M
      R22(I,J)=Q(K)
44  R22(J,I)=R22(I,J)
      CALL MATINV(R22,NR,15,IERR)
      IF(IERR.EQ.1) GOTO 43
56  DO 45 I=1,NL
      DO 45 J=1,NR
      K=(J+M-1)*(J+M)/2+I
45  R12(I,J)=Q(K)
      DO 40 I=1,NL
      DO 40 J=1,NL
      K=J*(J-1)/2+I
      R11(I,J)=Q(K)
40  R11(J,I)=R11(I,J)
      CALL MATINV(R11,NL,27,IERR)
      IF(IERR.EQ.1) GOTO 39
36  DO 46 I=1,NL
      DO 46 J=1,NR
      PRO(I,J)=0.0
      DO 46 K=1,NL
46  PRO(I,J)=PRO(I,J)+R11(I,K)*R12(K,J)
      DO 47 I=1,NR
      DO 47 J=1,NR
      PRO1(I,J)=0.0
      DO 47 K=1,NL
47  PRO1(I,J)=PRO1(I,J)+R12(K,I)*PRO(K,J)
      DO 48 I=1,NR
      DO 48 J=1,NR
      PRO2(I,J)=0.0
      DO 48 K=1,NR
48  PRO2(I,J)=PRO2(I,J)+R22(I,K)*PRO1(K,J)
      DO 49 I=1,NR
      DO 49 J=1,NR
      VEC(I,J)=0.0
      IF(I.EQ.J) VEC(I,J)=1.000
49  CONTINUE
      CALL EBERVC(NR,1,200,0.01,0.001,1000.0,15,1)
      TEMP=-100.0
      DO 50 J=1,NR
      IF(TEMP.GT.PRO2(J,J)) GOTO 50
      TEMP=PRO2(J,J)
      JJ=J
50  CONTINUE
      CANON=SQRT(PRO2(JJ,JJ))
      DIF=CANON-ROOT
      ROOT=CANON
      WRITE(6,52) IPOWER,ROOT
52  FORMAT(1H,10X,24H THE DEGREE IS EQUAL TO I2,5X,23H THE CANONICAL
      1ROOT IS F10.4)
      IF(DIF.LT.0.05.OR.ROOT.GE.0.95000) GOTO 51
27  CONTINUE
51  WRITE(6,53) IPOWER,ROOT
53  FORMAT(1H0,10X,57H THE DEGREE OF THE MOST PREDICTABLE SURFACE IS
      1EQUAL TO I2,3X,48H THE CORRESPONDING CANONICAL ROOT IS EQUAL TO
      1F7.4//)
      NR1=NR-1
      DO 171 I=1,NR1
      JP=I+1
      DO 171 J=JP,NR
      IF(PRO2(I,I).GE.PRO2(J,J)) GOTO 171

```

```

TEMP=PRQ2(I,I)
PRQ2(I,I)=PRQ2(J,J)
PRQ2(J,J)=TEMP
DO 174 K=1,NR
TEMP=VEC(K,J)
VEC(K,J)=VEC(K,1)
174 VEC(K,1)=TEMP
171 CONTINUE
TOTALX=XMAX-XMIN
TOTALY=YMAX-YMIN
INDEX=TOTALY/TOTALX*50.0
DELTA=TOTALX/50.0
TX=50.0/TOTALX
TY=FLOAT(INDEX)/TOTALY
DO 172 JJ=1,NR
INDEX1=1
PRQ2(JJ,JJ)=SQRT(PRQ2(JJ,JJ))
WRITE(6,173) PRQ2(JJ,JJ)
173 FORMAT(1H1,10X,37H TREND SURFACE FOR THE CANONICAL ROOT,2X,F8.4//)
WRITE(6,114)
114 FORMAT(1H0,10X,34H THE EQUATION OF THE TREND SURFACE//)
DO 54 I=1,NL
E(I)=0.0
DO 54 J=1,NR
54 E(I)=E(I)+PRQ(I,J)*VEC(J,JJ)
RR=0.0
DO 55 I=1,NL
E(I)=E(I)/PRQ2(JJ,JJ)
55 RR=RR+E(I)*E(I)
DO 57 I=1,NL
57 E(I)=E(I)/SQRT(RR)
J3=0
IF(M.GT.ITERM) GOTO 59
DO 60 J=1,M
J2=J3+1
J3=J2+2
60 WRITE(6,58) (VARIAT(J1),J1=J2,J3),VEC(J,JJ)
58 FORMAT(1H ,5X,3A4,3X,F6.3)
GOTO 112
59 DO 132 J=1,M
J2=J3+1
J3=J2+2
132 WRITE(6,58) (VARIAT(J1),J1=J2,J3),E(J)
112 DO 64 I=1,ITERM,10
IPRINT=I+9
LIMIT=ITERM
IF(ITERM.GT.IPRINT) LIMIT=IPRINT
WRITE(6,115)
115 FORMAT(//)
WRITE(6,62) (TERM(J),J=1,LIMIT)
62 FORMAT(1H0,10(6X,A4))
IF(M.GT.ITERM) GOTO 65
61 WRITE(6,63) (E(IK),IK=1,LIMIT)
63 FORMAT(1H0,10F10.4//)
GOTO 64
65 WRITE(6,63) (VEC(J,JJ),J=1,LIMIT)
64 CONTINUE
WRITE(6,97)
97 FORMAT(1H0,40H NOTE X4Y2=X**4*Y**2,X3=X**3,AND SO ON)
BSUM=0.0

```

```

CSUM=0.0
BSS=0.0
CSS=0.0
BCR=0.0
DO 72 NSAMPL=1,N
L=0
A(1,1)=1.0
DO 73 I=1,IPOWER
DO 74 J=1,I
A(J,I+1)=A(J,I)*DM(NSAMPL,M+1)
L=L+1
74 P(L)=A(J,I+1)
A(I+1,I+1)=A(I,I)*DM(NSAMPL,M+2)
L=L+1
73 P(L)=A(I+1,I+1)
108 B(NSAMPL)=0.0
C(NSAMPL)=0.0
IF(M.GT.ITERM) GOTO 75
DO 76 J=1,ITERM
76 B(NSAMPL)=B(NSAMPL)+E(J)*P(J)
DO 77 I=1,M
77 C(NSAMPL)=C(NSAMPL)+VEC(I,JJ)*DM(NSAMPL,I)
GOTO 31
75 DO 78 J=1,ITERM
78 B(NSAMPL)=B(NSAMPL)+VEC(J,JJ)*P(J)
DO 79 I=1,M
79 C(NSAMPL)=C(NSAMPL)+E(I)*DM(NSAMPL,I)
81 BSUM=BSUM+B(NSAMPL)
BSS=BSS+B(NSAMPL)**2
CSUM=CSUM+C(NSAMPL)
CSS=CSS+C(NSAMPL)**2
72 BCR=BCR+B(NSAMPL)*C(NSAMPL)
DENON=S*BSS-BSUM**2
ALPHA=(BSS*CSUM-BSUM*BCR)/DENON
BETA=(S*BCR-BSUM*CSUM)/DENON
DO 133 I=1,N
B(I)=ALPHA+BETA*B(I)
133 RESIDU(I)=C(I)-B(I)
S2=0.0
DO 116 I=1,N
116 S2=S2+RESIDU(I)
S2=-1.0*S2/S
DO 117 I=1,N
117 RESIDU(I)=RESIDU(I)+S2
WRITE(6,118) S2
118 FORMAT(1H0,10X,55H THE CONSTANT OF THE TREND SURFACE EQUATION IS E
1QUAL TO,F10.4)
WRITE(6,80)
80 FORMAT(1H1,13H X-COORDINATE,5X,13H Y-COORDINATE,5X,15H OBSERVED VA
1LUE,5X,17H CALCULATED VALUE,5X,9H RESIDUAL///)
WRITE(6,82) ((DM(I,M+1),DM(I,M+2),C(I),B(I),RESIDU(I)),I=1,N)
82 FORMAT(1H ,F10.4,8X,F10.4,8X,F10.4,12X,F10.4,8X,F10.4)
DO 66 LENGTH=1,INDEX
Y=YMAX-DELTA*(FLOAT(LENGTH)-1.0)
DO 66 LWIDTH=1,50
X=XMIN+DELTA*(FLOAT(LWIDTH)-1.0)
L=0
A(1,1)=1.0
DO 67 I=1,IPOWER
DO 68 J=1,I

```

```

      A(J,I+1)=A(J,I)*X
      L=L+1
68  P(L)=A(J,I+1)
      A(I+1,I+1)=A(I,I)*Y
      L=L+1
67  P(L)=A(I+1,I+1)
107 POLY(LENGTH,LWIDTH)=S2
      IF(M.GT.ITERM) GOTO 69
      DO 70 J=1,ITERM
70  POLY(LENGTH,LWIDTH)=POLY(LENGTH,LWIDTH)+E(J)*P(J)
      GOTO 66
69  DO 71 J=1,ITERM
71  POLY(LENGTH,LWIDTH)=POLY(LENGTH,LWIDTH)+VEC(J,J)*P(J)
66  POLY(LENGTH,LWIDTH)=ALPHA+BETA*POLY(LENGTH,LWIDTH)
      PMAX=-100000.0
      PMIN=100000.0
      DO 83 I=1,N
      PMAX=AMAX1(PMAX,B(I))
      PMIN=AMIN1(PMIN,B(I))
83  CONTINUE
      DIFF=PMAX-PMIN
86  GRAD=DIFF/10.0
      DO 88 LENGTH=1,INDEX
      DO 88 LWIDTH=1,50
      DO 121 I=1,10
      IGRAD=I
      DISC=GRAD*(FLOAT(I)-1.0)+PMIN
      IF(DISC.GE.POLY(LENGTH,LWIDTH)) GOTO 123
121 CONTINUE
      IGRAD=10
123 IPOLY(LENGTH,LWIDTH)=DOT(IGRAD)
88  CONTINUE
      DO 134 I=1,N
      DTEMPX=(DM(I,M+1)-XMIN)*TX
      DTEMPY=(YMAX-DM(I,M+2))*TY
      MAPING(I,1)=DTEMPX
      MAPING(I,2)=DTEMPY
      IF(MAPING(I,1).EQ.0) MAPING(I,1)=1
      IF(MAPING(I,2).EQ.0) MAPING(I,2)=1
134 CONTINUE
      DO 137 I=1,INDEX
      DO 137 J=1,50
      DO 138 K=1,N
      IF(MAPING(K,1).EQ.J.AND.MAPING(K,2).EQ.I) GOTO 139
138 CONTINUE
      GOTO 137
139 IPOLY(I,J)=SAMPLE
137 CONTINUE
150 SCALE=TOTALX*4.0/100.0*FEET
      MSCALE=SCALE
      WRITE(6,90) MSCALE
90  FORMAT(1H1,35X,5H ----,18,5H FEET,5X,18H * SAMPLE LOCALITY///)
153 WRITE(6,91)
91  FORMAT(1H ,13X,105H *****
1*****
      WRITE(6,92) ((IPOLY(I,J),J=1,50),I=1,INDEX)
92  FORMAT(1H ,13X,2H *,101X,2H */14X,2H *,50A2,1X,2H *)
      WRITE(6,124)
124  FORMAT(1H ,13X,2H *,101X,2H *)
      WRITE(6,91)

```

```

WRITE(6,122)
122 FORMAT(1H0,10X,7H LEGEND/)
DO 109 I=1,10
  DISC=GRAD*(FLOAT(I)-1.0)+PMIN
109 WRITE(6,110) (DOT(I),DISC)
110 FORMAT(1H0,11X,A2,2H =,F8.3)
  IF(INDEX1.EQ.2) GOTO 172
  PMAX=-100000.0
  PMIN=100000.0
  DO 151 I=1,N
    PMAX=AMAX1(PMAX,RESIDU(I))
    PMIN=AMIN1(PMIN,RESIDU(I))
151 CONTINUE
  GRAD=(PMAX-PMIN)/10.0
  DO 161 I=1,N
    DO 159 J=1,10
      JDOT=J
      DISC=GRAD*(FLOAT(J)-1.0)+PMIN
      IF(DISC.GE.RESIDU(I)) GOTO 160
159 CONTINUE
      JDOT=9
160 SIG(I)=DOT(JDOT)
161 CONTINUE
  DO 152 I=1,INDEX
    DO 152 J=1,50
      DO 157 K=1,N
        IF(MAPING(K,1).EQ.J.AND.MAPING(K,2).EQ.I) GOTO 156
        IPOLY(I,J)=BLANK
157 CONTINUE
        GOTO 152
156 IPOLY(I,J)=SIG(K)
152 CONTINUE
  INDEX1=2
  WRITE(6,158)
158 FORMAT(1H1,10X,17H THE RESIDUAL MAP//)
  GOTO 153
172 CONTINUE
100 STOP
END

```

```

SUBROUTINE EBERVC(N,IN,NBMAX,EPS,EPS1,EF,NN,IND)
COMMON AV(15,15),A(15,15)
DO 16 II=1,IN
  EPS=EPS/EF
  EPS1=EPS1/EF
  NB=0
18 DR=0.0
  DI=0.0
  DO 17 I=2,N
    IJ=I-1
    DO 17 J=1,IJ
      C=A(I,J)+A(J,I)
      D=A(I,I)-A(J,J)
      IF(EPS.LE.ABS(C)) GOTO 23
21 CC=1.0
    SS=0.0
    GOTO 22
23 CC=D/C
    SIG=SIGN(1.0,CC)
    COT=CC+SIG*SQRT(1.0+CC*CC)
    SS=SIG/SQRT(1.0+COT*COT)
    CC=SS*COT
    DR=DR+1.0
22 E=A(I,J)-A(J,I)
    IF(EPS.GT.ABS(E)) GOTO 31
    CO=CC*CC-SS*SS
    SI=2.0*SS*CC
    H=0.0
    G=0.0
    HJ=0.0
    DO 40 K=1,N
      IF(K.EQ.I) GOTO 40
      IF(K.EQ.J) GOTO 40
      H=H+A(I,K)*A(J,K)-A(K,I)*A(K,J)
      S1=A(I,K)*A(I,K)+A(K,J)*A(K,J)
      S2=A(J,K)*A(J,K)+A(K,I)*A(K,I)
      G=G+S1+S2
      HJ=HJ+S1-S2
40 CONTINUE
    D=D*CO+C*SI
    H=2.0*H*CO-HJ*SI
    F=(2.0*E*D-H)/(4.0*(E*E+D*D)+2.0*G)
    IF(EPS1.GT.ABS(F)) GOTO 31
    CH=1.0/SQRT(1.0-F*F)
    SH=F*CH
    DI=DI+1.0
    GOTO 36
31 CH=1.0
    SH=0.0
36 C1=CH*CC-SH*SS
    C2=CH*CC+SH*SS
    S1=CH*SS+SH*CC
    S2=SH*CC-CH*SS
    IF((ABS(S1)+ABS(S2)).EQ.0.0) GOTO 17
    DO 52 L=1,N
      A1=A(L,I)
      A2=A(L,J)
      A(L,I)=C2*A1-S2*A2
      A(L,J)=C1*A2-S1*A1
      IF(IND.LT.0) GOTO 52

```

```

      A1=AV(L,I)
      A2=AV(L,J)
      AV(L,I)=C2*A1-S2*A2
      AV(L,J)=C1*A2-S1*A1
52  CONTINUE
      DO 53 L=1,N
      A1=A(I,L)
      A2=A(J,L)
      A(I,L)=C1*A1+S1*A2
      A(J,L)=C2*A2+S2*A1
      IF(IND.GT.0) GOTO 53
      A1=AV(I,L)
      A2=AV(J,L)
      AV(I,L)=C1*A1+S1*A2
      AV(J,L)=C2*A2+S2*A1
53  CONTINUE
17  CONTINUE
      IF((DR+DI).LT.0.5) GOTO 16
      NB=NB+1
      IF(NB.NE.NBMAX) GOTO 18
16  CONTINUE
      EPS=EPS*EF**IN
      EPS1=EPS1*EF**IN
      IF(IND.LE.0) GOTO 70
      DO 80 I=1,N
      SUM=0.0
      DO 81 J=1,N
81  SUM=SUM+AV(J,I)**2
      SUM=SQRT(SUM)
      DO 82 J=1,N
82  AV(J,I)=AV(J,I)/SUM
80  CONTINUE
      RETURN
70  DO 90 I=1,N
      SUM=0.0
      DO 91 J=1,N
91  SUM=SUM+AV(I,J)**2
      SUM=SQRT(SUM)
      DO 92 J=1,N
92  AV(I,J)=AV(I,J)/SUM
90  CONTINUE
      RETURN
      END

```

```

C      SUBROUTINE MATINV(A,N,NN,IERR)
C      ADAPTED FROM MULTIVARIATE PROCEDURES FOR THE BEHAVIOURAL
C      SCIENCES BY COOLEY AND LOHNES, P.198.
C
      DOUBLE PRECISION A(NN,NN),PIVOT(27),AMAX
      DIMENSION IPIVOT(27),INDEX(27,2)
      EQUIVALENCE (IROW,JROW),(ICOLUMN,JCOLUMN),(AMAX,T,SWAP)
      IERR=0
      DETERM=1.0
      DO 20 J=1,N
20    IPIVOT(J)=0
      DO 550 I=1,N
      AMAX=0.0
      DO 105 J=1,N
      IF(IPIVOT(J)-1) 60,105,60
60    DO 100 K=1,N
      IF(IPIVOT(K)-1) 80,100,740
80    IF(DABS(AMAX)-DABS(A(J,K))) 85,100,100
85    IROW=J
      ICOLUMN=K
      AMAX=A(J,K)
100   CONTINUE
105   CONTINUE
      IPIVOT(ICOLUMN)=IPIVOT(ICOLUMN)+1
      IF(IROW-ICOLUMN) 140,260,140
140   DETERM=-DETERM
      DO 200 L=1,N
      SWAP=A(IROW,L)
      A(IROW,L)=A(ICOLUMN,L)
200   A(ICOLUMN,L)=SWAP
260   INDEX(I,1)=IROW
      INDEX(I,2)=ICOLUMN
      PIVOT(I)=A(ICOLUMN,ICOLUMN)
      DETERM=DETERM*PIVOT(I)
      IF(PIVOT(I).GT.-0.0005.AND.PIVOT(I).LT.0.0005) GOTO 760
      A(ICOLUMN,ICOLUMN)=1.000
      DO 350 L=1,N
350   A(ICOLUMN,L)=A(ICOLUMN,L)/PIVOT(I)
      DO 550 L1=1,N
      IF(L1-ICOLUMN) 400,550,400
400   T=A(L1,ICOLUMN)
      A(L1,ICOLUMN)=0.0
      DO 450 L=1,N
450   A(L1,L)=A(L1,L)-A(ICOLUMN,L)*T
550   CONTINUE
      DO 710 I=1,N
      L=N+1-I
      IF(INDEX(L,1)-INDEX(L,2)) 630,710,630
630   JROW=INDEX(L,1)
      JCOLUMN=INDEX(L,2)
      DO 705 K=1,N
      SWAP=A(K,JROW)
      A(K,JROW)=A(K,JCOLUMN)
      A(K,JCOLUMN)=SWAP
705   CONTINUE
710   CONTINUE
740   RETURN
760   IERR=1
      RETURN
      END

```

APPENDIX V. Input for sample problem of canonical trend surface.

CANONICAL TREND ANALYSIS ON PERMIAN SYSTEM FROM KANSAS AND COLORADO P J LEE

30 4 3 211200

SAND SHALE CARBONATE EVAPORITE

(2F5.1, 5X, 4F5.0)

185-	260	608	365	148	20	75
235-	285	640	224	304	14	98
260-	230	464	104	242	18	100
450-	220	532	157	238	0	137
550-	230	562	120	316	0	126
555-	140	530	30	461	0	39
20-	295	447	293	116	12	26
115-	330	844	451	311	42	40
230-	340	906	337	432	60	77
310-	355	845	266	350	24	205
290-	380	915	295	355	43	222
360-	400	1139	179	643	20	297
370-	365	1118	180	568	0	370
385-	420	1224	207	758	11	248
480-	345	1162	130	659	13	360
510-	330	1003	224	542	21	216
555-	310	721	229	400	12	80
620-	300	775	223	477	28	47
115-	430	614	255	272	28	59
225-	495	702	237	341	39	85
260-	500	933	275	435	41	182
310-	485	1001	348	450	17	186
425-	440	1204	277	610	10	307
410-	510	1144	310	520	12	302
380-	550	1048	362	510	12	164
430-	530	1114	246	528	32	308
420-	550	1023	295	501	18	209
570-	460	955	267	502	24	162
575-	510	1005	271	637	8	89
340-	580	1126	270	558	68	230

APPENDIX VI. Output for sample problem of canonical trend surface.

CANONICAL TREND ANALYSIS ON PERMIAN SYSTEM FROM KANSAS AND COLORADO P J LEE

	MEAN	STANDARD DEVIATION
SAND	247.567	87.018
SHALE	439.467	155.699
CARBONATE	21.567	16.850
EVAPORITE	168.200	101.715

COVARIANCE MATRIX				THE SAMPLE SIZE IS	30
SAND	1.000				
SHALE	-0.138	1.000			
CARBONATE	0.462	-0.047	1.000		
EVAPORITE	-0.117	0.663	-0.097	1.000	

RECORD OF SUCCESSIVE EVALUATION TREND SURFACE DEGREE

THE DEGREE IS EQUAL TO 1	THE CANONICAL ROOT IS	0.7804
THE DEGREE IS EQUAL TO 2	THE CANONICAL ROOT IS	0.8810
THE DEGREE IS EQUAL TO 3	THE CANONICAL ROOT IS	0.9464

THE DEGREE OF THE MOST PREDICTABLE SURFACE IS EQUAL TO 3
THE CORRESPONDING CANONICAL ROOT IS EQUAL TO 0.9464

TREND SURFACE FOR THE CANONICAL ROOT 0.9464

THE EQUATION OF THE TREND SURFACE

SAND	0.516
SHALE	0.408
CARBONATE	-0.104
EVAPORITE	0.746

X	Y	X2	XY	Y2	X3	X2Y	XY2	Y3
-0.4031	-0.9149	0.0146	-0.0048	-0.0145	-0.0001	0.0003	0.0002	0.0000

NOTE X4Y2=X**4*Y**2,X3=X**3,AND SO ON

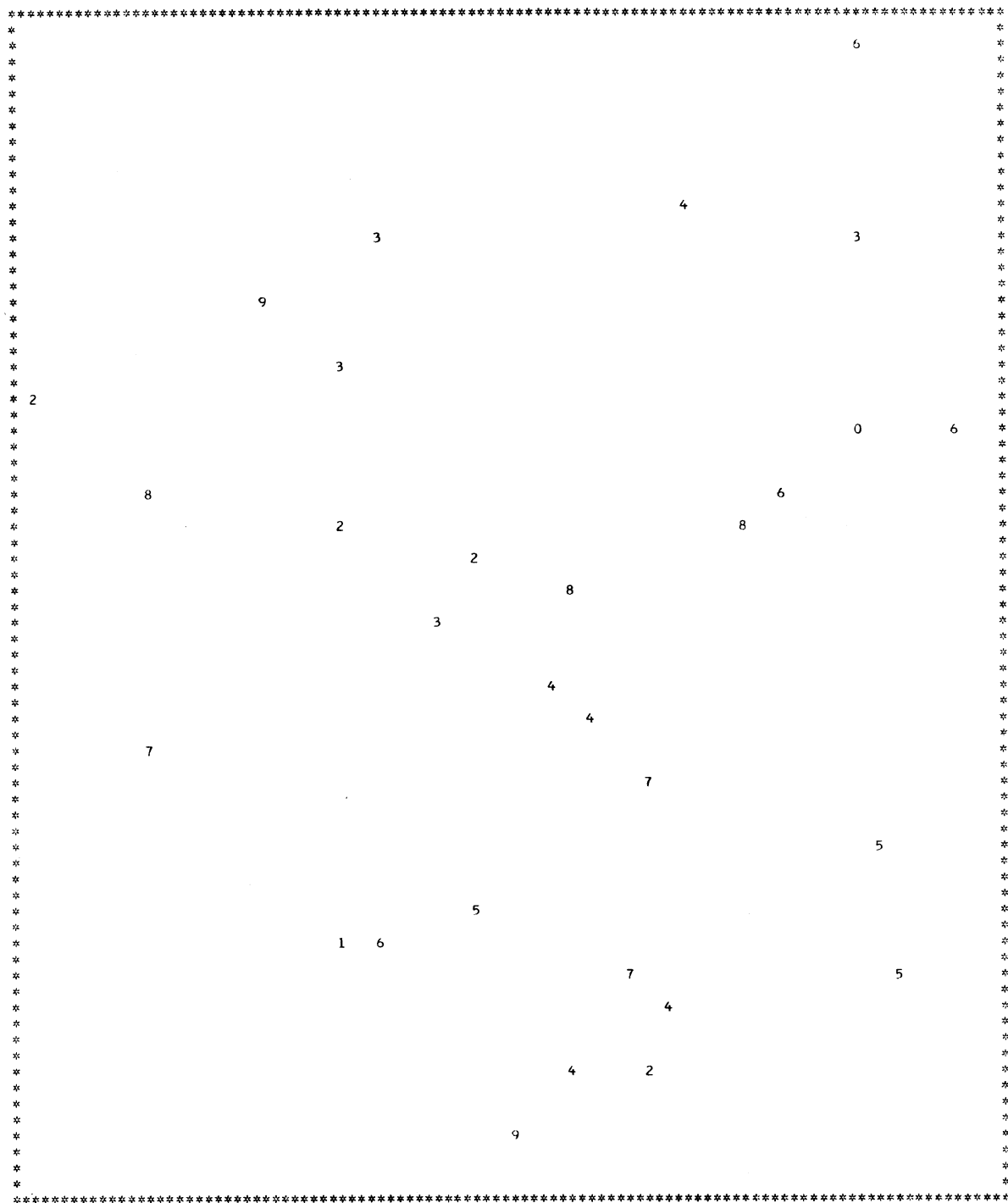
THE CONSTANT OF THE TREND SURFACE EQUATION IS EQUAL TO 0.0000

X-COORDINATE	Y-COORDINATE	OBSERVED VALUE	CALCULATED VALUE	RESIDUAL
18.5000	-26.0000	-0.7406	-1.2937	0.5532
23.5000	-28.5000	-0.9628	-0.6816	-0.2812
26.0000	-23.0000	-1.8469	-1.5947	-0.2521
45.0000	-22.0000	-1.1607	-1.0923	-0.0684
55.0000	-23.0000	-1.2566	-1.0149	-0.2416
55.5000	-14.0000	-2.0489	-2.2093	0.1604
2.0000	-29.5000	-1.5615	-1.1965	-0.3650
11.5000	-33.0000	-0.1959	-0.8965	0.7006
31.0000	-35.5000	0.1300	0.5782	-0.4481
23.0000	-34.0000	-0.3948	-0.0700	-0.3248
36.0000	-40.0000	1.0806	1.1523	-0.0716
29.0000	-38.0000	0.3227	0.6376	-0.3148
37.0000	-36.5000	1.5488	0.9287	0.6201
38.5000	-42.0000	1.2438	1.3327	-0.0888
48.0000	-34.5000	1.3371	0.6505	0.6866
51.0000	-33.0000	0.4828	0.3324	0.1504
55.5000	-31.0000	-0.8015	-0.2234	-0.5780
62.0000	-30.0000	-0.9761	-1.1118	0.1357
11.5000	-43.0000	-1.2350	-1.4280	0.1930
22.5000	-49.5000	-1.0382	-0.5006	-0.5375
26.0000	-50.0000	0.1325	0.0103	0.1223
31.0000	-48.5000	0.7820	0.7993	-0.0172
42.5000	-44.0000	1.7104	1.4494	0.2611
41.0000	-51.0000	1.6215	1.3960	0.2255
38.0000	-55.0000	0.8916	0.9637	-0.0721
43.0000	-53.0000	1.1837	1.3404	-0.1567
42.0000	-55.0000	0.7637	1.1873	-0.4235
57.0000	-46.0000	0.2185	0.2740	-0.0554
57.5000	-51.0000	0.1589	0.1423	0.0166
34.0000	-58.0000	0.6106	0.1394	0.4713

[illegible]

34

THE RESIDUAL MAP



LEGEND

0 = -0.578	5 = 0.061
1 = -0.450	6 = 0.189
2 = -0.322	7 = 0.317
3 = -0.194	8 = 0.445
4 = -0.067	9 = 0.573

TREND SURFACE FOR THE CANONICAL ROOT 0.8671

THE EQUATION OF THE TREND SURFACE

SAND 0.757
SHALE -0.115
CARBONATE 0.616
EVAPORITE -0.184

X	Y	X2	XY	Y2	X3	X2Y	XY2	Y3
0.1807	-0.9832	-0.0060	0.0049	-0.0230	0.0001	0.0001	0.0001	-0.0002

NOTE $X4Y2 = X**4*Y**2$, $X3 = X**3$, AND SO ON

THE CONSTANT OF THE TREND SURFACE EQUATION IS EQUAL TO 0.0001

X-COORDINATE	Y-COORDINATE	OBSERVED VALUE	CALCULATED VALUE	RESIDUAL
18.5000	-26.0000	1.3449	0.9334	0.4116
23.5000	-28.5000	-0.2565	0.8108	-1.0671
26.0000	-23.0000	-1.1130	-0.5538	-0.5590
45.0000	-22.0000	-1.3743	-2.2745	0.9003
55.0000	-23.0000	-1.7330	-1.1140	-0.6190
55.5000	-14.0000	-2.4639	-2.5063	0.0424
2.0000	-29.5000	0.5376	0.8094	-0.2717
11.5000	-33.0000	2.8431	1.9043	0.9388
31.0000	-35.5000	0.2478	0.2509	-0.0031
23.0000	-34.0000	2.3547	1.2650	1.0898
36.0000	-40.0000	-1.0349	-0.3683	-0.6665
29.0000	-38.0000	1.1608	0.5450	0.6159
37.0000	-36.5000	-1.8355	-0.5313	-1.3042
38.5000	-42.0000	-1.1153	-0.6325	-0.4827
48.0000	-34.5000	-1.8430	-1.3810	-0.4620
51.0000	-33.0000	-0.3863	-1.3241	0.9374
55.5000	-31.0000	-0.3232	-0.8622	0.5390
62.0000	-30.0000	0.2137	0.7124	-0.4986
11.5000	-43.0000	0.6193	1.2072	-0.5878
22.5000	-49.5000	0.7679	0.9118	-0.1438
26.0000	-50.0000	0.9279	0.7713	0.1562
31.0000	-48.5000	0.6670	0.3568	0.3103
42.5000	-44.0000	-0.5421	-0.9449	0.4029
41.0000	-51.0000	-0.1074	-0.2303	0.1230
38.0000	-55.0000	0.6022	0.6296	-0.0273
43.0000	-53.0000	0.0507	0.0125	0.0383
42.0000	-55.0000	0.1637	0.4818	-0.3179
57.0000	-46.0000	0.2239	-0.5634	0.7875
57.5000	-51.0000	-0.2924	0.2331	-0.5254
34.0000	-58.0000	1.6959	1.4533	0.2427

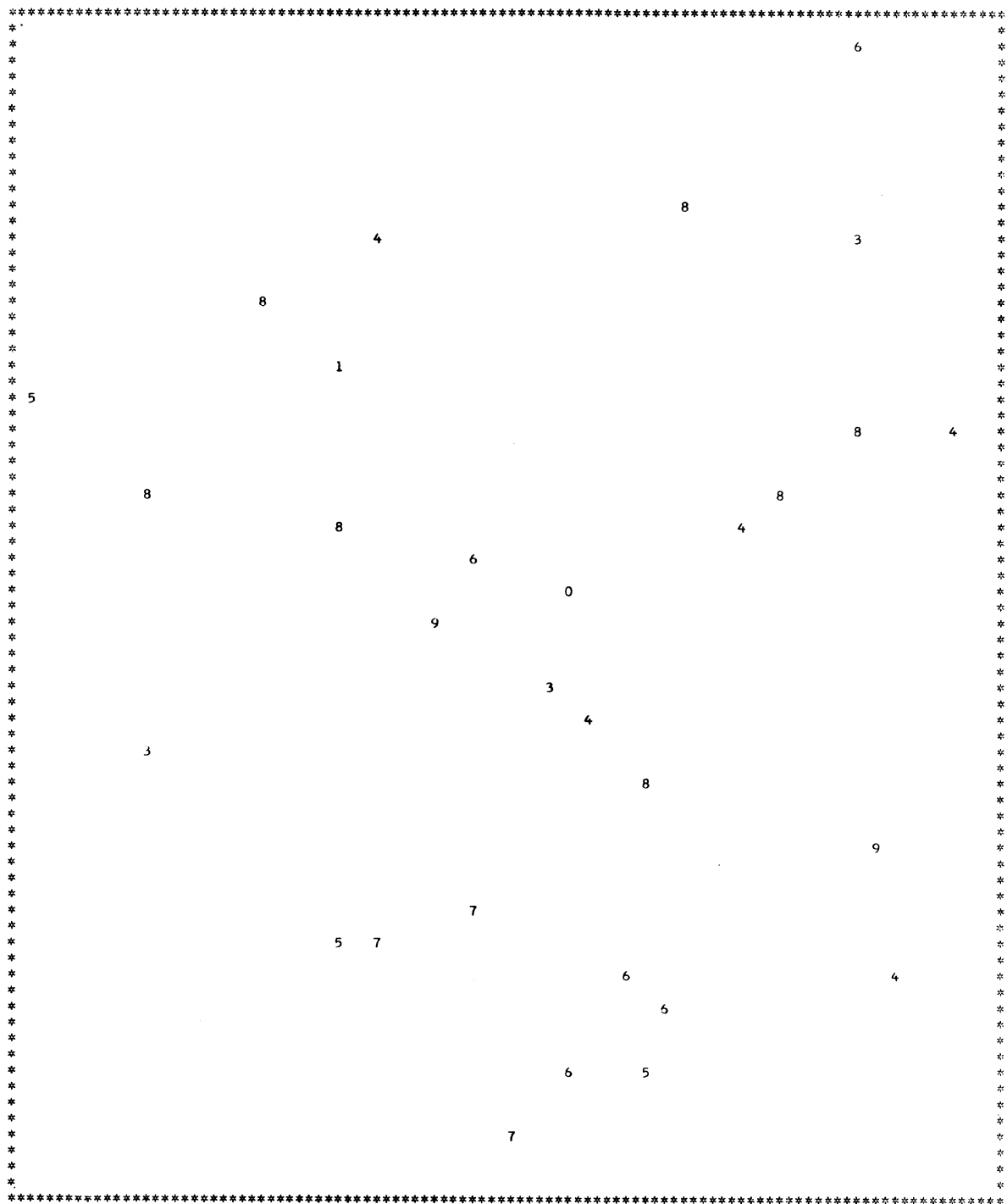
* SAMPLE LOCALITY

[illegible]

LEGEND

0 = -2.506	5 = -0.301
1 = -2.065	6 = 0.140
2 = -1.624	7 = 0.581
3 = -1.183	8 = 1.022
4 = -0.742	9 = 1.463

THE RESIDUAL MAP



LEGEND

0 = -1.304	5 = -0.107
1 = -1.065	6 = 0.132
2 = -0.825	7 = 0.372
3 = -0.586	8 = 0.611
4 = -0.347	9 = 0.850

TREND SURFACE FOR THE CANONICAL ROOT 0.7282

THE EQUATION OF THE TREND SURFACE

SAND 0.087
SHALE 0.737
CARBONATE -0.093
EVAPORITE -0.663

X	Y	X2	XY	Y2	X3	X2Y	XY2	Y3
0.5857	-0.8101	-0.0120	0.0220	-0.0058	0.0002	0.0001	0.0004	0.0001

NOTE X4Y2=X**4*Y**2,X3=X**3,AND SO ON

THE CONSTANT OF THE TREND SURFACE EQUATION IS EQUAL TO 0.0000

X-COORDINATE	Y-COORDINATE	OBSERVED VALUE	CALCULATED VALUE	RESIDUAL
18.5000	-26.0000	-0.6466	-0.3713	-0.2753
23.5000	-28.5000	-0.1656	-0.3185	0.1529
26.0000	-23.0000	-0.6146	-0.6986	0.0841
45.0000	-22.0000	-0.7220	-0.6460	-0.0760
55.0000	-23.0000	-0.3179	0.1317	-0.4496
55.5000	-14.0000	0.8461	0.6746	0.1715
2.0000	-29.5000	-0.5064	-0.4545	-0.0520
11.5000	-33.0000	0.3179	0.0321	0.2858
31.0000	-35.5000	-0.6587	-0.2108	-0.4479
23.0000	-34.0000	0.4360	-0.0525	0.4885
36.0000	-40.0000	0.0642	-0.1698	0.2341
29.0000	-38.0000	-0.8221	-0.0318	-0.7402
37.0000	-36.5000	-0.6552	-0.2978	-0.3575
38.5000	-42.0000	1.0063	-0.1361	1.1424
48.0000	-34.5000	-0.2810	-0.2781	-0.0030
51.0000	-33.0000	0.1535	-0.1789	0.3324
55.5000	-31.0000	0.4225	0.1336	0.2890
62.0000	-30.0000	0.9078	0.9758	-0.0680
11.5000	-43.0000	-0.1094	0.0236	-0.1330
22.5000	-49.5000	-0.0310	-0.0656	0.0346
26.0000	-50.0000	-0.1913	-0.0558	-0.1354
31.0000	-48.5000	0.0596	-0.0132	0.0729
42.5000	-44.0000	-0.0038	-0.0632	0.0594
41.0000	-51.0000	-0.3755	0.0794	-0.4549
38.0000	-55.0000	0.5290	0.0069	0.5221
43.0000	-53.0000	-0.5515	0.1703	-0.7219
42.0000	-55.0000	0.0926	0.1523	-0.0596
57.0000	-46.0000	0.3426	0.7942	-0.4516
57.5000	-51.0000	1.5506	1.1355	0.4151
34.0000	-58.0000	-0.0762	-0.2171	0.1409

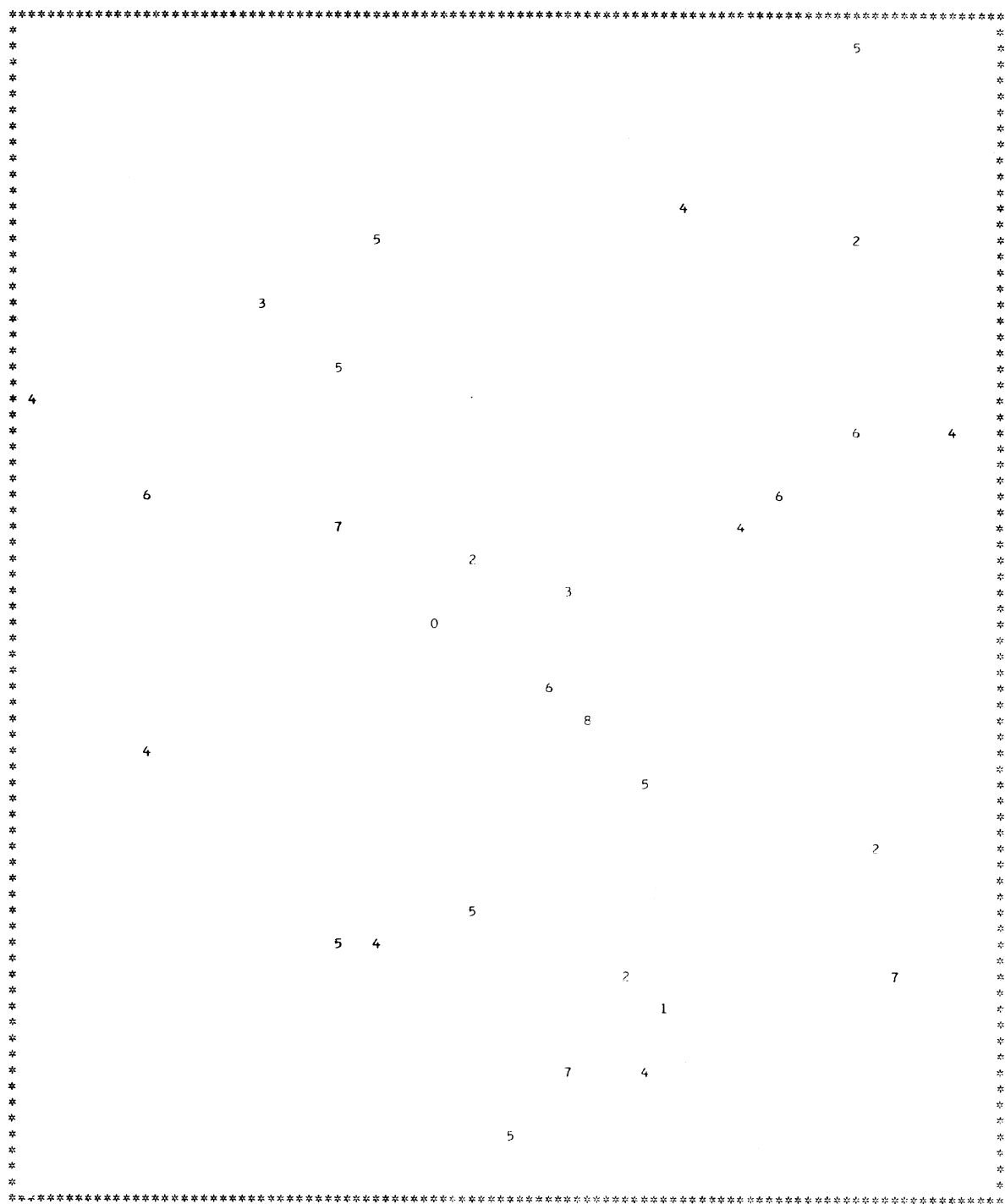
----- 506979 FEET * SAMPLE LOCALITY

[illegible]

LEGEND

0 = -0.699	5 = 0.218
1 = -0.515	6 = 0.402
2 = -0.332	7 = 0.585
3 = -0.148	8 = 0.769
4 = 0.035	9 = 0.952

THE RESIDUAL MAP



LEGEND

0 = -0.740	5 = 0.201
1 = -0.552	6 = 0.389
2 = -0.364	7 = 0.578
3 = -0.175	8 = 0.766
4 = 0.013	9 = 0.954

TREND SURFACE FOR THE CANONICAL ROOT 0.5201

THE EQUATION OF THE TREND SURFACE

SAND -0.630
 SHALE 0.139
 CARBONATE 0.762
 EVAPORITE 0.057

X	Y	X2	XY	Y2	X3	X2Y	XY2	Y3
0.6705	-0.7415	-0.0124	0.0074	-0.0164	0.0001	-0.0001	-0.0001	-0.0002

NOTE X4Y2=X**4*Y**2,X3=X**3,AND SO ON

THE CONSTANT OF THE TREND SURFACE EQUATION IS EQUAL TO 0.0000

X-COORDINATE	Y-COORDINATE	OBSERVED VALUE	CALCULATED VALUE	RESIDUAL
18.5000	-26.0000	-1.2328	-0.2893	-0.9434
23.5000	-28.5000	-0.3318	-0.0378	-0.2940
26.0000	-23.0000	0.6634	-0.0629	0.7263
45.0000	-22.0000	-0.5172	0.2222	-0.7394
55.0000	-23.0000	-0.1860	0.3255	-0.5115
55.5000	-14.0000	0.5458	0.0780	0.4678
2.0000	-29.5000	-1.1296	-1.4474	0.3178
11.5000	-33.0000	-0.7343	-0.3789	-0.3554
31.0000	-35.5000	-0.0825	0.0575	-0.1400
23.0000	-34.0000	1.0335	0.0287	1.0048
36.0000	-40.0000	0.6789	-0.0443	0.7233
29.0000	-38.0000	0.5811	0.0690	0.5121
37.0000	-36.5000	-0.2589	-0.0080	-0.2509
38.5000	-42.0000	0.1443	-0.1176	0.2619
48.0000	-34.5000	0.7665	-0.0287	0.7952
51.0000	-33.0000	0.2631	0.0354	0.2277
55.5000	-31.0000	-0.3830	0.1606	-0.5435
62.0000	-30.0000	0.4344	0.3629	0.0715
11.5000	-43.0000	0.0267	0.2790	-0.2523
22.5000	-49.5000	0.7307	0.6357	0.0950
26.0000	-50.0000	0.6843	0.5205	0.1638
31.0000	-48.5000	-0.9140	0.2142	-1.1282
42.5000	-44.0000	-0.5064	-0.2343	-0.2722
41.0000	-51.0000	-0.7378	-0.1446	-0.5932
38.0000	-55.0000	-1.2004	0.1929	-1.3932
43.0000	-53.0000	0.6405	-0.1678	0.8083
42.0000	-55.0000	-0.4269	-0.0294	-0.3975
57.0000	-46.0000	0.0217	-0.4124	0.4341
57.5000	-51.0000	-0.6515	-0.4988	-0.1527
34.0000	-58.0000	2.0783	0.7207	1.3576

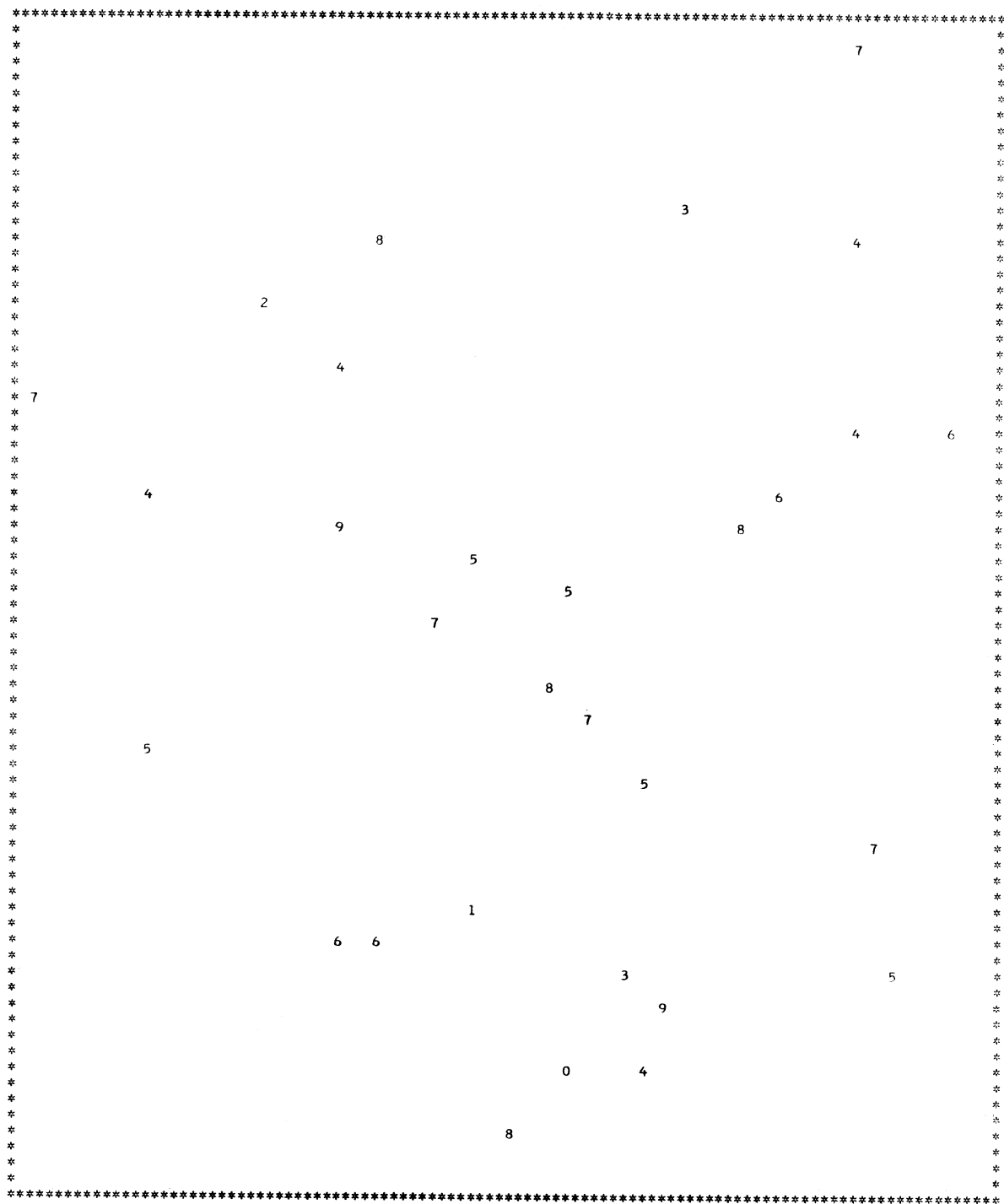
---- 506879 FEET * SAMPLE LOCALITY

[illegible]

LEGEND

0 = -1.447	5 = -0.363
1 = -1.231	6 = -0.147
2, = -1.014	7 = 0.070
3 = -0.797	8 = 0.287
4 = -0.580	9 = 0.504

THE RESIDUAL MAP



LEGEND

0 = -1.393	5 = -0.018
1 = -1.116	6 = 0.257
2 = -0.843	7 = 0.532
3 = -0.568	8 = 0.807
4 = -0.293	9 = 1.082

KANSAS GEOLOGICAL SURVEY COMPUTER PROGRAM
THE UNIVERSITY OF KANSAS, LAWRENCE

PROGRAM ABSTRACT

Title (If subroutine state in title):

Canonical correlation program

Date: August 1966

Author, organization: P.J. Lee, Freshwater Institute, Winnipeg 19, Canada

Direct inquiries to: Dr. D.F. Merriam

Name: Address: Kansas Geological Survey
Lawrence, Kansas 66044

Purpose/description: Computes canonical correlation coefficient and canonical variates between
two sets of variables. Bartlett's statistic is used to test the statistical significance of the ca-
nonical roots.

Mathematical method:

Restrictions, range: Accepts up to 99999 samples having up to 30 variables in each set.

Computer manufacturer: IBM Model: System/ 360 Model 65

Programming language: FORTRAN IV (G)

Memory required: 65 K bytes K Approximate running time: Less than 2 minutes for the given example

Special peripheral equipment required: None

Remarks (special compilers or operating systems, required word lengths, number of successful runs, other ma-
chine versions, additional information useful for operation or modification of program)

KANSAS GEOLOGICAL SURVEY COMPUTER PROGRAM
THE UNIVERSITY OF KANSAS, LAWRENCE

PROGRAM ABSTRACT

Title (If subroutine state in title):

Canonical trend-surface program

Date: July 1966

Author, organization: P.J. Lee, Freshwater Institute, Winnipeg 19, Canada

Direct inquiries to: Dr. D.F. Merriam

Name: Address: Kansas Geological Survey
Lawrence, Kansas 66044

Purpose/description: Computes canonical trend surface for a set of variables over an area with irregular sampling grid. Trend map and residual map are printed by printer.

Mathematical method:

Restrictions, range: Accepts up to 300 samples having up to 15 geologic variables, polynomial order up to 6.

Computer manufacturer: IBM Model: System/ 360 Model 65

Programming language: FORTRAN IV(G)

Memory required: 101 K bytes K Approximate running time: About 2 minutes for the given example

Special peripheral equipment required: None

Remarks (special compilers or operating systems, required word lengths, number of successful runs, other machine versions, additional information useful for operation or modification of program)

COMPUTER CONTRIBUTIONS

1. Mathematical simulation of marine sedimentation with IBM 7090/7094 computers, by J.W.Harbaugh, 1966.
2. A generalized two-dimensional regression procedure, by J.R.Dempsey, 1966.
3. FORTRAN IV and MAP program for computation and plotting of trend surfaces for degrees 1 through 6, by Mont O'Leary, R.H.Lippert, and O.T.Spitz, 1966.
4. FORTRAN II program for multivariate discriminant analysis using an IBM 1620 computer, by J.C.Davis and R.J.Sampson, 1966.
5. FORTRAN IV program using double Fourier series for surface fitting of irregularly spaced data, by W.R.James, 1966.
6. FORTRAN IV program for estimation of cladistic relationships using the IBM 7040, by R.L.Bartcher, 1966.
7. Computer applications in the earth sciences: Colloquium on classification procedures, edited by D.F.Merriam, 1966.
8. Prediction of the performance of a solution gas drive reservoir by Muskat's Equation, by Apolonio Baca, 1967.
9. FORTRAN IV program for mathematical simulation of marine sedimentation with IBM 7040 or 7094 computers, by J.W.Harbaugh and W.J.Wahlstedt, 1967.
10. Three-dimensional response surface program in FORTRAN II for the IBM 1620 computer, by R.J.Sampson and J.C.Davis, 1967.
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