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A SURFACE-FITTING PROGRAM SUITABLE FOR TESTING GEOLOGICAL MODELS WHICH INVOLVE AREALLY-DISTRIBUTED DATA

by
E. H. Timothy Whitten

TECHNICAL REPORT NO. 2
of
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Northwestern University
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CORRECTION FOR TECHNICAL REPORT NO. 2

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Please make this correction in your copy of Technical Report No. 2, E. H. T. Whitten: "A surface-fitting program suitable for testing geological models which involve areally-distributed data", 1963.

Page 45, line 18, should read

040061000007.000000001.000007000006.000000001.0000064

instead of

040061000002.000000000.500004000002.500000000.5000054

Northwestern University

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Prefatory Remarks

This report is the first of a series of computer program manuals arising from a continuing study of computer applications in the earth and environmental sciences, including geology, geography, geophysics, geochemistry, and environmental engineering. In some of these subjects, notably oceanography, atmospheric science, and solid-earth geophysics, computer capability has advanced far beyond that in the more classical fields of geology and geography, as well as in such aspects of environmental science as soil mechanics and sanitary engineering. Our study is concerned mainly with these more classical fields in which computer utilization is less far advanced.

Our project has as its purposes the evaluation of developments in computer capability in our fields through assessment of present activities; and an obligation to make available in the public domain a series of computer programs especially adapted to the needs of workers in our fields. The first purpose is being met through conferences and literature search; and the second is being met by reports such as this, which will include programs arising from our own studies, as well as program reports contributed by others active in the field.

The IBM 709 program described here is based on one of the earliest programs developed in the Department of Geology at Northwestern University. It is almost "classical" in that it grew from an early machine-language version on the basic IBM 650, later modified to SOAP II, to its present version in FORTRAN for the IBM 709. Copies of the program in various stages of development have been widely distributed to interested workers. Dr. Whitten, who has developed the program in its later stages, including double-precision computation, has very kindly prepared this manuscript, and has illustrated it with examples from his own work on igneous rocks. The program is used without modification for studies of stratigraphic, sedimentary, and other kinds of mappable data. An extension of the program, including visual trend-surface map output, is scheduled for distribution later in 1963.

W. L. Garrison

W. C. Krumbein

TABLE OF CONTENTS

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ABSTRACT

The Fortran listing and program flow charts are given in full. The method of utilizing the surface-fitting program is described in detail with the aid of an actual example.

INTRODUCTION

Geological problems commonly involve large numbers of observations which have been made at different map-locations. In order to test a geological response model on the basis of field observations, an objective quantitative method must be employed to integrate the data and to synthesize a picture of the areal variability. Some geological problems must be considered in a three-dimensional or poly-dimensional framework (e.g., three spatial dimensions together with time). However, many problems can be examined profitably in terms of a two-dimensional analysis (or a series of two-dimensional analyses), and the present report is restricted to such cases.

If quantitative measurements (e.g., of specific gravity) have been made at numerous localities within a map-area, the areal variability can be expressed visually by isopleths (i.e., contour-type lines of equal value). It is widely recognized that such isopleths are highly subjective, and that different draughtsmen will develop wholly dissimilar isopleth maps without violation of the observed data. This situation could be rectified by interpolation of more and more observations; but in most practical field problems, the density of sample stations is prescribed by outside factors (which are

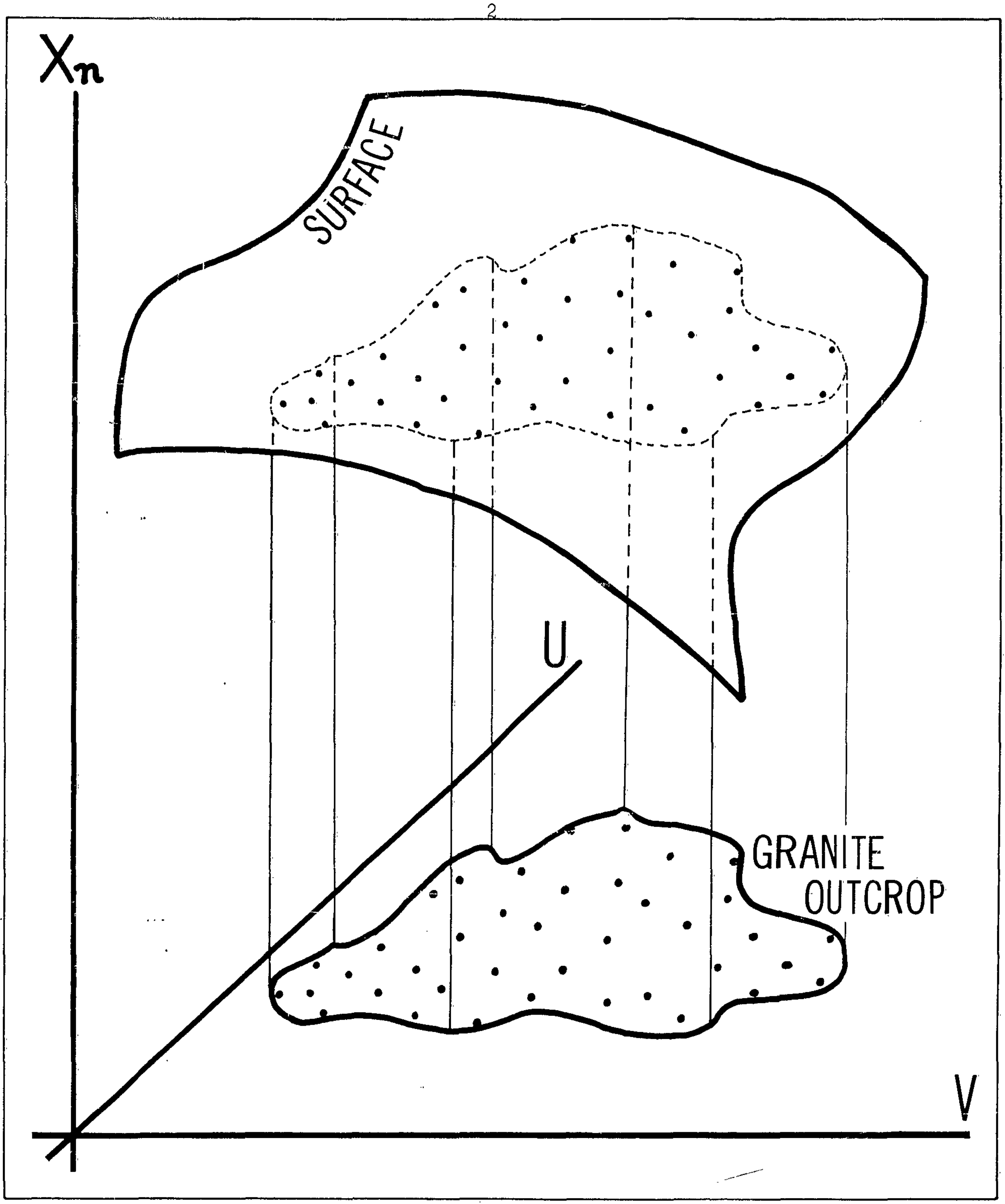


Figure 1: A hypothetical granite outcrop projected on to a computed mathematical surface, $X_n = f(U,V)$. Dots on the outcrop area indicate specimen localities for which values of X_n were observed (After Whitten, 1962, Fig. 1).

usually non-geological). In consequence, it is commonly useful to obtain an objective quantitative mathematical approximation to the areal variability shown by the observations.

The sample locations can be defined by two orthogonal geographic coordinates (independent variables, U and V). Ordinates may be erected at each U, V-location with heights proportional to the quantitative value of the property measured (dependent variable, X). In this way points representing X are located in three-dimensions and the variability of X can be approximated by a mathematical surface, $X=f(U,V)$, as shown in Figure 1. Various properties may have been measured (e.g., electrical resistivity, quartz-content, P_2O_5-content, etc.), so that a family of surfaces representing X_1, X_2, X_3,.... X_n can be developed.

Various types of function could be utilized to approximate the best mathematical surface, but polynomials have been used extensively with success. The present program uses the polynomial function:

$$X_n = a_0 + a_1U + a_2V + a_3U^2 + a_4UV + a_5V^2 + a_6U^3 + a_7U^2V + \ldots \quad \text{.....(i)}$$

To obtain the coefficients of the surface which most closely approximates the observed data, the conventional method of least squares is employed. In practice surfaces of successively higher degree are computed; the linear (first degree) surface

$$X_n = b_0 + b_1U + b_2V \quad \text{.....(ii)}$$

then the linear plus quadratic surface (second degree)

$$X_n = c_0 + c_1U + c_2V + c_3U^2 + c_4UV + c_5V^2 \quad \text{......(iii)}$$

and so on. Successive surfaces of higher degree (linear, linear plus quadratic, linear plus quadratic plus cubic,....) account for larger proportions of the total sum of squares of the observed data values (X_n). The proportion of the total sum of squares accounted for by a surface provides some measure of its "closeness" or "goodness" of fit.

Commonly it is convenient to use the algebraic polynomial expression to plot isopleths on the surface within the whole map-area. Naturally, the distinction between such isopleths and those drawn with respect to the observed data should be kept in mind clearly. The computed isopleths provide a useful method of assaying the regional trend inherent in the data. In many geological situations, such trends are masked by the local variability of the observed data.

When the regional variability has been approximated by a mathematical surface, valuable geological information can also frequently be obtained by noting and mapping the departures of individual observations from the computed surface.

DEVELOPMENT OF THE METHOD AND TERMINOLOGY

For two-dimensional graphs, some of the problems of approximating a curve to a set of data points have long been recognized. It is common practice to utilize the quantitative method of least squares to develop the regression line. This method has been extended to mapped data and the technique is referred to as trend surface analysis. Thus, a linear surface (Equation ii) corresponds to a regression line in the two-dimensional case. The method of computation is simple in principle, but the arithmetic is extremely tedious and was virtually impossible before the advent of high-speed computing machines.

Oldham and Sutherland (1955) demonstrated the value of orthogonal polynomials (DeLury, 1950) in the estimation of regional effects indicated by mapped data, while the paper on trend surface analysis by Grant (1957) may be considered definitive. Grant was mainly concerned with geophysical data available on a rectangular grid, but he showed that coefficients for the polynomial equation (i) can be estimated for irregularly-spaced data. The present program is designed for irregularly-spaced data (i.e., observations not restricted to rectangular geographic grid intersections). For data drawn from sample stations on a U,V-grid, Grant defined <u>trend</u> and <u>residual</u> on the basis of a Z^2-array, where $Z^2_{a_k}$ <u>represented the proportion</u> of the total sum of squares of the mapped variable (X_n) accounted for by the a_k-th polynomial coefficient in Equation (i). Z^2-terms which contribute significantly to the total sum of squares determine the coefficients to be incorporated in the <u>complete trend</u>. The remaining Z^2-terms refer to those <u>coefficients which</u> comprise the <u>residual</u>. A typical Z^2-array is shown in Table 1. It <u>will be noticed</u> that the boundary (solid line) between the Z^2-terms contributing to the complete trend and to the residual is irregular. Although Grant suggested

TABLE 1

PART OF Z^2-ARRAY*

		N	LINEAR	QUADRATIC	CUBIC	QUARTIC	QUINTIC	SEXTIC
	309,300 a_{0}	97,110 a_{1}	17,690 a_{3}	2,189 a_{6}	1,700 a_{10}	30 a_{15}	371 a_{21}	1 a_{28}
N	288,260 a_{2}	54,847 a_{4}	4,197 a_{7}	414 a_{11}	517 a_{16}	404 a_{22}	86 a_{29}	5 a_{37}
LINEAR	100,354 a_{5}	2,323 a_{8}	12,822 a_{12}	1,532 a_{17}	9 a_{23}	101 a_{30}	96 a_{38}	115 a_{47}
QUADRATIC	1,520 a_{9}	654 a_{13}	368 a_{18}	144 a_{24}	271 a_{31}	32 a_{39}	387 a_{48}	0 a_{58}
CUBIC	13 a_{14}	130 a_{19}	105 a_{25}	56 a_{32}	231 a_{40}	688 a_{49}	22 a_{59}	61 a_{70}
QUARTIC	1,245 a_{20}	0 a_{26}	492 a_{33}	0 a_{41}	190 a_{50}	168 a_{60}	26 a_{71}	12 a_{83}
QUINTIC	20 a_{27}	9 a_{34}	235 a_{42}	123 a_{51}	433 a_{61}	865 a_{72}	9 a_{84}	42 a_{97}
SEXTIC	618 a_{35}	221 a_{43}	126 a_{52}	25 a_{62}	395 a_{73}	129 a_{85}	289 a_{98}	146 a_{112}
SEPTIC	90 a_{44}	77 a_{53}	280 a_{63}	2 a_{74}	0 a_{86}	42 a_{99}	731 a_{113}	29 a_{128}
OCTIC	30 a_{54}	13 a_{64}	48 a_{75}	102 a_{87}	181 a_{100}	3 a_{114}	61 a_{129}	383 a_{145}

*Adapted from Grant (1957, p. 319)

some statistical tests, there is no generally-accepted procedure for defining this line; hence, some might choose a different boundary line such, for example, as the broken line shown on the array.

The method described here (Krumbein, 1959) for computing polynomial coefficients with respect to irregularly-spaced data points does not include preparation of a Z^2-array, or isolation of each separate coefficient. The linear coefficients (Equation ii), the linear plus quadratic coefficients (Equation iii), the linear plus quadratic plus cubic coefficients, etc., are computed separately. Since the complete trend defined by Grant (1957) may embrace some, but not necessarily all, terms of several degrees, existing methods for irregularly-spaced data do not permit isolation of the complete trend.[1] In consequence, a surface (e.g., the linear plus quadratic surface) is referred to as a partial trend surface on the assumption that it accounts for some unspecified portion of the complete trend. When higher degree surfaces (e.g., linear through sextic) are considered, partial trend surface is likely to be a misnomer; the equation probably contains all the complete trend terms in addition to some residual terms. Whitten (1959) referred to partial trend surfaces as trend components; and this usage has been followed in numerous publications (e.g., Allen and Krumbein, 1962), although Krumbein (1959) referred to individual polynomial coefficients as components. In view of the inadequacy of partial trend surface, it was suggested that trend component be employed in its place (Whitten, 1963).

Whitten (1959) used deviation to refer to that variability not included in a partial trend surface computed for irregularly-spaced data; another word was necessary because characteristically these terms are different from those comprising the residual in Grant's terminology.

Krumbein (1959) extended Grant's (1957) method for use with irregularly-spaced data. The mathematics are outlined with respect to the computed linear surface $X_{n\ comp.} = b_0 + b_1U + b_2V$ of Equation (ii).

If $X_{n_{ij\,obs}}$ is the observed value at the U_i, V_j-location, then the deviation at this point is $(X_{n_{ij\,obs}} - X_{n_{ij\,comp}})$.

[1]This program has proved a useful tool in its present form, but it can be extended to determine the contribution associated with each coefficient (cf., Mandelbaum, 1963).

To obtain the least squares fit, the sum of squares of the deviations must be minimized. Thus,

$$\sum\left(X_{n_{i\,j\,obs}} - X_{n_{i\,j\,comp}}\right)^2 = \sum\left(X_{n_{obs}} - b_0 - b_1U - b_2V\right)^2 \quad .....(iv)$$

is minimized. It can be shown (see Hoel, 1947, p. 90) that these sums of squares are a function of b_0, b_1, and b_2 only, so Equation (iv) can be expressed as $F(b_0, b_1, b_2)$. To minimize $F(b_0, b_1, b_2)$ it is necessary that

$$\frac{\partial F}{\partial b_0} = \frac{\partial F}{\partial b_1} = \frac{\partial F}{\partial b_2} = 0 \quad .....(v)$$

These partial derivatives are

$$\left.\begin{aligned} \partial F/\partial b_0 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-1) = 0 \\ \partial F/\partial b_1 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-U) = 0 \\ \partial F/\partial b_2 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-V) = 0 \end{aligned}\right\} \quad .....(vi)$$

These expressions reduce to the three normal equations:

$$\left.\begin{aligned} b_0N + b_1\Sigma U + b_2\Sigma V &= \Sigma X_{n_{obs}} \\ b_0U + b_1\Sigma U^2 + b_2\Sigma UV &= \Sigma UX_{n_{obs}} \\ b_0V + b_1\Sigma UV + b_2\Sigma V^2 &= \Sigma VX_{n_{obs}} \end{aligned}\right\} \quad .....(vii)$$

where N is the number of U_i, V_j-locations at which data were obtained. Converting Equations (vii) to matrix form, we have

$$\begin{bmatrix} N & \Sigma U & \Sigma V \\ \Sigma U & \Sigma U^2 & \Sigma UV \\ \Sigma V & \Sigma UV & \Sigma V^2 \end{bmatrix} \cdot \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} \Sigma X_{n_{obs}} \\ \Sigma UX_{n_{obs}} \\ \Sigma VX_{n_{obs}} \end{bmatrix} \quad .....(viii)$$

To obtain the least squares fit, the sum of squares of the deviations must be minimized. Thus,

$$\sum\left(X_{n_{ij\,obs}} - X_{n_{ij\,comp}}\right)^2 = \sum\left(X_{n_{obs}} - b_0 - b_1U - b_2V\right)^2 \quad \text{.....(iv)}$$

is minimized. It can be shown (see Hoel, 1947, p. 90) that these sums of squares are a function of b_0, b_1, and b_2 only, so Equation (iv) can be expressed as $F(b_0, b_1, b_2)$. To minimize $F(b_0, b_1, b_2)$ it is necessary that

$$\frac{\partial F}{\partial b_0} = \frac{\partial F}{\partial b_1} = \frac{\partial F}{\partial b_2} = 0 \quad \text{.....(v)}$$

These partial derivatives are

$$\left.\begin{aligned} \partial F/\partial b_0 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-1) = 0 \\ \partial F/\partial b_1 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-U) = 0 \\ \partial F/\partial b_2 &= \Sigma 2(X_{n_{obs}} - b_0 - b_1U - b_2V)\cdot(-V) = 0 \end{aligned}\right\} \quad \text{.....(vi)}$$

These expressions reduce to the three normal equations:

$$\left.\begin{aligned} b_0N + b_1\Sigma U + b_2\Sigma V &= \Sigma X_{n_{obs}} \\ b_0U + b_1\Sigma U^2 + b_2\Sigma UV &= \Sigma UX_{n_{obs}} \\ b_0V + b_1\Sigma UV + b_2\Sigma V^2 &= \Sigma VX_{n_{obs}} \end{aligned}\right\} \quad \text{.....(vii)}$$

where N is the number of U_i, V_j-locations at which data were obtained. Converting Equations (vii) to matrix form, we have

$$\begin{bmatrix} N & \Sigma U & \Sigma V \\ \Sigma U & \Sigma U^2 & \Sigma UV \\ \Sigma V & \Sigma UV & \Sigma V^2 \end{bmatrix} \cdot \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} \Sigma X_{n_{obs}} \\ \Sigma UX_{n_{obs}} \\ \Sigma VX_{n_{obs}} \end{bmatrix} \quad \text{.....(viii)}$$

Since the $[U, V]$ matrix and the column vector $[X_{n_{obs.}}]$ are known from the original data, Equation (viii) can be solved to derive the required coefficients by multiplication of both sides by the inverse of the $[U, V]$ matrix. Then:

$$\begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = [U, V]^{-1} \cdot \begin{bmatrix} \Sigma X_{n_{obs}} \\ \Sigma UX_{n_{obs}} \\ \Sigma VX_{n_{obs.}} \end{bmatrix} \quad .....(ix)$$

The present FORTRAN program is designed to compute the polynomial linear coefficients by use of Equation (ix). Similar equations can be developed for coefficients of surfaces of degree two, three, four,....., and p. The present program is restricted to computation of degrees one, two and three. For the linear plus quadratic plus cubic surface (degree 3), Equation (viii) takes the form shown in Equation (x).

It would appear that the method can be extended to surfaces of higher degree provided that the symmetrical $[U, V]$ matrices can be inverted satisfactorily, or that other adequate methods for solving the simultaneous equations are available.

Inversion of matrices similar to that in Equation (x) involve several problems. In the course of extensive testing the matrix inversion routine incorporated in this program has always provided adequate inverse matrices when the computation is effected in double precision (i.e., with sixteen significant figures). The program can be extended readily for determination of higher degree polynomial surfaces, and the existing matrix inversion routine commonly yields good results up to degree 5. For degree 6 and above, an alternative method is necessary and the matrix-scaling procedure suggested by Mandelbaum (1963) provides one possible method. For a large range of geological problems, surfaces up to degree 3 provide adequate trend components. In fact, experience has shown that, in many cases, use of surfaces of higher degree than three, includes in the trend some of the variability which is more appropriately considered as part of the deviation.

To assess the geological significance of a computed trend component, it is useful to develop the confidence intervals on the surface. A method for determination of such

$$
\begin{bmatrix}
N & \Sigma U & \Sigma V & \Sigma U^2 & \Sigma UV & \Sigma V^2 & \Sigma U^3 & \Sigma U^2V & \Sigma UV^2 & \Sigma V^3 \\
\Sigma U & \Sigma U^2 & \Sigma UV & \Sigma U^3 & \Sigma U^2V & \Sigma UV^2 & \Sigma U^4 & \Sigma U^3V & \Sigma U^2V^2 & \Sigma UV^3 \\
\Sigma V & \Sigma UV & \Sigma V^2 & \Sigma U^2V & \Sigma UV^2 & \Sigma V^3 & \Sigma U^3V & \Sigma U^2V^2 & \Sigma UV^3 & \Sigma V^4 \\
\Sigma U^2 & \Sigma U^3 & \Sigma U^2V & \Sigma U^4 & \Sigma U^3V & \Sigma U^2V^2 & \Sigma U^5 & \Sigma U^4V & \Sigma U^3V^2 & \Sigma U^2V^3 \\
\Sigma UV & \Sigma U^2V & \Sigma UV^2 & \Sigma U^3V & \Sigma U^2V^2 & \Sigma UV^3 & \Sigma U^4V & \Sigma U^3V^2 & \Sigma U^2V^3 & \Sigma UV^4 \\
\Sigma V^2 & \Sigma UV^2 & \Sigma V^3 & \Sigma U^2V^2 & \Sigma UV^3 & \Sigma V^4 & \Sigma U^3V^2 & \Sigma U^2V^3 & \Sigma UV^4 & \Sigma V^5 \\
\Sigma U^3 & \Sigma U^4 & \Sigma U^3V & \Sigma U^5 & \Sigma U^4V & \Sigma U^3V^2 & \Sigma U^6 & \Sigma U^5V & \Sigma U^4V^2 & \Sigma U^3V^3 \\
\Sigma U^2V & \Sigma U^3V & \Sigma U^2V^2 & \Sigma U^4V & \Sigma U^3V^2 & \Sigma U^2V^3 & \Sigma U^5V & \Sigma U^4V^2 & \Sigma U^3V^3 & \Sigma U^2V^4 \\
\Sigma UV^2 & \Sigma U^2V^2 & \Sigma UV^3 & \Sigma U^3V^2 & \Sigma U^2V^3 & \Sigma UV^4 & \Sigma U^4V^2 & \Sigma U^3V^3 & \Sigma U^2V^4 & \Sigma UV^5 \\
\Sigma V^3 & \Sigma UV^3 & \Sigma V^4 & \Sigma U^2V^3 & \Sigma UV^4 & \Sigma V^5 & \Sigma U^3V^3 & \Sigma U^2V^4 & \Sigma UV^5 & \Sigma V^6
\end{bmatrix}
\cdot
\begin{bmatrix} d_0 \\ d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \\ d_6 \\ d_7 \\ d_8 \\ d_9 \end{bmatrix}
=
\begin{bmatrix} \Sigma X_{n_{obs}} \\ \Sigma UX_{n_{obs}} \\ \Sigma VX_{n_{obs}} \\ \Sigma U^2X_{n_{obs}} \\ \Sigma UVX_{n_{obs}} \\ \Sigma V^2X_{n_{obs}} \\ \Sigma U^3X_{n_{obs}} \\ \Sigma U^2VX_{n_{obs}} \\ \Sigma UV^2X_{n_{obs}} \\ \Sigma V^3X_{n_{obs}} \end{bmatrix}
$$

..... Equation (x)

N.B. The broken lines indicate the smaller U,V-matrices appropriate to degrees 1 and 2.

surfaces was described by Krumbein (1963). For many purposes the sums of squares associated with the computed surfaces provide useful guides to the significance of trend components and deviations. The method of computing these values is described below.

If $\bar{X}_{n_{obs}}$ is the mean value of a set of observed values $X_{n_{obs}}$, then the deviation from the mean at the ij-th point is $\left(X_{n_{ij_{obs}}} - \bar{X}_{n_{obs}}\right)$, as shown in Figure 2A. The sum of the squares of all the deviations is defined as the total sum of squares of the observed X_n, i.e.,

$$\sum^{N} (X_{n_{obs}} - \bar{X}_{n_{obs}})^2 \qquad .....(xi)$$

This expression is not in the easiest form for computation; it can be shown (see Dixon and Massey, 1957, p. 19) that Equation (xi) is equivalent to:

$$\sum^{N} X^2_{n_{obs}} - \left(\frac{\sum^{N} X_{n_{obs}}}{N}\right)^2 \qquad .....(xii)$$

In this form the total sum of squares of the observed data can be computed very easily.

The sum of squares of the computed values, $X_{n_{comp}}$, is obtained in a similar way. The distance from the mean of the observed values, $\bar{X}_{n_{obs}}$, to the trend component (measured normal to the U, V-plane) at the ij-th datum-point is $(X_{n_{ij_{comp}}} - \bar{X}_{n_{obs}})$, as shown on Figure 2B. Hence, the sum of the squares of the computed values is:

$$\Sigma(X_{n_{comp}} - \bar{X}_{n_{obs}})^2 = \Sigma X^2_{n_{comp}} - \left(\frac{\Sigma X_{n_{comp}}}{N}\right)^2 \qquad .....(xiii)$$

Since $\bar{X}_{n_{obs}} = \bar{X}_{n_{comp}}$, the sum of squares of the deviations from the trend component (see Figure 2C) is given

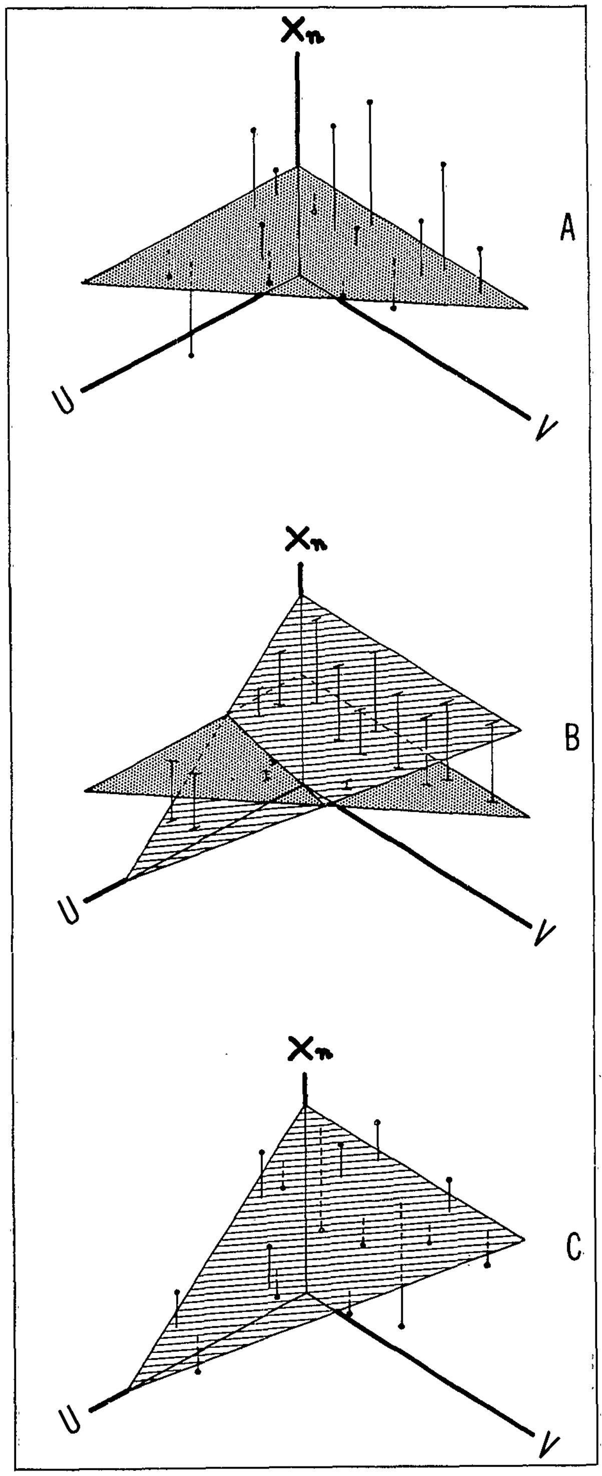


Figure 2: Plane with dots is $\bar{X}_{n_{obs}}$ and plane with ruled lines is degree 1 (linear) computed trend component. A few representative observed points (X_n) are shown as large dots.

by:

$$\Sigma(X_{n_{obs}} - X_{n_{comp}})^2 = \Sigma X^2_{n_{deviation}} \qquad \text{......(xiv)}$$

The proportion of the total variability accounted for by a trend component can now be expressed as a percentage. Thus, by using values derived from Equations (xii) and (xiii), a linear surface accounts for:

$$\frac{(\text{Sum of squares of the computed } X_{n_{linear}})}{(\text{Total sum of squares of the observed } X_n)} \times 100 \text{ per cent.} \qquad (xv)$$

of the total variability, where $X_{n_{linear}}$ are values of X_n computed for the linear trend component. Similar expressions can be evaluated for surfaces of each degree by use of the Equations (xii) and (xiii).

TREND SURFACES IN TESTS OF GEOLOGICAL MODELS

Within the physical sciences it is common practice to test the validity of conceptual process-response models with newly-acquired data. This technique is being used more widely in the earth sciences (e.g., Miller and Ziegler, 1958; Hurley, et al., 1962; Krumbein, 1962A; Ringwood, 1962A, 1962B; Sloss, 1962; Wyllie, 1962). However, few process-response models for igneous, sedimentary, or metamorphic rocks have been evaluated explicitly, and in most cases the critical response and process factors are not clearly defined.

In problems which involve areally distributed data, trend surface analysis can be of considerable use in testing geological models. As an example of a petrogenetic model in igneous geology, a magmatic granite massif may be considered. According to most theories a magma cools inwards from the walls and downwards from the roof. Such cooling would tend to develop an annular pattern of mineralogical variation when the pluton is examined in a random sub-horizontal section (exposed surface). Metastable high temperature mineral phases would be preserved where the magma froze rapidly (e.g., near the margins of the granite). Hence, cafemic silicate minerals would be more abundant at the margins of the pluton, and lower temperature quartzo-feldspathic

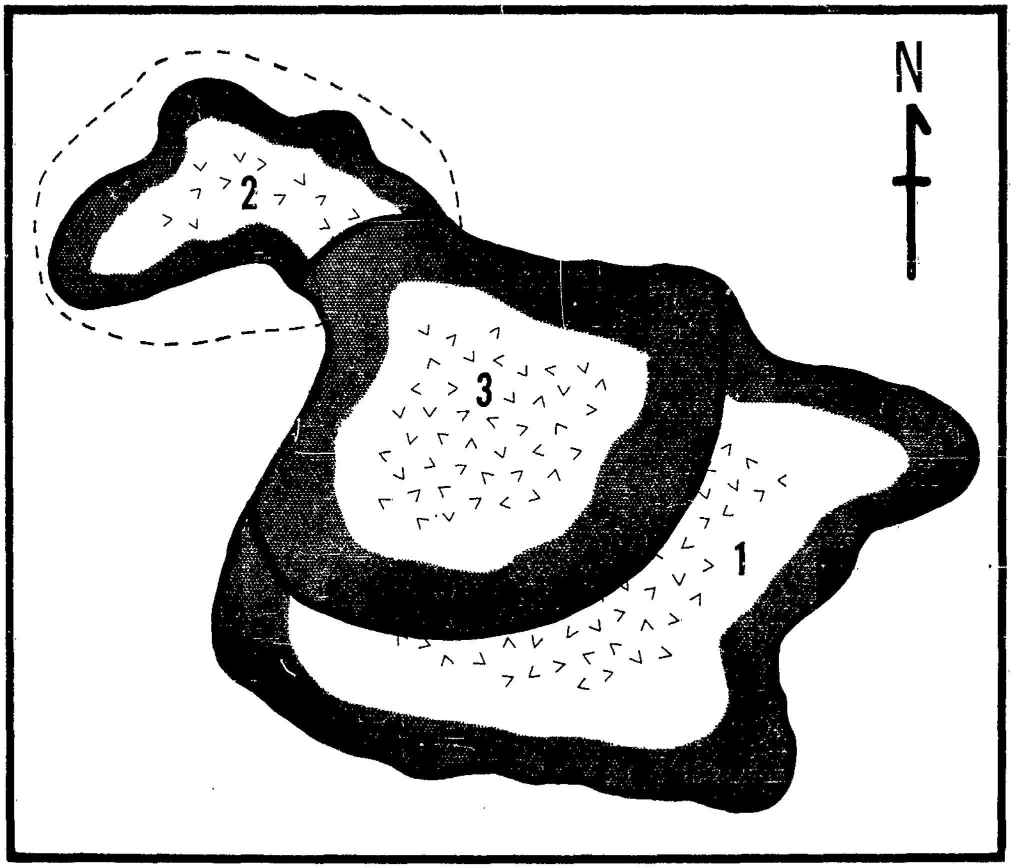


Figure 3: Map illustrating multiple intrusion model. See text for explanation

minerals near the center. Such fractionation would result in both a chemical zonation and also a concentric pattern of density variation within the intrusion. Individual minerals might also show variation within the massif. For example, more anorthitic plagioclase might be expected in the rapidly-chilled marginal zones, and be associated there with potassic feldspars with high temperature optics. These phenomena would also result in zonally-arranged textural differences within the pluton.

The process model for a cooling magmatic pluton can be augmented to include multiple intrusion. Each separately-intruded unit would tend to be annular. The youngest intrusion would be expected to show a complete sequence of gradational annular zones, while the concentric zones of older masses are likely to be transected by the later units. The actual contacts between successive units might not be determined easily in the field.

Figure 3 represents a conceptual model for the multiple intrusion hypothesis. One intrusion would result in a single zonal arrangement. In the figure it is supposed that an initial intrusion (1) occurred in the southeast, followed by a younger mass (2) in the northwest. Both of these masses responded to the cooling systems by development of an annular pattern of mineralogical zonation. The last event represented in Figure 3 involved intrusion of a third pluton (3), which transected the earlier masses (1 and 2). Hence, the last intrusion (3) has complete zones, whereas the earlier ones (1 and 2) are incomplete.

Other models could be erected on the basis of different petrogenetic hypotheses. However, as an illustration, the magmatic multiple intrusion conceptual model will be examined and tested with respect to an actual example.

The Lacorne granitoid complex, Quebec, recently described by Dawson and Whitten (1962), affords a convenient example. Some recent work suggested that the Lacorne massif comprises a single intrusion, and some that it is a multiple intrusion. According to the latter view, several discrete units occur in the northwestern area. These divergent views can be tested quantitatively in terms of the conceptual model (Figure 3).

Quantitative modal data have been accumulated from a wide range of U, V-locations. Figure 4 shows isopleths drawn to illustrate the areal variation of color index over the whole Lacorne massif. Commonly, with this type

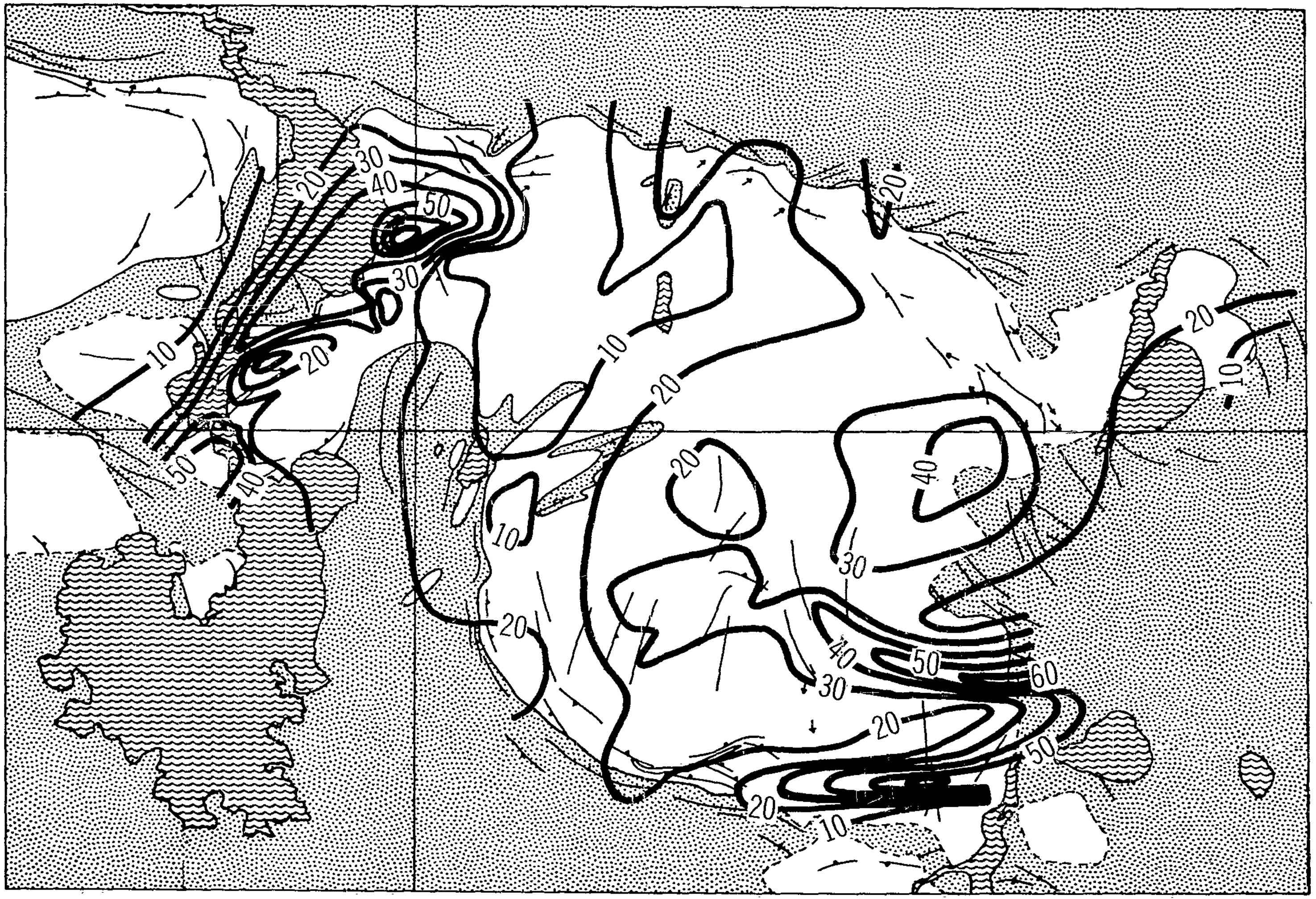


Figure 4: Isopleths with respect to color index data for the Lacorne granitic massif, Quebec, Canada (after Dawson and Whitten, 1962, Fig. 2).

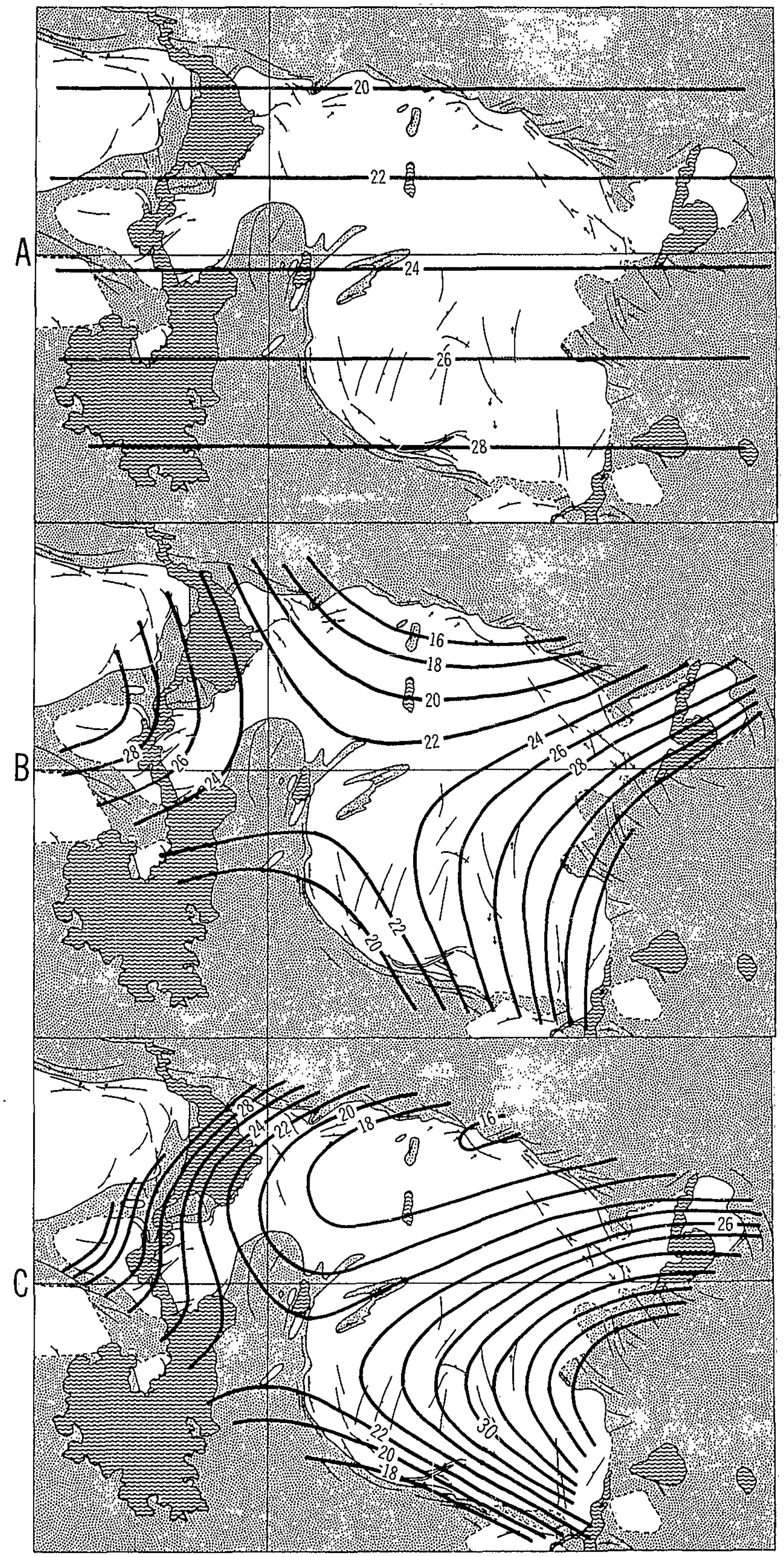


Figure 5: Trend components for color index data in the Lacorne granitic massif, Quebec, Canada. A. linear component (accounts for 2.3 per cent. of the total sum of squares). B. degree 2 component (accounts for [illegible] per cent. of the total sum of squares). C. degree 3 component (accounts for 11.6 per cent. of the total sum of squares). (After Dawson and Whitten, 1962, Fig. 4).

of data, local variability tends to mask the regional gradients. An objective method of screening-out the local effects, and of estimating the regional trend, is desirable. If polynomial surfaces are computed with respect to the color index data, the trends become reasonably clear. By simultaneous analysis of all the data from the complex, the single intrusion model can be tested first. Thus, Figure 5 shows the degree 1, degree 2, and degree 3 trend components; these surfaces account for progressively larger proportions of the total sum of squares of the observed dependent variable (color index). Because there is no concentric pattern of variation, Figure 5C is completely at variance with the model which involves a single intrusion of magma. In fact, as Dawson and Whitten (1962) pointed out, this pattern is anomalous when compared with the mineralogical variation found in most other granitic massifs, and it suggests multiple intrusion.

Recent detailed mapping by Brett (1960) suggested that a marked compositional change occurs in the area between the strongly developed maximum and minimum illustrated in Figure 5C. Although margins of separate intrusions were not defined, Brett's 1:12,000 map showed hornblende granite to the southeast, and muscovite granodiorite to the northwest, of the line of compositional change. Also a zone of biotite granodiorite was mapped along the junction, but Brett did not map definite contacts or state whether this is a discrete intrusion or a portion of either of the other two possible units.

In order to test the multiple intrusion model, the color index data from the entire Lacorne mass were divided into two groups corresponding to the geographic areas northwest and southeast of the zone mapped by Brett. Figure 6A shows the two degree 3 trend components. Although eccentric, both areas now possess a markedly concentric regional pattern. This augurs well for the correctness of the model, although the more mafic interior of both areas is rather unusual by comparison with other granites.

Thus, this first test suggests that the multiple intrusion hypothesis may be correct. The specific geographic domains which have been isolated can be incorporated in a slightly more refined model, which must be tested by quantitative analysis of some additional variables. Modal quartz percentage can be determined easily, and the trend components for this variable are shown in Figure 6B. These maps appear to corroborate the model; in particular, strong support is provided by the concentric pattern in the eastern

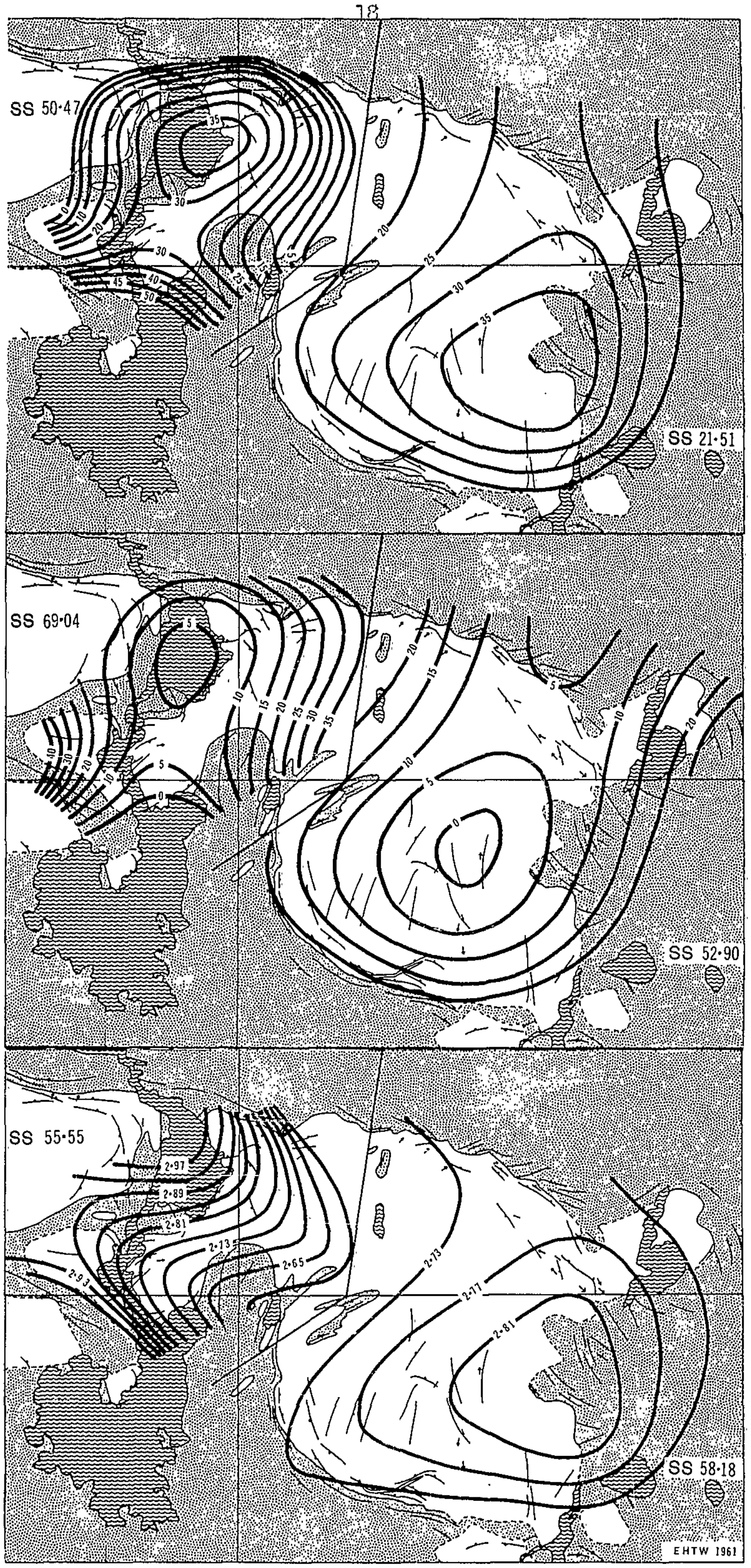


Figure 6: Degree 3 trend components for data from the southeastern and northwestern parts of the Lacorne massif taken separately. The percentage of the total sum of squares accounted for by the surface for each part of the massif is indicated as SS. A. color index; B. quartz percentage; C. specific gravity. (After Dawson and Whitten, 1962, Fig. 11).

part of the Lacorne massif. However, the pattern is unlike that of most other granite massifs because the quartz content is lowest in the center, and is thus the opposite of what is commonly believed to be the case in most granite massifs.

The usefulness of Figure 6B as an independent check of the validity of the model is questionable because quartz percentage and color index are both percentage data which have a strong negative correlation (cf., Chayes, 1960). Thus, there would appear to be a strong inherent negative correlation between these two trend components (Figure 6A and 6B), so that the quartz percentage surface does not provide an independent reason for believing that the model is correct.

The disharmony between the trends shown by (a) these two supposed granites, and (b) the variation which appears to be general in most other granite masses, suggests that additional testing is necessary before confidence can be expressed in the correctness of the model. Additional variables, which are not subject to the closed table restraints inherent in the volumetric modal data, can provide further evidence. Density of the rocks is a suitable variable for which trend surfaces are illustrated in Figure 6C. Now there is no semblance of a concentric pattern in the northwest area, so it is doubtful whether a simple single intrusion exists there. The eastern area maintains a concentric pattern compatible with that for the color index data (Figure 6A) and does not compromise the validity of the model for that area.

With this information in hand, careful review of the outcrops might reveal previously-unnoticed characteristics which support the concept that the eastern mass is a discrete intrusion. Because of the nature of the exposures, it is possible that the necessary detail could not be obtained. However, numerous other variables could be measured and subjected to trend analysis. The variety of variables which have already been expressed in quantitative terms in assessing the areal variability of different granites was reviewed by Whitten (1963A); other variables could undoubtedly be measured to advantage. The areal variability of the temperature of crystallization within the Lacorne massifs might provide valuable information in support or contradiction of the model. Although he did not analyze the results with trend surfaces, Carter (1962) constructed a thermal isopleth map for the Venås granite, Norway, which indicated the lowest temperatures at which equilibrium between co-existing feldspars was attained during cooling of

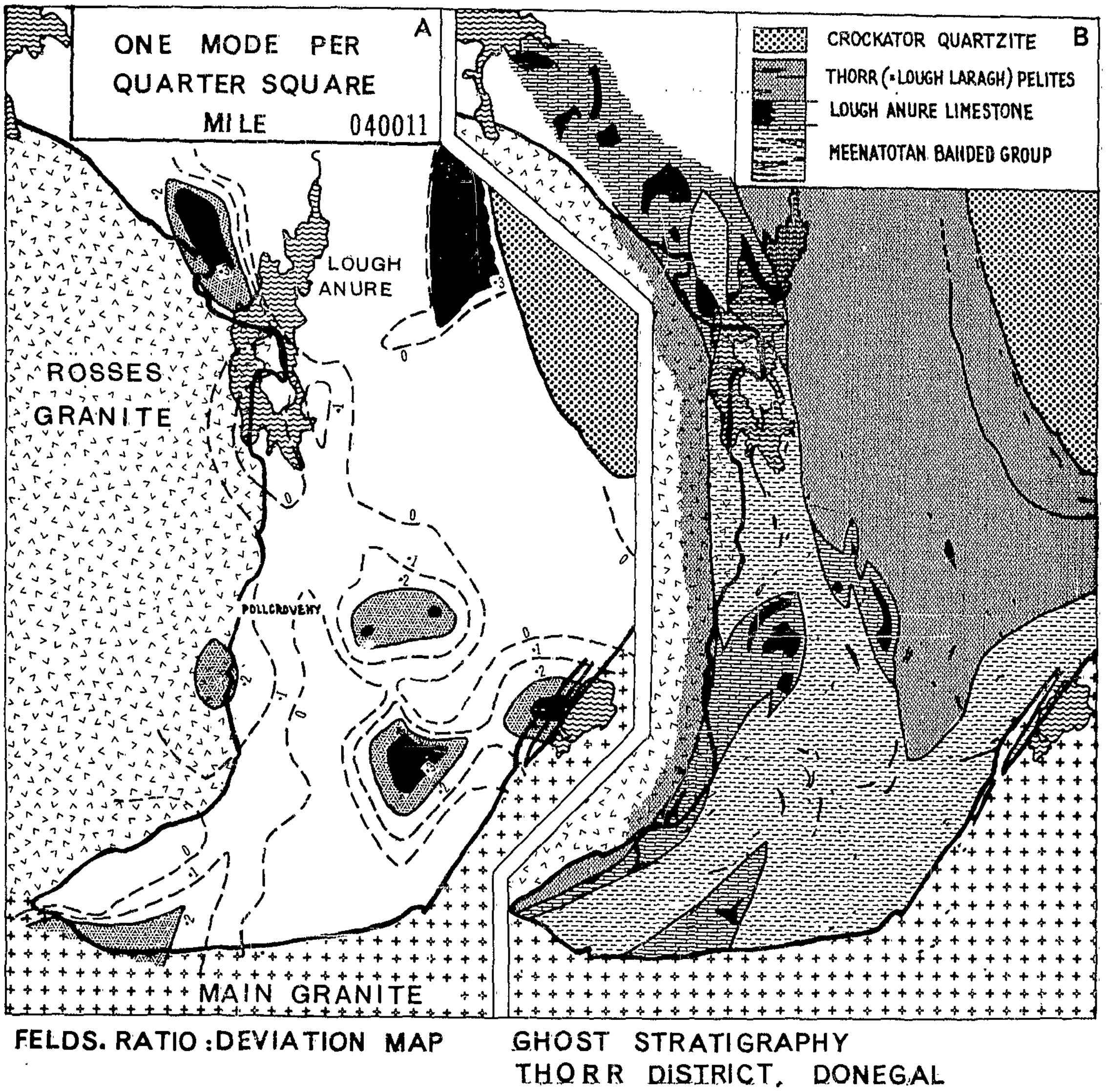


Figure 7: Comparison of palimpsestic ghost stratigraphy and ghost stratigraphy in the 'older granite' of Donegal, Thorr district, County Donegal, Eire. A. Positive deviations from the degree 2 trend component for the microcline to plagioclase ratio within granite samples. B. Ghost anticline defined by metasedimentary rocks enclosed within the granite and based on data from Pitcher (1953A; 1953B) and Pitcher and Read (1959). (After Whitten, 1960, Fig. 5).

the magma. Again, the areal variability of alkali feldspar optics, which was studied in several Russian granites by Marfunin (1962), might produce direct evidence bearing on the multiple intrusion model for the Lacorne massif.

The models discussed above are susceptible to test with trend surface maps because the regional variation across each unit is involved. Comparable tests which involve deviations from the regional trends are also important in development of a complete petrogenetic process-response model; this is true for problems in many widely different fields of geological inquiry, but, initially, the case of magmatic granitic intrusions is discussed.

For the classical model involving intrusion of a homogeneous fluid, which was thoroughly mixed before slow cooling and crystallization, the essential variability would be regional (with respect to the total intrusion). Local deviations from the regional areal variability (trend) would be essentially random. Deviations might be expected to arise from errors or inexact measurements during analysis of the samples and from analogous factors unrelated to the regional picture. Again, assimilation or contamination at the margins of an intrusion might result in local endometamorphic modification of the granite. On these bases a petrogenetic process-response model would predict that the deviations are essentially random over a major part of the intrusion.

Data with which this model can be tested are surprisingly sparse. However, Figure 7 shows the deviations from the degree 2 trend component for the ratio of microcline to plagioclase in the 'older granite' of Donegal, Ireland (Whitten, 1960). This map contradicts the model because the deviations show a distinct pattern. Just prior to publication of this map, Pitcher and Read (1959) established conclusively that relics of a known stratigraphic succession of Precambrian metasedimentary rocks are preserved throughout this granite in their pre-granite positions; these relics define a ghost antiform. Hence, the deviations mapped by Whitten (1960) may be referred to as palimpsestic ghost stratigraphy and as a palimpsestic ghost antiform which are defined by local variations in the mineralogical composition of the granitic rock. This facet of the quantitative response model involves revision of the proposed conceptual process model for this particular granite. Precambrian metasedimentary rocks which were where the granite is now must have radically affected the composition of the granite. Hence, any model involving intrusion of magma must involve tranquil conditions during which the liquid developed inhomogeneity prior to crystallization. Alternatively, some totally different petrogenetic sequence of events might have been involved, in which case any magmatic model would be proved incorrect by careful quantitative analysis of the appropriate variables (response model). With financial support of the National Science Foundation Grant G. 19633 quantitative data for numerous additional variables are being assembled for this Irish granite with a view to testing exhaustively various petrogenetic models.

The granite controversy (e.g., Read, 1957) is mainly involved with the validity of rival petrogenetic process models -- those which invoke magmatic hypotheses and those which invoke various granitizational processes. Qualitative evaluation appears to be insufficient to resolve the controversy. Quantitative tests of specific models would seem to offer a real opportunity for resolution of this debate. Probably for some granites a magmatic model will prove adequate, but for others it may not. At the present time it is unknown whether the type of response model identified and partially described for the 'older granite' of Donegal is unique, or whether it is representative of common relationships. Deviation maps for the Malsburg granite, Germany, (Whitten, 1962) show that published K_2O and Na_2O analyses yield a strongly defined NW.-SE. deviation pattern. This relationship was totally unsuspected from the existing process models. Hence, current petrological and petrogenetical concepts about this particular granite probably require revision. On the basis of such a revision, a new model could be constructed, while the modal and chemical data recently published by Leible (1959), Mehnert (1960), Mehnert and Willgallis (1961), and Rein (1961) would form an initial basis for quantitative tests of the new model.

Wadsworth (1963) studied the areal variability of textural variables in the Twelve-foot Fall quartz diorite, Wisconsin, with the aid of trend surface analysis. Work with many additional types of variables must supplement analyses of the standard modal and chemical measurements if an adequate response model is to be constructed.

At present many qualitative and subjective judgments about the composition and variability of rock masses have to be relied upon in petrogenetic theory. If adequate data can be made available, trend surface and deviation maps provide objective estimates which are valuable as firm foundations for evaluation of petrogenetic models for granite bodies.

Although this discussion has been illustrated by granites, it must be emphasized that trend surface and deviation maps have value in many other fields of the earth sciences. The earliest deviation maps were published for stratigraphic facies maps by Krumbein (1956, 1962B), Grant (1957) showed that positive deviations based on observed Bouguer anomalies are associated with sub-surface sulphide mineralization. On the basis of deviation maps prepared for the heavy mineral content of the top Ashdown Pebble Bed, England, Allen and Krumbein (1962) developed a paleogeographic reconstruction (process model) for the Wealden area.

Most geological problems are susceptible to quantitative analysis. Commonly, the philosophy of objectives in geological mapping is not clear. As Chayes and Suzuki (1963) suggested, greater clarity could result from closer definition of the objective (cf., Whitten, 1963B). In many cases the objective will remain obscure until the processes involved, and the responses to these processes, are expressed quantitatively in the context of a unifying model. The model will have to be modified as more is learned of the processes and the responses associated with particular geological problems. In studies of present-day sedimentation, both the processes and the responses can commonly be analysed. The processes involved in the formation of granites are essentially conjectural. In the erection of process-response models for the genesis of granites magmatic, granitizational, or some other processes may be involved. The validity of such models has to be assessed solely on the results of quantitative analysis of the many attributes of the response products (the granitic rocks).

The present program provides a useful method of evaluating the quantitative behavior of response characteristics, and hence, of testing petrogenetic and other geologic models.

DEVELOPMENT OF THE FORTRAN PROGRAMS

Professors W. C. Krumbein and D. Harris prepared a surface-fitting program in MACHINE LANGUAGE for the Basic IBM 650 in 1957. This program would compute degree 1, 2, and 3 trend components with respect to four dependent variables, and it effected the calculations in single precision. This program was rewritten in SOAP and filed in the IBM London Library by Krumbein and C. Faulkner in 1960 under file number 60705, and was subsequently catalogued under the number 8.3.001 in IBM New York Library.

In June, 1961, Mr. R. Axelrod began re-writing the program for Krumbein in FORTRAN language for use on the IBM 709. By February, 1962, Whitten had converted the entire FORTRAN program to double precision and extended it for simultaneous use with eight variables. In addition, Whitten prepared the program designated as Part II in this report for use in conjunction with the main surface-fitting program.

Apart from these main steps in the evolution of this program, minor revisions have been made continuously. Throughout this work the staff of the Northwestern University Computing Center have given much advice; special mention should be made of assistance given by Mrs. O.G. Benson and Mr. H. Rymer of Northwestern University, and by Miss S. Hitz and Dr. C. Faulkner of IBM.

Financial support for this work has been received from the Graduate School of Northwestern University, the National Science Foundation (grant to Whitten, Project Number G-19633), and the Office of Naval Research (Contract Nonr-1228(26); Task no. 389-135). This continuing assistance is gratefully acknowledged.

OUTLINE OF THE PROGRAM AND CAPACITY

The present program is designed to operate with one to eight sets of mapped variables (dependent variables). There is no upper limit to the number of data-points which can be utilized. The lower limit to the number of data-points is prescribed by the distribution of the data-points and the precision with which the surface must be defined. However, as an empirical guide, at least three times the number of data-points as the number of coefficients should be used.

Computation of the polynomial coefficients is facilitated if the axes are oriented so as to reduce unintentional alignment of the U and V values of the data-points. Commonly, the origin is placed at the top left-hand corner of the map, so that U increases downwards and V from left to right. This choice was based on preservation of a sense of direction in the map similar to that used for gridded data, which are commonly analysed as rows and columns starting from the upper left (Krumbein, 1960,

p. 360). It is advantageous to maintain this orientation, although others can be found in the literature.

The FORTRAN program can be considered conveniently as a series of sections, thus:

PART I

Phase 1 - Preparation of the $[U, V]$ matrix and the column vector $[X_n]$.

Phase 2 - Inversion of the degree 1, 2, and 3 $[U, V]$ matrices.

Phase 3 - Multiplication of the inverse matrices and column vectors $[X_n]$ to obtain the degree 1, 2, and 3 coefficients.

Phase 4 - Use of the coefficients to compute values of X_n at each datum-point and to calculate the deviations at each of these map-points.

Phase 5 - Preparation of the sums of squares summary for the surfaces of each degree.

PART II

Use of the coefficients to calculate a network of computed values over the entire map-area.

The actual FORTRAN program is listed in Appendix I, and the flow charts are shown in Figures 8 and 9.

It will be noticed that most of the operations in Part I are completed in double precision, which insures use of sixteen significant figures. This is necessary because use of eight significant figures only (single precision) introduces serious rounding errors at several stages of the program.

In practice Part II is an invaluable adjunct to the main surface-fitting program (Part I) because commonly it is difficult to draw isopleths accurately on the basis of values computed at the observed data-locations only. Isopleths for the computed surfaces are mathematical curves. These are drafted more easily if a network of computed values is laid over an area somewhat greater than that from which the observed data were collected. With Part II, values can be computed for a rectangular grid of up to 35 points in both the U and the V directions. The simple calculations involved in Part II do not require double precision.

PREPARATION TO RUN THE PROGRAM

(PART I)

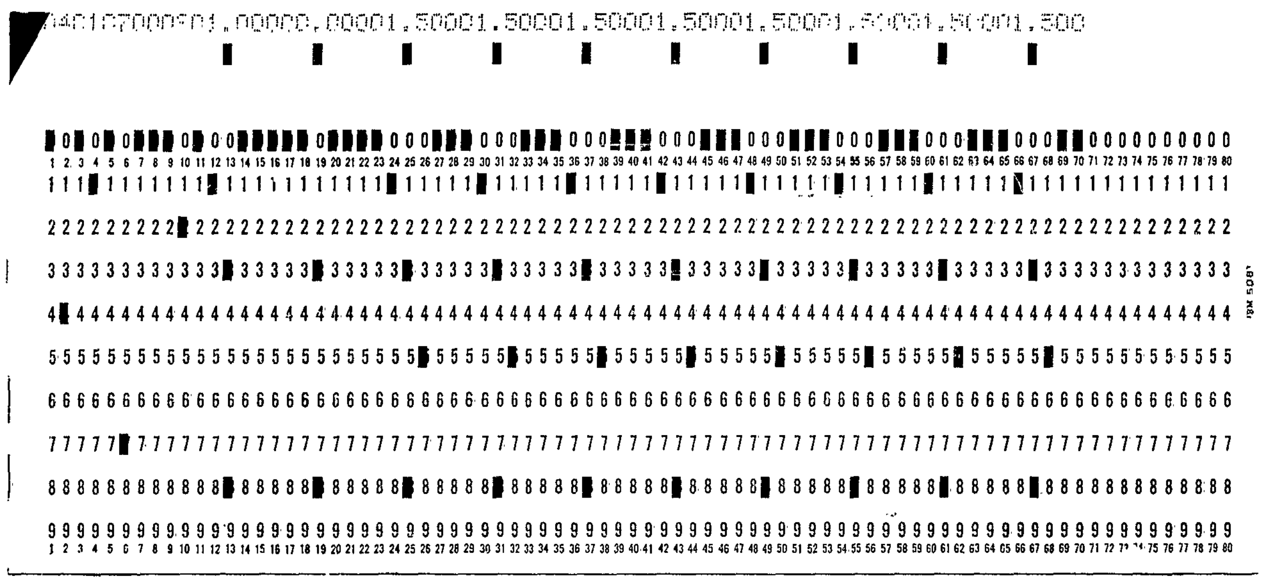
Data cards:

A separate data card is used for each sample location; the U,V-coordinates and the data for one through eight dependent variables recorded at each locality are included on the same 80-column IBM card. The format requires:

Columns 1	through	6	- Project number (either numeric or alphabetic)
7	"	10	- Sample point identification (either numeric or alphabetic)
11	"	16	- Geographic coordinate U (an independent variable)
17	"	22	- Geographic coordinate V (an independent variable)
23	"	28	- Dependent variable X_1
29	"	34	- Dependent variable X_2

Succeeding groups of six columns accommodate X_3 through X_8. Columns 71 through 80 are left blank.

A typical card with eight dependent variables (all identical for illustration) would have the following appearance:



Each variable should be expressed to the same number of decimal places. It is often convenient to punch the decimal on the data cards but this is optional as the position of the decimal is specified on the second master card. The program cannot accommodate 'no data,' because a blank space is interpreted as a zero observation. The program sets no limit to the number of data cards (and thus to the number of U,V-locations).

If less than eight dependent variables are involved, more space can be used on the data card for each variable; although the format of columns 1 through 10, and 71 through 80 remain unchanged. For example, if four dependent variables are involved, each variable could be assigned to 10-digit words, so that U occupies columns 11-20, V columns 21-30, etc.

The data deck:

The data deck is assembled in the following manner:

1. *DATA

2. Four TITLE CARDS

3. Two MASTER CARDS

4. Deck of data cards

5. One NINES CARD

6. Deck of data cards (exact duplicate set of 4 above)

7. One NINES CARD (exact duplicate of 5 above)

If more than one problem is to be executed with this program in the same run, successive decks may be assembled according to 2 through 7 above, and be placed behind 7 of the first deck. Any number of successive problems can be executed in this manner.

It will be noticed that two identical data decks (4 to 6 above) are required. This permits an unlimited number of geographic locations to be employed, and this benefit outweighs the slight inconvenience of duplicating the data cards. The program could be modified to store the data card information ready for second reading (B in Flow Sheet, Figure 1); this would obviate the need for a second deck of data cards, but involve a limit on the number of data cards which could be accommodated.

Title cards:

The format is (9 A6) so numeric and alphabetic characters can be utilized; typical cards might have the following form:

1 WHITTEN PROJECT 040060

0 MODAL DATA FOR LACORNE PLUTON, QUEBEC

0 X1 = QTZ; X2 = COLOR INDEX; X3 = FELD. RATIO

0 LQC-TREND SURFACES, N = 48

Master cards:

The first card has the format (A6, A4, I1, F1.0) and must provide the following information:

Columns 1 through 10 - Project control number (numeric or alphabetic characters) identified as NPROJ1 and NPROJ2

Column 11 - Number of dependent variables (1 through 8) identified as NX

Column 12 - Insert 1 if require coefficient cards to be punched by program in addition to list of coefficients printed automatically. If cards are not required, leave column blank. Identified in program as PCHCO.

The second master card has a format of (10X, 10A6), and the statement is identified in the program as VFT (variable format statement). The card is prepared as follows:

Columns 1 through 10 - Project control number (numeric or alphabetic characters) not used in program, but used to identify this card.

Columns 11 on - Statement of the format employed for the data cards. A typical statement would be (6XA4,10F6.3), which implies that (i) columns 1 through 6 of data card are not read, (ii) columns 7 through 10 are read and contain numeric or alphabetic sample point identification, and (iii) columns 11 onwards contain 10 words of 6 letters all expressed to 3 decimal places (this would be appropriate for U, V, and eight X_n). With U, V, and two X_n entered to two decimal places in 10-letter words, the statement would be (6XA4,4F10.2).

Thus, a typical set of two master cards might be

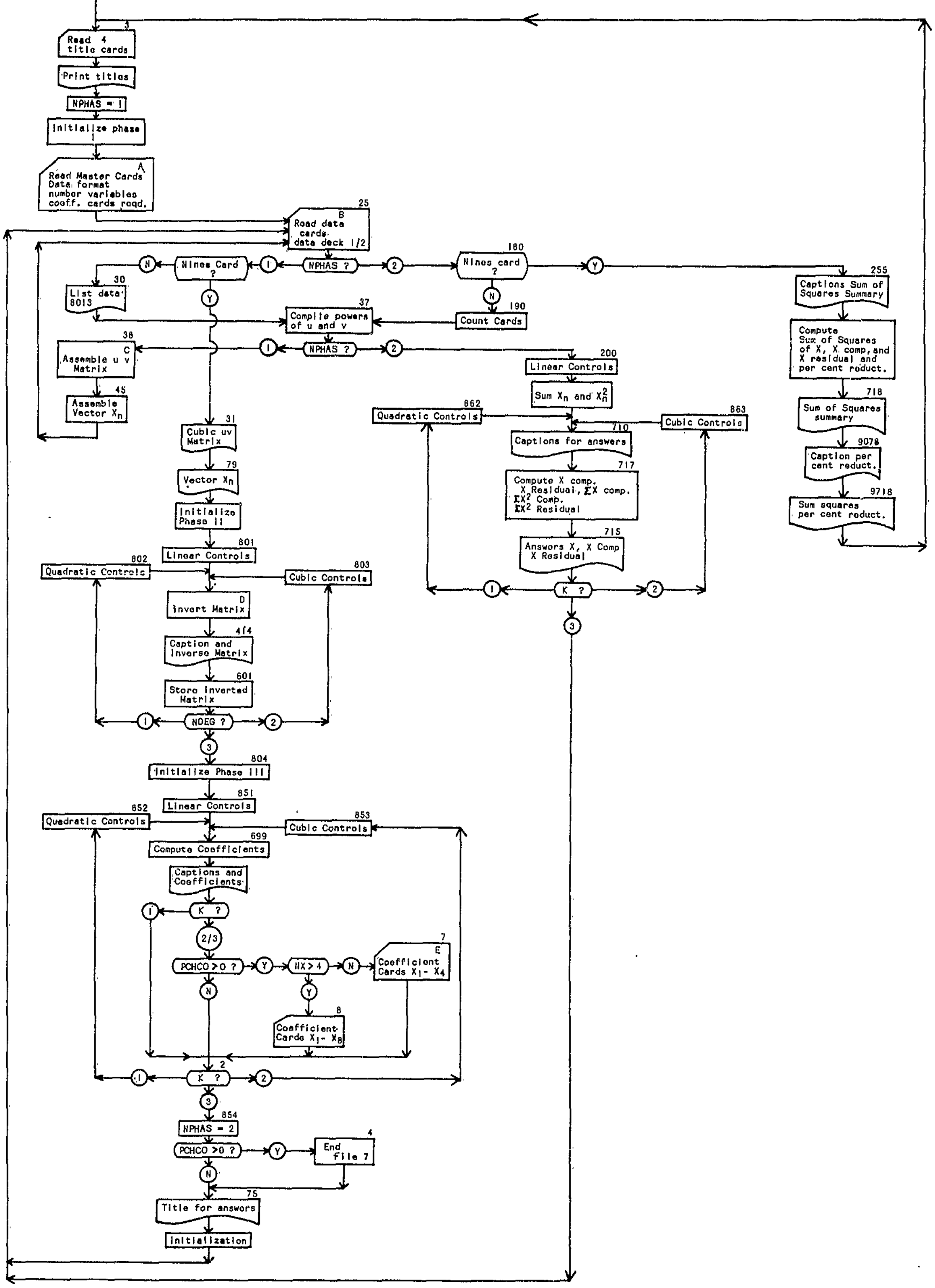
040060000041 (i.e., four variables and coefficient
0400600000(6XA4,10F6.3) cards wanted)

(Note: the format statement specifies the same number of decimal places for the variables U, V and X_n).

Nines card:

The program searches for the value 99999. to indicate that all data cards have been read. When U, V, and X_n are

Figure 8: Flow Chart for Part I of the program.



expressed as six-letter words, the nines card requires 99999. in columns 11 through 16. If ten-letter words are employed 000099999. is punched in columns 11 through 20, and similarly for any other word length 99999. is punched in the U-position of the data cards.

In this FORTRAN program all input is read from Tape 5. Output is put on Tape 6 when printed listing is required and on Tape 7 when card output is requested.

OPERATION OF THE PROGRAM

(PART I)

The sequence of operations can be read from the flow sheet (Figure 8). This sequence and the output of the program is outlined below.

For purposes of illustration, identical values are used for X_1, X_2.....X_8 at each datum-location in the following example. This has been done solely because the illustrative output is more easy to read, but in practice the several X_n may be completely independent, although each is a dependent variable with respect to U and V.

The four title cards are read first and this information is immediately printed out as shown in Table 2.

Following some initialization, the information contained on the two master cards is read and stored for use throughout the program (point A on flow sheet, Figure 8).

The program now begins to read the first deck of data cards and assembles the [U,V] matrix and the column vector $[X_n]$. During initialization NPHAS was set equal to 1, so that as each data card is read the information is immediately printed out on one line. The powers and products of U and V for this datum-location are then computed (37 in program listing) and stored in the 10 x 10 matrix P(I,J) (point C of flow sheet, Figure 1) and the column vector B(I,J). This column vector $[X_n]$is actually a matrix of size 10 x NX, where NX is defined by the number of dependent variables, so the matrix actually stores one column vector for each dependent variable (X_n).

Then the second data card is read; the additional information is added to that already in the P(I,J) and B(I,J) matrices Successive data cards are dealt with until the nines card is

TABLE 2

WHITTEN PROJECT 0401070000

PROBLEM TO ILLUSTRATE PROGRAM

X1 THRU X8 ALL IDENTICAL SYNTHETIC

LQC DOUBLE PRECISION 8 VARS.

TABLE 3

DATA

CONTROL	U	V	X1	X2	X3	X4	X5	X6	X7	X8
0001	0.	0.	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0002	1.000	0.	1.500	1.500	1.500	1.500	1.500	1.500	1.500	1.500
0003	2.000	0.	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0004	3.000	0.	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0005	0.	1.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0006	1.000	1.000	2.500	2.500	2.500	2.500	2.500	2.500	2.500	2.500
0007	2.000	1.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
0008	3.000	1.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0009	0.	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0010	1.000	2.000	2.500	2.500	2.500	2.500	2.500	2.500	2.500	2.500
0011	2.000	2.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
0012	3.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0013	0.	3.000	0.020	0.020	0.020	0.020	0.020	0.020	0.020	0.020
0014	1.000	3.000	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
0015	2.000	3.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
0016	3.000	3.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0017	0.	4.000	0.	0.	0.	0.	0.	0.	0.	0.
0018	1.000	4.000	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
0019	2.000	4.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0020	3.000	4.000	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500

TABLE 4

UV CUBIC

1	0.20000000E 02 0.12000000E 03	0.30000000E 02 0.18000000E 03	0.40000000E 02 0.13999999E 03	0.70000000E 02 0.18000000E 03	0.59999999E 02 0.40000000E 03
2	0.30000000E 02 0.18000000E 03	0.70000000E 02 0.48999999E 03	0.59999999E 02 0.36000000E 03	0.18000000E 03 0.41999999E 03	0.13999999E 03 0.60000000E 03
3	0.40000000E 02 0.40000000E 03	0.59999999E 02 0.36000000E 03	0.12000000E 03 0.41999999E 03	0.13999999E 03 0.60000000E 03	0.18000000E 03 0.14160000E 04
4	0.70000000E 02 0.41999999E 03	0.18000000E 03 0.13800000E 04	0.13999999E 03 0.98000000E 03	0.48999999E 03 0.10800000E 04	0.36000000E 03 0.13999999E 04
5	0.59999999E 02 0.60000000E 03	0.13999999E 03 0.98000000E 03	0.18000000E 03 0.10800000E 04	0.36000000E 03 0.13999999E 04	0.41999999E 03 0.21240000E 04
6	0.12000000E 03 0.14160000E 04	0.18000000E 03 0.10800000E 04	0.40000000E 03 0.13999999E 04	0.41999999E 03 0.21240000E 04	0.60000000E 03 0.52000000E 04
7	0.18000000E 03 0.10800000E 04	0.48999999E 03 0.39700000E 04	0.36000000E 03 0.27600000E 04	0.13800000E 04 0.29400000E 04	0.98000000E 03 0.36000000E 04
8	0.13999999E 03 0.13999999E 04	0.36000000E 03 0.27600000E 04	0.41999999E 03 0.29400000E 04	0.98000000E 03 0.36000000E 04	0.10800000E 04 0.49560000E 04
9	0.18000000E 03 0.21240000E 04	0.41999999E 03 0.29400000E 04	0.60000000E 03 0.36000000E 04	0.10800000E 04 0.49560000E 04	0.13999999E 04 0.78000000E 04
10	0.40000000E 03 0.52000000F 04	0.60000000E 03 0.36000000E 04	0.14160000E 04 0.49560000E 04	0.13999999E 04 0.78000000E 04	0.21240000E 04 0.19560000E 05

TABLE 5

VECTOR X(S)

1	0.30019999E 02	0.30019999E 02	0.30019999E 02	0.30019999E 02	0.30019999E 02	0.30019999E 02	0.30019999E 02	0.30019999E 02
2	0.50000000E 02	0.50000000E 02	0.50000000E 02	0.50000000E 02	0.50000000E 02	0.50000000E 02	0.50000000E 02	0.50000000E 02
3	0.47059999E 02	0.47059999E 02	0.47059999E 02	0.47059999E 02	0.47059999E 02	0.47059999E 02	0.47059999E 02	0.47059999E 02
4	0.11499999E 03	0.11499999E 03	0.11499999E 03	0.11499999E 03	0.11499999E 03	0.11499999E 03	0.11499999E 03	0.11499999E 03
5	0.82000000E 02	0.82000000E 02	0.82000000E 02	0.82000000E 02	0.82000000E 02	0.82000000E 02	0.82000000E 02	0.82000000E 02
6	0.11117999E 03	0.11117999E 03	0.11117999E 03	0.11117999E 03	0.11117999E 03	0.11117999E 03	0.11117999E 03	0.11117999E 03
7	0.29000000E 03	0.29000000E 03	0.29000000E 03	0.29000000E 03	0.29000000E 03	0.29000000E 03	0.29000000E 03	0.29000000E 03
8	0.18600000E 03	0.18600000E 03	0.18600000E 03	0.18600000E 03	0.18600000E 03	0.18600000E 03	0.18600000E 03	0.18600000E 03
9	0.20400000E 03	0.20400000E 03	0.20400000E 03	0.20400000E 03	0.20400000E 03	0.20400000E 03	0.20400000E 03	0.20400000E 03
10	0.30853999E 03	0.30853999E 03	0.30853999E 03	0.30853999E 03	0.30853999E 03	0.30853999E 03	0.30853999E 03	0.30853999E 03

TABLE 6

INVERTED MATRIX OF DEGREE 1

1	0.23999999E-00	-0.59999999E-01	-0.49999999E-01
2	-0.59999999E-01	0.39999999E-01	-0.
3	-0.49999999E-01	-0.	0.24999999E-01

TABLE 7

INVERTED MATRIX OF DEGREE 2

1	0.54142857E 00	-0.33000000E-00	-0.28285714E-00	0.49999999E-01	0.59999999E-01	0.35714285E-01
2	-0.33000000E-00	0.56999999E 00	0.59999999E-01	-0.15000000E-00	-0.39999999E-01	-0.
3	-0.28285714E-00	0.59999999E-01	0.35571428E-00	-0.	-0.30000000E-01	-0.71428571E-01
4	0.49999999E-01	-0.15000000E-00	-0.	0.49999999E-01	0.	0.
5	0.59999999E-01	-0.39999999E-01	-0.30000000E-01	0.	0.20000000E-01	0.
6	0.35714285E-01	-0.	-0.71428571E-01	0.	0.	0.17857143E-01

reached at the end of the data deck, by which time a complete list of the data cards has been made in the format shown in Table 3.

Immediately the nines card is read, the program calls for a print out of P(I,J), which comprises the [U,V] degree 3 matrix (see Equation x). This information is listed in floating point with the first row of the matrix across the page in two lines identified by 1. Subsequent rows are identified by 2, 3, 4,.....10 (see Table 4).

The column vectors for each X_n are then printed in floating point (Table 5). The ten entries of each column are listed down the page (identified by 1, 2, 3,.....10), and successive columns across the page correspond to X_1, X_2, X_3,.....X_8 (those for X_6 through X_8 being listed on a second line).

Initialization for Phase 2 of Part I is then completed and the program reads control statements in preparation for inversion of the linear 3 x 3 [U,V] matrix (D in flow sheet). The linear [U,V] matrix comprises the top left 3 x 3 block of the 10 x 10 matrix stored in P(I,J). The inverted 3 x 3 matrix, called A(I,J) in the program, is printed out in floating point as shown in Table 6. This inverted matrix, A(I,J), is stored in Y(I,J,NDEG), in which NDEG is defined as 1 (degree 1).

The program proceeds to 802 and reads the degree 2 controls before returning to the matrix inversion routine (D on the flow chart) to invert the degree 2 matrix, i.e., the top left 6 x 6 section of the main [U,V] matrix, P(I,J). The inverted 6 x 6 matrix, A(I,J), is printed out in floating point (see Table 7) and stored in Y(I,J,NDEG) with the degree, NDEG, defined as 2. The sixth column of A(I,J) is listed on a lower line.

Proceeding to 803, the degree 3 controls (including NDEG = 3) are read and the whole 10 x 10 P(I,J) matrix is inverted. The inverse A(I,J) is printed out and stored in Y(I,J,NDEG). Each row of A(I,J) requires two lines to print out as shown in Table 8. Because P(I,J) is always symmetrical about the principal diagonal, the degree 1, 2, and 3 inverse matrices, A(I,J), should also be symmetrical about their principal diagonal. The lists of the three inverted matrices enable the symmetry of each matrix to be

TABLE 8

INVERTED MATRIX OF DEGREE 3

1	0.80500000E 00 0.22499999E-00	-0.87238095E 00 -0.33333333E-01	-0.76916666E 00 -0.49999999E-01	0.30000000E-00 -0.42857143E-01	0.38142857E-00 -0.20833333E-01
2	-0.87238095E 00 -0.42857143E-01	0.39815872E 01 0.52222222E 00	0.38142857E-00 0.15000000E-00	-0.27999999E 01 0.28571428E-01	-0.60428571E 00 -0.66260929E-16
3	-0.76916666E 00 -0.10958333E 01	0.38142857E-00 0.29211201E-15	0.21790277E 01 0.24999999E-01	-0.49999999E-01 0.85714285E-01	-0.44785714E-00 0.14930555E-00
4	0.30000000E-00 -0.29605947E-15	-0.27999999E 01 -0.50000000E 00	-0.49999999E-01 -0.49999999E-01	0.23999999E 01 0.	0.15000000E-00 0.49343245E-16
5	0.38142857E-00 0.85714285E-01	-0.60428571E 00 -0.65527830E-15	-0.44785714E-00 -0.74999999E-01	0.15000000E-00 -0.57142857E-01	0.47357143E-00 -0.30310851E-16
6	0.22499999E-00 0.67500000E 00	-0.42857143E-01 0.30051843E-31	-0.10958333E 01 0.	-0.13523329E-30 -0.21428571E-01	0.85714285E-01 -0.10416666E-00
7	-0.33333333E-01 0.	0.52222222E 00 0.11111110E-00	-0. 0.	-0.49999999E-00 -0.	0. -0.
8	-0.49999999E-01 0.14802973E-15	0.15000000E-00 0.19737298E-15	0.24999999E-01 0.24999999E-01	-0.49999999E-01 -0.	-0.74999999E-01 -0.24671622E-16
9	-0.42857143E-01 -0.21428571E-01	0.28571428E-01 -0.20034562E-31	0.85714285E-01 -0.	0.90155531E-31 0.14285714E-01	-0.57142857E-01 0.21147105E-16
10	-0.20833333E-01 -0.10416666E-00	0. -0.	0.14930555E-00 -0.	0. 0.	-0. 0.17361110E-01

TABLE 9

COEFFS DEGREE 1

1	0.18517999E 01 0.18517999E 01	0.18517999E 01 0.18517999E 01	0.18517999E 01 0.18517999E 01	0.18517999E 01	0.18517999E 01
2	0.19880000E-00 0.19880000E-00	0.19880000E-00 0.19880000E-00	0.19880000E-00 0.19880000E-00	0.19880000E-00	0.19880000E-00
3	-0.32449999E-00 -0.32449999E-00	-0.32449999E-00 -0.32449999E-00	-0.32449999E-00 -0.32449999E-00	-0.32449999E-00	-0.32449999E-00

TABLE 10

COEFFS DEGREE 2

1	0.10831428E 01 0.10831428E 01	0.10831428E 01 0.10831428E 01	0.10831428E 01 0.10831428E 01	0.10831428E 01	0.10831428E 01
2	0.88699999E 00 0.88699999E 00	0.88699999E 00 0.88699999E 00	0.88699999E 00 0.88699999E 00	0.88699999E 00	0.88699999E 00
3	0.84711428E 00 0.84711428E 00	0.84711428E 00 0.84711428E 00	0.84711428E 00 0.84711428E 00	0.84711428E 00	0.84711428E 00
4	-0.24900000E-00 -0.24900000E-00	-0.24900000E-00 -0.24900000E-00	-0.24900000E-00 -0.24900000E-00	-0.24900000E-00	-0.24900000E-00
5	0.29399999E-01 0.29399999E-01	0.29399999E-01 0.29399999E-01	0.29399999E-01 0.29399999E-01	0.29399999E-01	0.29399999E-01
6	-0.30392857E-00 -0.30392857E-00	-0.30392857E-00 -0.30392857E-00	-0.30392857E-00 -0.30392857E-00	-0.30392857E-00	-0.30392857E-00

checked by the operator.[2]

Because NDEG = 3, after storing the inverted 10 x 10 cubic matrix, the program proceeds to 804 and initializes for Phase 3. Now the program is ready to solve Equation (ix) for the polynomial coefficients; the degree 1, 2 and 3 coefficients are obtained by successive operations. At 851 the linear controls are read, and multiplication of parts of the stored Y and B matrices develops linear coefficients in the matrix C(I,J,K). These are listed in floating point notation with the three coefficients (b_0, b_1, and b_2) in columns (Table 9); successive columns relate to variables X_1 through X_8 (with X_6 through X_8 on a lower line).

Since K = 1 the machine, after listing the linear coefficients, reads the degree 2 controls at 852 and returns to 699 to compute the degree 2 coefficients which are stored in the same C(I,J,K) matrix. The program follows the same looping so that the six coefficients are listed in columns (Table 10). K is now 2, so the program goes to 12 to test whether card output is required.

If coefficient cards are required for Part II of the program PCHCO will have been set at 1 on the second master card. If the number (NX) of dependent variables (X_n) is four or less the machine proceeds to 7 and puts instructions on Tape 7 for the punching of six cards, i.e., one for each coefficient c_0, c_1,.....c_6. The format of these cards insures that:

Columns 1 through 6	- Project number of program (NPROJ1).
Column 7	- Degree of surface where 2 indicates degree 2, and 3 degree 3
Column 8	- 1, which designates that coefficients of group X_1 through X_4 are involved.
Columns 9 and 10	- Numbers cards of each degree in correct order, successive cards being 1, 2, 3, ...

[2] As an additional check, the program could be modified either to
(a) invert the inverse matrix, A(I,J); this should recompute the original matrix P(I,J), or
(b) multiply the original matrix, P(I,J), by the computed inverse, A(I,J); the product should be a close approach to the unit matrix.

Columns 11 through 25 - Coefficients for variable X_1

Columns 26 through 40 - Coefficients for variable X_2

Columns 41 through 55 - Coefficients for variable X_3

Columns 56 through 70 - Coefficients for variable X_4

If there are five to eight variables NX is greater than 4 and the program goes to 8, instead of 7, so that two sets of coefficient cards are punched. The first set contains variables X_1 through X_4 identified by 1 in column 8, and the second contains X_5 through X_8 and is identified by 2 in column 8. The format of these cards is otherwise the same, and in both cases the coefficients are given in floating point.

The degree 2 controls made K = 2, so the program proceeds to 853 and reads the degree 3 controls (including K = 3). The degree 3 coefficients are computed and added to C(I,J,K); these coefficients (d_1, d_2, d_3, d_4, d_5,.....d_{10}) are listed in columns (Table 11). Cards are punched when PCHCO is 1, with the format detailed above for the degree 2.

K is now 3 so the program moves to 854 where NPHAS is changed to 2 and phases 4 and 5 are initiated. Following initialization, the first data card is read (at 25) for the second time (B on Flow Sheet). In practice it is the first card of the second (duplicate) data deck which is read. Proceeding to 190, the data cards are counted, and then (returning to 37) powers and products of U and V are compiled for this first data card.

The linear controls required for computing the values of X_n on the trend surface at each U,V-grid point are read at 200. Each dependent observed variable (X_n) is stored in SUMX(L) and as subsequent data cards are read the values of X_n are added to SUMX(L) to derive the $\sum X_1$, $\sum X_2$,....., $\sum X_8$. Also, each dependent observed variable is squared and stored in SUMXQ(L) to develop the $\sum X_n^2$.

At 710 a brief caption stating the degree surface and the card number is listed in preparation for tabulation of the main answers.

At 717 the linear computed values of X_n at the U,V-point recorded on the first data card are calculated by solution of Equation (ii); namely,

TABLE 11

COEFFS DEGREE 3

1	0.10052714E 01 0.10052714E 01	0.10052714E 01 0.10052714E 01	0.10052714E 01 0.10052714E 01	0.10052714E 01	0.10052714E 01
2	-0.30275238E-00 -0.30275238E-00	-0.30275238E-00 -0.30275238E-00	-0.30275238E-00 -0.30275238E-00	-0.30275238E-00	-0.30275238E-00
3	0.24195071E 01 0.24195071E 01	0.24195071E 01 0.24195071E 01	0.24195071E 01 0.24195071E 01	0.24195071E 01	0.24195071E 01
4	0.65300000E 00 0.65300000E 00	0.65300000E 00 0.65300000E 00	0.65300000E 00 0.65300000E 00	0.65300000E 00	0.65300000E 00
5	0.16547143E-00 0.16547143E-00	0.16547143E-00 0.16547143E-00	0.16547143E-00 0.16547143E-00	0.16547143E-00	0.16547143E-00
6	-0.13942143E 01 -0.13942143E 01	-0.13942143E 01 -0.13942143E 01	-0.13942143E 01 -0.13942143E 01	-0.13942143E 01	-0.13942143E 01
7	-0.16733333E-00 -0.16733333E-00	-0.16733333E-00 -0.16733333E-00	-0.16733333E-00 -0.16733333E-00	-0.16733333E-00	-0.16733333E-00
8	-0.74499999E-01 -0.74499999E-01	-0.74499999E-01 -0.74499999E-01	-0.74499999E-01 -0.74499999E-01	-0.74499999E-01	-0.74499999E-01
9	0.21857142E-01 0.21857142E-01	0.21857142E-01 0.21857142E-01	0.21857142E-01 0.21857142E-01	0.21857142E-01	0.21857142E-01
10	0.17625000E-00 0.17625000E-00	0.17625000E-00 0.17625000E-00	0.17625000E-00 0.17625000E-00	0.17625000E-00	0.17625000E-00

TABLE 12

CONTROL PT		X OBS	X COMP	DEVIATION
DEGREE 1 CARD 1				
0001	X1	1.00000	1.85180	-0.85180
0001	X2	1.00000	1.85180	-0.85180
0001	X3	1.00000	1.85180	-0.85180
0001	X4	1.00000	1.85180	-0.85180
0001	X5	1.00000	1.85180	-0.85180
0001	X6	1.00000	1.85180	-0.85180
0001	X7	1.00000	1.85180	-0.85180
0001	X8	1.00000	1.85180	-0.85180
DEGREE 2 CARD 1				
0001	X1	1.00000	1.08314	-0.08314
0001	X2	1.00000	1.08314	-0.08314
0001	X3	1.00000	1.08314	-0.08314
0001	X4	1.00000	1.08314	-0.08314
0001	X5	1.00000	1.08314	-0.08314
0001	X6	1.00000	1.08314	-0.08314
0001	X7	1.00000	1.08314	-0.08314
0001	X8	1.00000	1.08314	-0.08314
DEGREE 3 CARD 1				
0001	X1	1.00000	1.00527	-0.00527
0001	X2	1.00000	1.00527	-0.00527
0001	X3	1.00000	1.00527	-0.00527
0001	X4	1.00000	1.00527	-0.00527
0001	X5	1.00000	1.00527	-0.00527
0001	X6	1.00000	1.00527	-0.00527
0001	X7	1.00000	1.00527	-0.00527
0001	X8	1.00000	1.00527	-0.00527
DEGREE 1 CARD 2				
0002	X1	1.50000	2.05060	-0.55060
0002	X2	1.50000	2.05060	-0.55060
0002	X3	1.50000	2.05060	-0.55060
0002	X4	1.50000	2.05060	-0.55060
0002	X5	1.50000	2.05060	-0.55060
0002	X6	1.50000	2.05060	-0.55060
0002	X7	1.50000	2.05060	-0.55060
0002	X8	1.50000	2.05060	-0.55060
DEGREE 2 CARD 2				
0002	X1	1.50000	1.72114	-0.22114
0002	X2	1.50000	1.72114	-0.22114
0002	X3	1.50000	1.72114	-0.22114
0002	X4	1.50000	1.72114	-0.22114
0002	X5	1.50000	1.72114	-0.22114
0002	X6	1.50000	1.72114	-0.22114
0002	X7	1.50000	1.72114	-0.22114
0002	X8	1.50000	1.72114	-0.22114
DEGREE 3 CARD 2				
0002	X1	1.50000	1.18819	0.31181
0002	X2	1.50000	1.18819	0.31181
0002	X3	1.50000	1.18819	0.31181
0002	X4	1.50000	1.18819	0.31181
0002	X5	1.50000	1.18819	0.31181
0002	X6	1.50000	1.18819	0.31181
0002	X7	1.50000	1.18819	0.31181
0002	X8	1.50000	1.18819	0.31181

$$X = b_0 + b_1U + b_2V,$$

with the aid of the linear coefficients stored in C(I,J,K) and the powers of U and V compiled at 37 in T(I). The computed values are stored in XCP(L,K). These computed values, XCP(L,K), are subtracted from the observed values of X_n on the first data card. The differences are the deviations at this U,V-point, and are stored in RESD(L,K).

As successive data cards are read, the computed values are calculated and added to SXCP(L,K) to provide the sum of the computed X_n. Similarly, both the computed values and the deviations are squared, and successive squares are added to, and stored in, SXCPQ(L,K) and SRESQ(L,K), respectively.

The principal answers relating to the first datum-point are now listed in fixed point. The observed value (X OBS) of X_1, the computed value (X COMP), and the deviation are listed across the page, and the values for X_2, X_3,..... follow on successive lines.

The linear controls at 200 defined K = 1 so the program proceeds to 862 where the degree 2 controls are read (including K = 2). The degree 2 equations(iii) are now solved with values from the first data card, and the steps enumerated above are repeated to develop degree 2 values which are stored in the same matrices with the linear values. On re-reaching 715 the observed, computed, and deviation values of X_n are listed for each dependent variable.

The program loops to 863 and reads the degree 3 controls (including K = 3) and returns to 717 again to solve the degree 3 polynomial equation for values of X_n. A similar set of values as for the degree 1 and 2 surfaces is computed, and the degree 3 answers for the first U,V-point are listed in the form shown in Table 12.

Since K = 3, the program loops back to 25 (B on the Flow Sheet) to read the second data card. The degree 1, 2 and 3 answers for the second U,V-point are prepared and listed (Table 12), and the new values are added to the matrices being used for summation, i.e., SUMX(L), SUMXQ(L), SXCP(L,K), etc.

It will be noticed that the sample number is listed at the extreme left of the answer tabulation.

The program keeps looping back to 25 until all the data cards have been read. When the second nines card is

TABLE 13

SUMS OF SQUARES

	X OBS	X COMP	DEVIATION
DEGREE 1			
X1	16.44038	5.20005	11.24033
X2	16.44038	5.20005	11.24033
X3	16.44038	5.20005	11.24033
X4	16.44038	5.20005	11.24033
X5	16.44038	5.20005	11.24033
X6	16.44038	5.20005	11.24033
X7	16.44038	5.20005	11.24033
X8	16.44038	5.20005	11.24033
DEGREE 2			
X1	16.44038	11.65615	4.78423
X2	16.44038	11.65615	4.78423
X3	16.44038	11.65615	4.78423
X4	16.44038	11.65615	4.78423
X5	16.44038	11.65615	4.78423
X6	16.44038	11.65615	4.78423
X7	16.44038	11.65615	4.78423
X8	16.44038	11.65615	4.78423
DEGREE 3			
X1	16.44038	13.95289	2.48749
X2	16.44038	13.95289	2.48749
X3	16.44038	13.95289	2.48749
X4	16.44038	13.95289	2.48749
X5	16.44038	13.95289	2.48749
X6	16.44038	13.95289	2.48749
X7	16.44038	13.95289	2.48749
X8	16.44038	13.95289	2.48749

TABLE 14

PERCENT OF SUM OF SQUARES ACCOUNTED FOR BY EACH SURFACE

	LINEAR	QUADRATIC	CUBIC
X1	31.62972	70.89951	84.86964
X2	31.62972	70.89951	84.86964
X3	31.62972	70.89951	84.86964
X4	31.62972	70.89951	84.86964
X5	31.62972	70.89951	84.86964
X6	31.62972	70.89951	84.86964
X7	31.62972	70.89951	84.86964
X8	31.62972	70.89951	84.86964

reached at the end of the deck, the nines test (180) causes the program to branch to 255. Titles for the sums of squares summaries are now listed and the required values are computed in accordance with Equations (xii) through (xv). These values are stored under the following names:

SSX(L)	:	total sum of squares of the observed data
SSXCP(L,K)	:	sum of squares of the computed values
SSRES(L,K)	:	sum of squares of the deviations
SSXCR(L,K)	:	percentage of total variability accounted for by each trend component.

These values are computed for each dependent variable and (except in the case of SSX(L)) for each degree.

On reaching 718 the first three of these sets of values are listed across the page; values for X_1, X_2, X_3,..... are written on successive lines (Table 13). Degree 1 (linear) values are given first for all variables, then degrees 2 and 3 (linear plus quadratic, and linear plus quadratic plus cubic, respectively).

The percentage sums of squares accounted for by each surface are then tabulated in fixed point notation for each degree and all dependent variables (Table 14).

When this listing is completed, the program loops back to 3 and is ready to begin the next completely new problem. There is no limit to the number of successive problems which can be run.

PREPARATION TO RUN THE PROGRAM

(PART II)

The data deck:

The data deck is assembled in the following manner:

1. *DATA

2. Four TITLE CARDS

3. One MASTER CARD

4. Deck of data cards

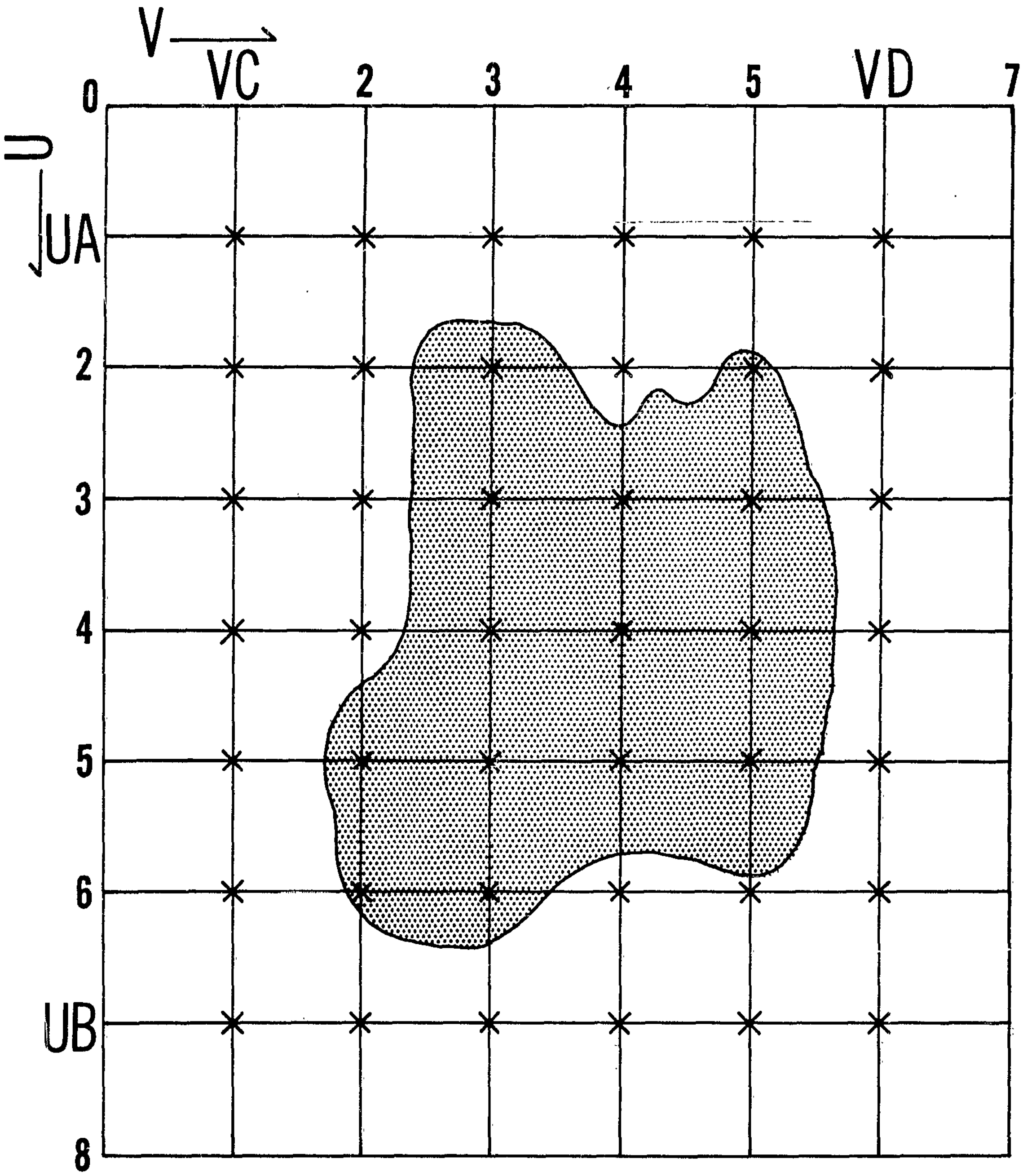


Figure 9: Example of an U,V-grid for a small intrusion. For explanation see text.

If more than one problem is to be executed with this program in the same run, successive decks may be assembled according to 2 through 4 above, and placed behind 4 of the first deck. Any number of successive problems can be executed in this manner.

Title cards:

The format is (12A6) so that numeric and alphabetic characters can be utilized; typical cards might have the following form:

1 WHITTEN PROJECT 040061

0 MODAL DATA FOR LA CORNE PLUTON, QUEBEC

0 X1 = QTZ; X2 = COLOR INDEX; X3 = FELD. RATIO

0 LQC-TREND SURFACES, UV-COMPUTED GRID

Master card:

This is a complex card which has the format (A6,2F10.3, I3,2F10.3,I3,I1) and it must provide the following information:

Columns 1 through 6 - Project control number (numeric or alphabetic characters) identified as NPROJ.

Columns 7 through 16 - The maximum U coordinate (UB on Figure 9) which must be expressed to three decimal places; identified as UB in the program.

Columns 17 through 26 - The minimum U coordinate (UA on Figure 9) which must be expressed to three decimal places; identified as UA in the program.

Columns 27 through 29 - The inclusive number of rows (identified as NU) of computed values required. The maximum number possible is 35.

Columns 30 through 39 - The maximum V coordinate (VD in program) expressed to three decimal places.

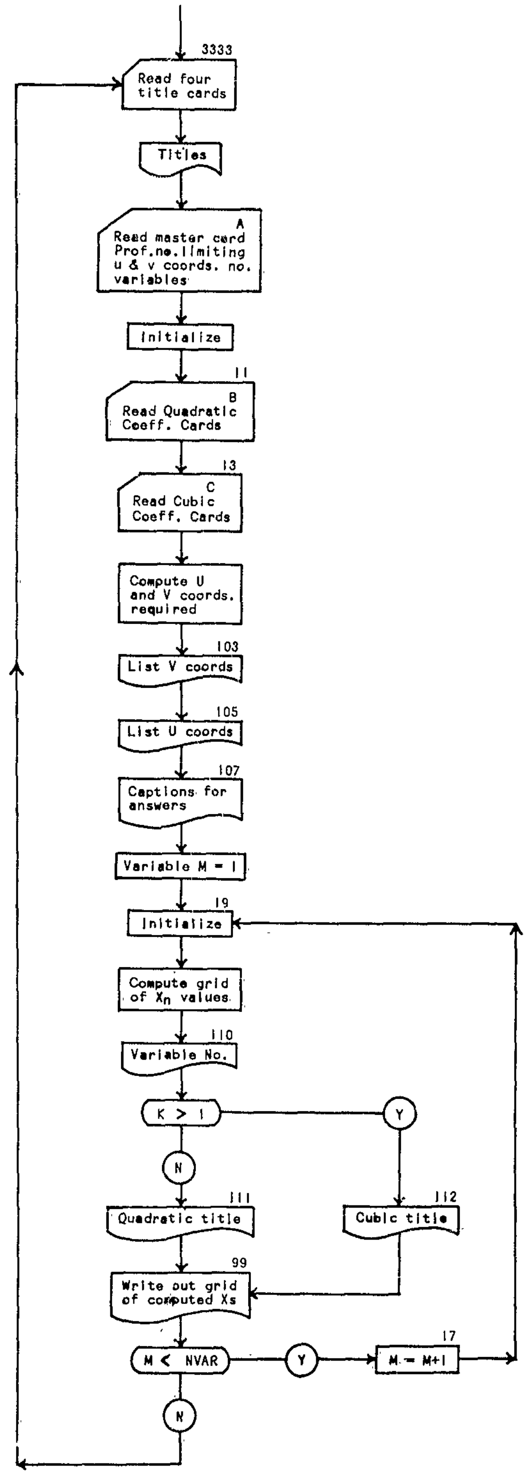


Figure 10: Flow chart for Part II of the program

Columns 40 through 49 - The minimum V coordinate (VC in program) expressed to three decimal places.

Columns 50 through 52 - The inclusive number of columns (identified as NV) of the computed values required. Maximum number possible is 35.

Column 53 - The number of dependent variables (X_n) which can be from one to four only.

As an example, to obtain computed values for four dependent variables at the points marked with a X in Figure 9 the master card must have the form:

040061000002.000000000.500004000002.500000000.5000054

Data cards:

These comprise the entire card output from Part I of the program. When from one to four dependent variables (X_n) were involved in Part I, the output cards comprise the new data deck without modification. This deck contains six degree 2, followed by ten degree 3, coefficient cards. If five to eight dependent variables were involved in Part I, the first, third, fifth,....., and thirty-first cards, which are identified by 1 in column 8, relate to variables X_1 through X_4 while the second, fourth, sixth,....., and thirty-second cards, which are identified by 2 in column 8, relate to variables X_5 through X_8 . In Part II it is necessary to run these two groups as successive separate problems (the master and title cards can of course be identical for both groups), because it will only accommodate four dependent variables at a time.

No nines cards are required.

OPERATION OF THE PROGRAM

(PART II)

The sequence of operations can be read from the flow sheet (Figure 10) and is described below. In this illustration, the card output from the illustration in Part I is assumed.

TABLE 15

WHITTEN PROJECT 040108

UV-COMPUTED VALUES

X1 THROUGH X4 IDENTICAL SYNTHETIC

PROBLEM TO ILLUSTRATE PROGRAM

TABLE 16

V-COORDINATES

0.
1.000
2.000
3.000
4.000

U-COORDINATES

0.
1.000
2.000
3.000

TABLE 17

UV-COMPUTED VALUES LISTED BY ROWS ACROSS MAP

QUADRATIC ANSWERS FIRST FOLLOWED BY CUBIC

VARIABLE X-1

QUADRATIC COMPUTED VALUES

U= 0.	1.083	1.626	1.562	0.889	-0.391
U= 1.000	1.721	2.294	2.258	1.615	0.364
U= 2.000	1.861	2.463	2.457	1.844	0.622
U= 3.000	1.503	2.135	2.158	1.574	0.382

CUBIC COMPUTED VALUES

U= 0.	1.005	2.207	1.677	0.475	-0.344
U= 1.000	1.188	2.503	2.130	1.127	0.552
U= 2.000	1.673	2.951	2.586	1.635	1.155
U= 3.000	1.456	2.549	2.042	0.993	0.459

VARIABLE X-2

QUADRATIC COMPUTED VALUES

U= 0.	1.083	1.626	1.562	0.889	-0.391

The four title cards are read first and this information is immediately printed out (Table 15).

The master card is read and the information stored. After initialization, six degree 2 coefficient cards (B in the flow sheet), and the ten degree 3 coefficient cards (C in the flow sheet), are read and stored in matrix COE(I,J). The U and V-coordinates for the required map-area are determined next. The interval between successive rows

UU = (UB - UA) / (UN - 1)

and successive columns

VV = (VD - VC) / (VN - 1)

are computed from information on the master card. These intervals are successively added to UA and VC and stored in UUM(I) and VVM(I), respectively. At 103 a list of the V-coordinates, VVM(I), and of the U-coordinates, UUM(I), is printed out (Table 16).

The captions for the computed grid of values is printed at 107. Then M (set as 1) defines which variable is involved in the following calculations. Using the coefficients stored in COE(I,J), and the U and V-coordinates stored in UUM(I) and VVM(I), respectively, the degree 2 and degree 3 polynomials are solved with respect to X_1 for each U,V-grid point. The values are stored in COMPX(I,J,K). This operation is effected by substituting appropriate values in Equation (i). The degree 2 values are then listed in fixed point to three decimal places by rows across the page, and the U-value of the row is identified in the left margin. The degree 3 values for X_1 are then listed in a similar manner (Table 17).

Following this listing, the program compares the number of variables (NVAR) stated on the master card with M. If there is still another variable, the program increments M to (M+1), loops back to 19, and initializes the COMPX(I,J,K) matrix. The coefficients for X_2 are then used to compute an array of values which are stored in COMPX(I,J,K) and listed. This process is repeated until values for all the X_n involved have been computed and listed. The program then loops back to 3333 to begin the next complete problem.

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APPENDIX I

```
      NORTHWESTERN UNIVERSITY GEOLOGY DEPARTMENT
C     SURFACE-FITTING PROGRAM FOR IRREGULARLY-SPACED MAP DATA
C     LINEAR, QUADRATIC, CUBIC - DOUBLE PRECISION - EIGHT VARIABLES
C     1957 KRUMBEIN AND HARRIS MACHINE LANGUAGE FOR BASIC IBM 650  4 VAR
C     1960 KRUMBEIN AND FAULKNER REWRITTEN IN SOAP FOR IBM 650 - 4 VARS
C     1961 AXELROD AND BENSON FOR KRUMBEIN REWRITTEN IN FORTRAN FOR
C          IBM 709 - FOUR VARIABLES AND SINGLE PRECISION
C     1962 WHITTEN EXTENDED TO DOUBLE PRECISION EIGHT VARIABLES AND
C          CARD OUTPUT FOR COEFFICIENTS FOR COMPUTING GRID OF UV-VALUES
      DIMENSION ZERO(2), ONE(2)
D     DIMENSION U(1), V(1)
      DIMENSION TIT1(9), TIT2(9), TIT3(9),TIT4(9),VFT(10)
D     DIMENSION X(8), T(10), B(10,8)
D     DIMENSION Y(10,10,3), C(10,8,3)
      DIMENSION XCP(8,3), RESD(8,3)
      DIMENSION SUMX(8), SUMXQ(8), SSX(8)
      DIMENSION SXCP(8,3), SXCPQ(8,3), SSXCP(8,3)
      DIMENSION            SRESQ(8,3), SSRES(8,3),SSXCR(8,3)
D     DIMENSION A(10,10),P(10,10)
      CARD1=1H1
      CARD2 = 1H2
      ONE(1) = 1.0
      ONE(2) = 0.0
    3 READ INPUT TAPE 5,72,TIT1,TIT2,TIT3,TIT4
      WRITE OUTPUT TAPE 6,72,TIT1,TIT2,TIT3,TIT4
   72 FORMAT (9A6)
C     * INITIALIZE PHASE ONE
      ZERO(1) = 0.0
      ZERO (2) = 0.0
    5 NPHAS=1
      DO 20 I=1,10
      DO 10 J=1,10
D  10 P(I,J) = ZERO
      DO 20 J = 1,8
D  20 B(I,J) = ZERO
      DO 904  I = 1,10
D 904 T(I) = ZERO
D     U = ZERO
D     V = ZERO
D     T(1)=1.0
C     READ MASTER CARDS
      READ INPUT TAPE 5,73,NPROJ1,NPROJ2,NX,PCHCD
   73 FORMAT (A6,A4,I1,F1.0)
      READ INPUT TAPE 5,11,VFT
   11 FORMAT (10X,10A6)
      WRITE OUTPUT TAPE 6,9,(I,I=1,NX)
    9 FORMAT(/20X4HDATA/20X4H----//5X7HCONTROL,4X1HU,10X1HV,X,8(9X1HX,I1
     1))
C     * ADD IN DATA
   25 READ INPUT TAPE 5,VFT,ID,U,V,(X(I), I = 1,NX)
      GO TO (27,180),NPHAS
   27 IF (U-99999.) 30,31,31
   30 CONTINUE
      WRITE OUTPUT TAPE 6, 8013,ID,U,V,(X(I),I = 1,NX)
 8013 FORMAT (5X, A4,10F11.3)
C     ASSEMBLE MATRIX
```

```
D   37 T(2)=U
D      T(3)=V
D      T(4)=U*U
D      T(5)=U*V
D      T(6)=V*V
D      T(7)=U*U*U
D      T(8)=U*U*V
D      T(9)=U*V*V
D      T(10)=V*V*V
       GO TO (38,200),NPHAS
    38 DO 45 I=1,10
       DO 40 J=1,10
D   40 P(I,J)=T(I)*T(J)+P(I,J)
       DO 45 J=1,NX
D   45 B(I,J)=X(J)*T(I)+B(I,J)
       GO TO 25
C      WRITE UV CUBIC MATRIX
    31 WRITE OUTPUT TAPE 6,78,
    78 FORMAT (////10X8HUV CUBIC/)
       DO 32 I=1,10
    32  WRITE OUTPUT TAPE 6,70,I,(P(I,J),J=1,10)
    70 FORMAT (/3XI2,5E20.8/(5X,5E20.8))
       WRITE OUTPUT TAPE 6,79,
C      WRITE OUT VECTOR XS
    79 FORMAT (//10X11HVECTOR X(S)/)
       DO 33 I=1,10
    33 WRITE OUTPUT TAPE 6,70,I,(B(I,J),J=1,NX)
C      BEGINNING PHASE TWO
       DO 501 I=1,10
       DO 501 J=1,10
       DO 501 K=1,3
D  501  Y(I,J,K) = ZERO
C      * CONTROL FOR INVERSION OF DATA MATRIX
       WRITE OUTPUT TAPE 6,74,
   801 MH=3
        NDEG =1
       GO TO 600
   802 MH=6
       NDEG =2
       GO TO 600
   803 MH=10
       NDEG =3
       GO TO 600
   600 DO 514 I=1,MH
       DO 514 J=1,MH
D  514 A(I,J)=P(I,J)
C       MATRIX INVERSION
       DO 414 K=1,MH
D      DIV = A(K,K)
D      A(K,K) = ONE
       DO 411 J=1,MH
D  411 A(K,J)=A(K,J)/DIV
       DO 414 I=1,MH
       IF(I-K)412,414,412
D  412 DIV = A(I,K)
D      A(I,K) = ZERO
```

```
      DO 413  J=1,MH
D 413 A(I,J)=A(I,J)-DIV*A(K,J)
  414 CONTINUE
      WRITE OUTPUT TAPE 6,900,NDEG
  900 FORMAT (/10X,26HINVERTED MATRIX OF DEGREE ,I1)
      DO 140 I=1,MH
  140 WRITE OUTPUT TAPE 6,70,I,(A(I,J),J=1,MH)
      DO 601 I=1,MH
      DO 601 J=1,MH
D 601 Y(I,J,NDEG) =A(I,J)
      GO TO (802,803,804) ,NDEG
C     INITIALIZE PHASE THREE
  804 DO 300 K=1,3
      DO 300 J=1,NX
      DO 300 I=1,10
D 300 C(I,J,K) = ZERO
C     COMPUTE COEFF
      WRITE OUTPUT TAPE 6,74,
   74 FORMAT (1H1)
  851 K=1
      MH=3
      GO TO 699
  852 K=2
      MH=6
      GO TO 699
  853 K=3
      MH=10
      GO TO 699
  699 DO 700 L=1,NX
      DO 700 I=1,MH
      DO 700 J=1,MH
D 700 C(I,L,K) = C(I,L,K) + Y(I,J,K) * B(J,L)
      WRITE OUTPUT TAPE 6,901,K
  901 FORMAT (/10X, 14HCOEFFS DEGREE ,I1)
      DO 703 I=1,MH
  703 WRITE OUTPUT TAPE 6,70,I,(C(I,L,K) , L=1,NX)
       GO TO (2,12,12),K
   12 IF (PCHCO) 1,2,1
    1 IF (NX-4) 7,7,8
    7 DO 9001      I =1,MH
 9001 WRITE OUTPUT TAPE 7,9000,NPROJ1,K,CARD1,I,(C(I,L,K),L=1,NX)
 9000 FORMAT (A6,I1,A1,I2,4E15.8)
      GO TO 2
    8 DO 9002 I=1,MH
 9002 WRITE OUTPUT TAPE 7,9000,NPROJ1,K,CARD1,I,(C(I,L,K),L=1,4),
     1                        NPROJ1,K,CARD2,I,(C(I,L,K),L=5,NX)
    2  GO TO (852,853,854) ,K
  854 NPHAS = 2
      IF (PCHCO) 4,6,4
    4 END FILE 7
C     BEGIN COMPUTING ANSWERS - PHASES FOUR AND FIVE
    6 WRITE OUTPUT TAPE 6,75,
   75 FORMAT(8H1CONTROL/3X2HPT,15X5HX OBS,14X6HX COMP,13X9HDEVIATION//)
      KCD = 0
      DO 705 L=1,NX
      DO 704 K=1,3
```

```
      SXCP(L,K) =0.0
      SXCPQ(L,K) =0.0
  704 SRESQ(L,K) =0.0
       SUMX(L) =0.0
  705 SUMXQ(L) =0.0
C     *  READ DATA
      GO TO 25
  180 IF (U - 99999.) 190,255,255
  190 KCD=KCD+1
      GO TO 37
C     *  COMPUTE X
  200 K=1
      MH=3
      DO 201 L=1,NX
      SUMX(L)=SUMX(L)+X(L)
  201 SUMXQ(L)=SUMXQ(L)+X(L)**2
      GO TO 710
  862 K=2
      MH=6
      GO TO 710
  863 K=3
      MH=10
      GO TO 710
  710 WRITE OUTPUT TAPE 6,902,K,KCD
  902 FORMAT (8H DEGREE ,I1,6H CARD ,I3)
      DO 715 L=1,NX
      XCP(L,K) =0.0
      DO 717 I=1,MH
  717 XCP (L,K) =C(I,L,K) * T(I) + XCP(L,K)
      RESD (L,K) =X(L)-XCP(L,K)
      SXCP(L,K) = SXCP(L,K) + XCP(L,K)
      SXCPQ(L,K) = SXCPQ(L,K) + XCP(L,K)**2
      SRESQ(L,K) = SRESQ(L,K) + RESD(L,K)**2
  715 WRITE OUTPUT TAPE 6,71,ID,L, X(L), XCP(L,K), RESD(L,K)
   71 FORMAT (2XA4,3H  X,I1,3F20.5)
       GO TO (862,863,864) ,K
  864 GO TO 25
  255 WRITE OUTPUT TAPE 6,76,
   76 FORMAT (1H1,15HSUMS OF SQUARES/20X5HX OBS, 14X,6HX COMP13X9HDEVIAT
     1ION//)
      CD=KCD
      DO 718 K=1,3
      WRITE OUTPUT TAPE 6,903,K
  903 FORMAT (/8H DEGREE ,I1)
      DO 718 L=1,NX
      SSX(L) =SUMXQ(L)-(SUMX(L)**2/CD)
      SSXCP(L,K) = SXCPQ(L,K) - (SXCP(L,K)**2/CD)
      SSRES(L,K) = SRESQ(L,K)
      SSXCR (L,K) = (SSXCP(L,K)/SSX(L))*100.0
  718 WRITE OUTPUT TAPE 6,77 ,L,SSX(L),SSXCP(L,K),SSRES(L,K)
      WRITE OUTPUT TAPE 6,9078,
 9078  FORMAT (///2X,55HPERCENT OF SUM OF SQUARES ACCOUNTED FOR BY EACH
 90781SURFACE/20X,6HLINEAR,13X,9HQUADRATIC,10X,5HCUBIC)
       DO 9718  L =1,NX
 9718 WRITE OUTPUT TAPE 6,77,L,(SSXCR(L,K),K = 1,3)
   77 FORMAT (6X3H  X,I1,3F20.5)
      GO TO 3
      END(1,0,0,0,0,0,0,0,0,1,0,0,0,0,0)
```

APPENDIX II

```
      NORTHWESTERN UNIVERSITY GEOLOGY DEPARTMENT
C     GRID OF COMPUTED VALUES FROM COEFFICIENTS OF LQC PROGRAM
C     PREPARED BY WHITTEN - JANUARY 1962
      DIMENSION UUM(35), VVM(35),COMPX(35,35,11)
      DIMENSION TIT1(12), TIT2(12), TIT3(12), TIT4(12), COE(20,4)
C     **READ TITLE CARDS
 3333 READ INPUT TAPE 5,101,TIT1,TIT2,TIT3,TIT4
      WRITE OUTPUT TAPE 6,101,TIT1, TIT2, TIT3, TIT4
  101 FORMAT (12A6)
C     ** READ MASTER CARD
      READ INPUT TAPE 5,1, NPROJ,UB,UA,NU,VD,VC,NV,NVAR
    1 FORMAT (A6,2F10.3,I3,2F10.3,I3,I1)
C     ** READ QUADRATIC COEFFICIENT CARDS
      DO 10 I= 1,20
      DO 10 J = 1,NVAR
   10 COE (I,J) = 0.0
      DO 11 I = 1,6
   11 READ INPUT TAPE 5,2, (COE (I,J), J = 1,NVAR)
    2 FORMAT (10X, 4E15.8)
C     ** READ CUBIC COEFFICENT CARDS
      DO 13 I = 11,20
   13 READ INPUT TAPE 5,3, (COE (I,J), J = 1,NVAR)
    3 FORMAT (10X, 4E15.8)
C     ** COMPUTE UV-MATRIX
      UN = NU
      VN = NV
      UU = (UB - UA)/(UN - 1.0)
      VV = (VD - VC)/(VN - 1.0)
      DO 14 I = 1, NU
   14 UUM(I) = UA + (UU*FLOATF(I -1))
      DO 15 I = 1, NV
   15 VVM(I) = VC + (VV*FLOATF(I-1))
      WRITE OUTPUT TAPE 6,103,
  103 FORMAT (//5X, 13HV-COORDINATES)
      WRITE OUTPUT TAPE 6,104,(VVM(I), I = 1,NV)
  104 FORMAT (//(5X,F7.3))
      WRITE OUTPUT TAPE 6,105,
  105 FORMAT (//5X,13HU-COORDINATES)
      WRITE OUTPUT TAPE 6,106,(UUM(I), I = 1,NU)
  106 FORMAT (//(5X,F7.3))
      WRITE OUTPUT TAPE 6,107,
  107 FORMAT(//5X,44HUV-COMPUTED VALUES LISTED BY ROWS ACROSS MAP//5X,
  107141HQUADRATIC ANSWERS FIRST FOLLOWED BY CUBIC)
      M = 1
   19 DO 12 K = 1,11,10
      DO 12 J = 1,NV
      DO 12 I = 1, NU
   12 COMPX (I,J,K) = 0.0
      DO 16 K = 1,11,10
      DO 16 J =1,NV
      DO 16 I = 1,NU
   16 COMPX(I,J,K) = COE (K,M) +(COE (K+1,M)*UUM(I))+(COE (K+2,M)*VVM(J)
   161)+(COE (K+3,M)*UUM(I)**2)+(COE (K+4,M)*UUM(I)*VVM(J))+(COE (K+5,M)
   162*VVM(J)**2) +(COE (K+6,M)*UUM(I)**3) +((COE (K+7,M)*UUM(I)**2)
   163*VVM(J))+((COE (K+8,M)*UUM(I))*VVM(J)**2)+(COE (K+9,M)*VVM(J)**3)
      WRITE OUTPUT TAPE 6,110,M
```

```
 110 FORMAT (///5X,11HVARIABLE X-,I1)
     DO 1000 K =1,11,10
     IF (K - 1) 111,111,112
 111 WRITE OUTPUT TAPE 6,113,
 113 FORMAT (//10X,25HQUADRATIC COMPUTED VALUES//)
     GO TO 99
 112 WRITE OUTPUT TAPE 6,114,
 114 FORMAT (//10X,21HCUBIC COMPUTED VALUES/)
  99 DO 1000 I =1,NU
1000 WRITE OUTPUT TAPE 6,102,UUM(I),(COMPX(I,J,K),J=1,NV)
 102 FORMAT (//2X,2HU=,F7.3,9F12.3/(11X,9F12.3))
     IF (M - NVAR) 17,3333,3333
  17 M = M + 1
     GO TO 19
     END(1,0,0,0,0,0,0,0,0,1,0,0,0,0,0)
```

LIST OF RECIPIENTS FOR #389135

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