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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
ONR Task No. 389-135
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OFFICE OF NAVAL RESEARCH
GEOGRAPHY BRANCH

Northwestern University
Evanston, Illinois

1963
CORRECTION FOR TECHNICAL REPORT NO. 2

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

Page 45, line 10, should read 0400610000001.0000000000.0000000000.0000000000.0000000000 instead of 040061000002.0000000000.5000000000.5000000000.5000000000.
Northwestern University
Evanston, Illinois

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F. H. Timothy Whitten

Technical Report No. 2
of
ONR Task No. 389-135
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Office of Naval Research
Geography Branch

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1963
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
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A SURFACE-FITTING PROGRAM SUITABLE FOR TESTING GEOLOGICAL MODELS WHICH INVOLVE AREALLY-DISTRIBUTED DATA

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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 onto 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 \( X_1, X_2, X_3, \ldots X_n \) 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:

\[
X_n = a_0 + a_1 U + a_2 V + a_3 U^2 + a_4 U V + a_5 V^2 + a_6 U^3 + a_7 U^2 V + \ldots (i)
\]

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

\[
X_n = b_0 + b_1 U + b_2 V \quad \ldots (ii)
\]

then the linear plus quadratic surface (second degree)

\[
X_n = c_0 + c_1 U + c_2 V + c_3 U^2 + c_4 U V + c_5 V^2 \quad \ldots (iii)
\]

and so on. Successive surfaces of higher degree (linear, linear plus quadratic, linear plus quadratic plus cubic, \ldots) 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 (1) 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 trend and residual on the basis of a $Z^2$-array, where $Z^2_{ak}$ represented the proportion of the total sum of squares of the mapped variable ($X_n$) accounted for by the $a_k$-th polynomial coefficient in Equation (1). $Z^2$-terms which contribute significantly to the total sum of squares determine the coefficients to be incorporated in the complete trend. The remaining $Z^2$-terms refer to those coefficients which comprise the residual. A typical $Z^2$-array is shown in Table 1. It will be noticed 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>
<thead>
<tr>
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<th>PART OF Z²-ARRAY*</th>
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<tr>
<td>N</td>
<td>LINEAR</td>
</tr>
<tr>
<td>---------</td>
<td>--------</td>
</tr>
<tr>
<td>309,300 a₀</td>
<td>30,300 a₁</td>
</tr>
<tr>
<td>288,260 a₂</td>
<td>54,847 a₄</td>
</tr>
<tr>
<td>100,354 a₅</td>
<td>2,323 a₈</td>
</tr>
<tr>
<td>1,520  a₉</td>
<td>654 a₁₃</td>
</tr>
<tr>
<td>1,245  a₁₄</td>
<td>130 a₁₉</td>
</tr>
<tr>
<td>20 a₂₀</td>
<td>0 a₂₆</td>
</tr>
<tr>
<td>20 a₂₇</td>
<td>9 a₃₄</td>
</tr>
<tr>
<td>618 a₃₅</td>
<td>221 a₄₃</td>
</tr>
<tr>
<td>90 a₄₄</td>
<td>77 a₅₃</td>
</tr>
<tr>
<td>30 a₅₄</td>
<td>13 a₶₄</td>
</tr>
</tbody>
</table>
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 ZP-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. 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

\[ X_n \text{ comp.} = b_0 + b_1U + b_2V \] of Equation (ii).

If \( X_{njobs} \) is the observed value at the \( U_i, V_j \)-location, then the deviation at this point is \( (X_{njobs} - X_{nj, comp}) \).

\(^1\)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).
where N is the number of \( \Lambda \)-locations at which data were obtained. Consequently, the matrix form we use is

\[
\begin{bmatrix}
\mathbf{sq}(\lambda_1x) \\
\mathbf{sq}(\lambda_2x) \\
\mathbf{sq}(\lambda_3x)
\end{bmatrix} = \begin{bmatrix}
\lambda_1 \\
\mathbf{A}_1 \\
\mathbf{A}_2
\end{bmatrix} \cdot \begin{bmatrix}
\mathbf{a}_1 \\
\mathbf{a}_2 \\
\mathbf{a}_3
\end{bmatrix} \cdot \begin{bmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\lambda_4 \\
\lambda_5 \\
\lambda_6
\end{bmatrix}
\]

These expressions reduce to the three normal equations:

\[
\begin{bmatrix}
\frac{\partial \mathbf{q}}{\partial \phi_1} \\
\frac{\partial \mathbf{q}}{\partial \phi_2} \\
\frac{\partial \mathbf{q}}{\partial \phi_3}
\end{bmatrix} = \begin{bmatrix}
\mathbf{a}_1 \\
\mathbf{a}_2 \\
\mathbf{a}_3
\end{bmatrix} \cdot \begin{bmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3
\end{bmatrix} + \begin{bmatrix}
\lambda_4 \\
\lambda_5 \\
\lambda_6
\end{bmatrix}
\]

These partial derivatives are

\[
\frac{\partial \mathbf{q}}{\partial \phi} = \frac{\lambda_1}{\partial \phi} \quad \frac{\partial \mathbf{q}}{\partial \phi} = \frac{\lambda_2}{\partial \phi} \quad \frac{\partial \mathbf{q}}{\partial \phi} = \frac{\lambda_3}{\partial \phi}
\]

Thus, the least-squares fit is obtained by minimizing the sum of squares of the residuals.
To obtain the least squares fit, the sum of squares of the deviations must be minimized. Thus,

$$\sum (x_{ni, obs} - x_{ni, comp})^2 = \sum (x_{n, obs} - b_0 - b_1U - b_2V)^2 \quad \text{(iv)}$$

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

$$\begin{align*}
\frac{\partial F}{\partial b_0} &= \Sigma 2(x_{n, obs} - b_0 - b_1U - b_2V).(-1) = 0 \\
\frac{\partial F}{\partial b_1} &= \Sigma 2(x_{n, obs} - b_0 - b_1U - b_2V).(-U) = 0 \\
\frac{\partial F}{\partial b_2} &= \Sigma 2(x_{n, obs} - b_0 - b_1U - b_2V).(-V) = 0
\end{align*} \quad \text{(vi)}$$

These expressions reduce to the three normal equations:

$$\begin{align*}
b_0 N + b_1 \Sigma U + b_2 \Sigma V &= \Sigma x_{n, obs} \\
b_0 U + b_1 \Sigma U^2 + b_2 \Sigma UV &= \Sigma u x_{n, obs} \\
b_0 V + b_1 \Sigma UV + b_2 \Sigma V^2 &= \Sigma v x_{n, obs}
\end{align*} \quad \text{(vii)}$$

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

$$\begin{bmatrix}
N & \Sigma U & \Sigma V \\
\Sigma U & \Sigma U^2 & \Sigma UV \\
\Sigma V & \Sigma UV & \Sigma V^2
\end{bmatrix} \begin{bmatrix}
b_0 \\
b_1 \\
b_2
\end{bmatrix} = \begin{bmatrix}
\Sigma x_{n, obs} \\
\Sigma u x_{n, obs} \\
\Sigma v x_{n, obs}
\end{bmatrix} \quad \text{(viii)}$$
Since the \([U, V]\) matrix and the column vector \([X_{nobs}]\) 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:

\[
\begin{bmatrix}
  b_0 \\
  b_1 \\
  b_2
\end{bmatrix} = \begin{bmatrix}
  U, V
\end{bmatrix}^{-1} \begin{bmatrix}
  \Sigma X_{nobs} \\
  \Sigma UX_{nobs} \\
  \Sigma VX_{nobs}
\end{bmatrix} \quad \ldots\ldots (ix)
\]

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, \ldots, 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).

\begin{equation}
\text{(x)}
\end{equation}

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
N.B. The broken lines indicate the smaller \( V \)-matrices appropriate to degrees 1 and 2.

\[
\begin{array}{c|cccccccc}
\text{sqo}_{u_x} & 6p & 9p & 3p & 7p & 4p & 8p & 5p & 2p & 1p & 0p \\
\hline
\text{sqo}_{u_x} & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & & & & \gamma_{A^3} & \gamma_{A_2} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & & & & & \gamma_{A^3} & \gamma_{A_2} \\
\text{sqo}_{u_x} & & & & & & & & & \gamma_{A^3} \\
\end{array}
\]
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 \( \bar{X}_{n, \text{obs}} \) is the mean value of a set of observed values \( X_{n, \text{obs}} \), then the deviation from the mean at the \( ij \)-th point is \( (X_{nij, \text{obs}} - \bar{X}_{n, \text{obs}}) \), 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.,

\[
\sum_{i=1}^{N} (X_{n, \text{obs}} - \bar{X}_{n, \text{obs}})^2 \quad \cdots \quad (\text{x})
\]

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

\[
\sum_{i=1}^{N} X_{n, \text{obs}}^2 - \left(\frac{\sum_{i=1}^{N} X_{n, \text{obs}}}{N}\right)^2 \quad \cdots \quad (\text{xi})
\]

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

\[
\sum (X_{n, \text{comp}} - \bar{X}_{n, \text{obs}})^2 = \sum X_{n, \text{comp}}^2 - \left(\frac{\sum X_{n, \text{comp}}}{N}\right)^2 \quad \cdots \quad (\text{xii})
\]

Since \( \bar{X}_{n, \text{obs}} = \bar{X}_{n, \text{comp}} \), the sum of squares of the deviations from the trend component (see Figure 2C) is given
Figure 2: Plane with dots is $X_n$ 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:

\[ \sum (X_{n\text{obs}} - X_{n\text{comp}})^2 = \sum X_n^2 \text{deviation} \quad \ldots \ldots (xIV) \]

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:

\[ \left( \frac{\text{Sum of squares of the computed } X_{n\text{linear}}}{\text{Total sum of squares of the observed } X_n} \right) \times 100 \text{ per cent.} \quad (xV) \]

of the total variability, where \( X_{n\text{linear}} \) 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; Wylie, 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, cemenitic 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 5: Trend components for color index data in the Lacrosse granite model, North America. A. Linear component (accounts for 2.3 per cent. of the total sum of squares). B. Degree 2 component (accounts for 5.5 per cent. of the total sum of squares). C. Degree 3 component (accounts for 11.8 per cent. of the total sum of squares). (After Hanson and Chilton, 1971, Fig. 6).
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 con-
centric 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 miner-
alogical 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 con-
tent 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 correla-
tion 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 pro-
vide 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 ob-
tained. 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 Whitton (1963A); other variables could un-
doubtedly 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-1288(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,
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 X₁

29 " 34 - Dependent variable X₂

Succeeding groups of six columns accommodate X₃ through X₈. 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, Il, Fl.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 NNX

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 PCCHCO.

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 Xn). With U, V, and two Xn 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 cards wanted)

0400600000(6XA4,10F6.3) cards wanted

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

Nines card:

The program searches for the value 999999 to indicate that all data cards have been read. When U, V, and Xn 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 \(X_1, X_2, \ldots, X_8\) 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 \(X_i\) 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 \(10 \times 10\) 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 \(10 \times NX\), 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.

Data

<table>
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<tr>
<th>CONTROL</th>
<th>U</th>
<th>V</th>
<th>X1</th>
<th>X2</th>
<th>X3</th>
<th>X4</th>
<th>X5</th>
<th>X6</th>
<th>X7</th>
<th>X8</th>
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<td>2.000</td>
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<td>2.000</td>
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</tbody>
</table>

TABLE 3

UV CUBIC

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<th>Value</th>
<th>X1</th>
<th>X2</th>
<th>X3</th>
<th>X4</th>
<th>X5</th>
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<th>X7</th>
<th>X8</th>
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<tbody>
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<td>0.21240000E 04</td>
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<td>0.49560000E 04</td>
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<tr>
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</tr>
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</tr>
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<td>0.13999999E 03</td>
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<td>0.49560000E 04</td>
</tr>
<tr>
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<td>0.49560000E 04</td>
</tr>
<tr>
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<td>0.21240000E 04</td>
<td>0.80000000E 04</td>
<td>0.49560000E 04</td>
</tr>
</tbody>
</table>
### TABLE 5

#### VECTOR $X(S)$

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### TABLE 6

#### INVERTED MATRIX OF DEGREE 1

<table>
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<tr>
<th></th>
<th>$0.23999999 \times 10^{-2}$</th>
<th>$-0.59999999 \times 10^{-1}$</th>
<th>$-0.49999999 \times 10^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>$0.$</td>
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<td>3</td>
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</tbody>
</table>

### TABLE 7

#### INVERTED MATRIX OF DEGREE 2

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<th>$0.49999999 \times 10^{-1}$</th>
<th>$0.59999999 \times 10^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
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<td>$0.59999999 \times 10^{-1}$</td>
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<td>$-0.39999999 \times 10^{-1}$</td>
</tr>
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<td>3</td>
<td>$-0.28285714 \times 10^{-1}$</td>
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<td>$-0.30000000 \times 10^{-1}$</td>
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<td>$0.$</td>
<td>$0.$</td>
</tr>
</tbody>
</table>
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 $3 \times 3$ $[U,V]$ matrix (D in flow sheet). The linear $[U,V]$ matrix comprises the top left $3 \times 3$ block of the $10 \times 10$ matrix stored in P(I,J). The inverted $3 \times 3$ 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 $6 \times 6$ section of the main $[U,V]$ matrix, P(I,J). The inverted $6 \times 6$ 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 $10 \times 10$ 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

<p>| | | | | |</p>
<table>
<thead>
<tr>
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<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<tr>
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<td>0.38142857e-00</td>
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<tr>
<td>3</td>
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<td>0.38142857e-00</td>
<td>0.37999999e+00</td>
<td>-0.42857143e-01</td>
</tr>
</tbody>
</table>

TABLE 9

COEFFS DEGREE 1

<p>| | | | |</p>
<table>
<thead>
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<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
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<td>0.18517999e-00</td>
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</tbody>
</table>

TABLE 10

COEFFS DEGREE 2

<p>| | | | | |</p>
<table>
<thead>
<tr>
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<th></th>
<th></th>
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TABLE 11

COEFFS DEGREE 3

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
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<tr>
<td>-3</td>
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<td>0.30792857e-00</td>
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</tr>
</tbody>
</table>
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. It
851 the linear controls are read, and multiplication of
parts of the stored Y and B matrices develops linear co-
cefficients in the matrix C(I,J,K). These are listed in floating
point notation with the three coefficients (b0, b1, and b2)
in columns (Table 9); successive columns relate to variables
X1 through X8 (with X8 through X8 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 (Xn) 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 c0, c1, ..., c6. The format of these cards insure
that:

Columns 1 through 6 - Project number of program (NPROJ).
Column 7 - Degree of surface where 2 indicates
degree 2, and 3 degree 3
Column 8 - 1, which designates that coefficients
of group X1 through X4 are involved.
Columns 9 and 10 - Numbers cards of each degree in cor-
rect order, successive cards being
1, 2, 3, ....

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 com-
puted inverse, A(I,J); the product should be a
close approach to the unit matrix.
Columns 11 through 25 - Coefficients for variable X₁
Columns 26 through 40 - Coefficients for variable X₂
Columns 41 through 55 - Coefficients for variable X₃
Columns 56 through 70 - Coefficients for variable X₄

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 X₁ through X₄ identified by 1 in column 8, and the second contains X₅ through X₈ 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 (d₁, d₂, d₃, d₄, d₅, ..., d₁₀) 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 Xn on the trend surface at each U,V-grid point are read at 200. Each dependent observed variable (Xn) is stored in SUMX(L) and as subsequent data cards are read the values of Xn are added to SUMX(L) to derive the \( \sum X_1, \sum X_2, ..., \sum X_9 \). Also, each dependent observed variable is squared and stored in SUMX²(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 Xn at the U,V-point recorded on the first data card are calculated by solution of Equation (11); namely,
### Table 11

<table>
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<th>PT</th>
<th>X OBS</th>
<th>X COMP</th>
<th>DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>0001 X1</td>
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<td>1.85180</td>
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<tr>
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<td>1.0000</td>
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<td>-0.85180</td>
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<tr>
<td>0001 X4</td>
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### Table 12

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<th>X COMP</th>
<th>DEVIATION</th>
</tr>
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</tr>
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<td>0001 X3</td>
<td>1.0000</td>
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<td>-0.08314</td>
</tr>
<tr>
<td>0001 X4</td>
<td>1.0000</td>
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<td>-0.08314</td>
</tr>
<tr>
<td>0001 X5</td>
<td>1.0000</td>
<td>1.08314</td>
<td>-0.08314</td>
</tr>
<tr>
<td>0001 X6</td>
<td>1.0000</td>
<td>1.08314</td>
<td>-0.08314</td>
</tr>
<tr>
<td>0001 X7</td>
<td>1.0000</td>
<td>1.08314</td>
<td>-0.08314</td>
</tr>
<tr>
<td>0001 X8</td>
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<td>1.08314</td>
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### Table 13

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<tbody>
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</tr>
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<tr>
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<td>-0.000527</td>
</tr>
<tr>
<td>0001 X5</td>
<td>1.0000</td>
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<td>-0.000527</td>
</tr>
<tr>
<td>0001 X6</td>
<td>1.0000</td>
<td>1.000527</td>
<td>-0.000527</td>
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<tr>
<td>0001 X7</td>
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<tr>
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### Table 14

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<th>DEVIATION</th>
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</thead>
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<tr>
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<td>-0.22114</td>
</tr>
<tr>
<td>0001 X3</td>
<td>1.5000</td>
<td>1.72114</td>
<td>-0.22114</td>
</tr>
<tr>
<td>0001 X4</td>
<td>1.5000</td>
<td>1.72114</td>
<td>-0.22114</td>
</tr>
<tr>
<td>0001 X5</td>
<td>1.5000</td>
<td>1.72114</td>
<td>-0.22114</td>
</tr>
<tr>
<td>0001 X6</td>
<td>1.5000</td>
<td>1.72114</td>
<td>-0.22114</td>
</tr>
<tr>
<td>0001 X7</td>
<td>1.5000</td>
<td>1.72114</td>
<td>-0.22114</td>
</tr>
<tr>
<td>0001 X8</td>
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<td>1.72114</td>
<td>-0.22114</td>
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### Table 15

<table>
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<th>X OBS</th>
<th>X COMP</th>
<th>DEVIATION</th>
</tr>
</thead>
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<td>0001 X1</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X2</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X3</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X4</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X5</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X6</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X7</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
<tr>
<td>0001 X8</td>
<td>1.5000</td>
<td>1.81819</td>
<td>0.31181</td>
</tr>
</tbody>
</table>
\[ X = b_0 + b_1 U + b_2 V, \]

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 \( X_2, X_3, \ldots \) follow on successive lines.

The linear controls at 200 defined \( K = 1 \) so the program proceeds to 362 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 363 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

<table>
<thead>
<tr>
<th>DEGREE 1</th>
<th>X OBS</th>
<th>X COMP</th>
<th>DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X2</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X3</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X4</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X5</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X6</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X7</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
<tr>
<td>X8</td>
<td>16.44038</td>
<td>5.20005</td>
<td>11.24033</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>DEGREE 2</th>
<th>X OBS</th>
<th>X COMP</th>
<th>DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X2</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X3</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X4</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X5</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X6</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X7</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
<tr>
<td>X8</td>
<td>16.44038</td>
<td>11.65615</td>
<td>4.78423</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>DEGREE 3</th>
<th>X OBS</th>
<th>X COMP</th>
<th>DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X2</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X3</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X4</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X5</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X6</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X7</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
<tr>
<td>X8</td>
<td>16.44038</td>
<td>13.95289</td>
<td>2.48749</td>
</tr>
</tbody>
</table>

TABLE 14

PERCENT OF SUM OF SQUARES ACCOUNTED FOR BY EACH SURFACE

<table>
<thead>
<tr>
<th>LINEAR</th>
<th>QUADRATIC</th>
<th>CUBIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X2</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X3</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X4</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X5</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X6</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X7</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
<tr>
<td>X8</td>
<td>31.62972</td>
<td>70.09951</td>
</tr>
</tbody>
</table>
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  LOC-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 (Xn) 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:

0400610000000.000000000.500000000.000000000

Data cards:

These comprise the entire card output from Part I of the program. When from one to four dependent variables (Xn) 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 X1 through X4 while the second, fourth, sixth, ...., and thirty-second cards, which are identified by 2 in column 8, relate to variables X5 through X8. 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

<table>
<thead>
<tr>
<th>V-COORDINATES</th>
<th>0.000</th>
<th>1.000</th>
<th>2.000</th>
<th>3.000</th>
<th>4.000</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-COORDINATES</td>
<td>0.000</td>
<td>1.083</td>
<td>1.626</td>
<td>1.562</td>
<td>0.889</td>
</tr>
<tr>
<td></td>
<td>1.000</td>
<td>1.721</td>
<td>2.294</td>
<td>2.258</td>
<td>1.615</td>
</tr>
<tr>
<td></td>
<td>2.000</td>
<td>1.861</td>
<td>2.463</td>
<td>2.457</td>
<td>1.846</td>
</tr>
<tr>
<td></td>
<td>3.000</td>
<td>1.963</td>
<td>2.135</td>
<td>2.158</td>
<td>1.574</td>
</tr>
</tbody>
</table>

### TABLE 17

UV-COMPUTED VALUES LISTED BY ROWS ACROSS MAP  
QUADRATIC ANSWERS FIRST FOLLOWED BY CUBIC  
VARIABLE X-1  
QUADRATIC COMPUTED VALUES

<table>
<thead>
<tr>
<th>U= 0.000</th>
<th>1.083</th>
<th>1.626</th>
<th>1.562</th>
<th>0.889</th>
<th>-0.391</th>
</tr>
</thead>
<tbody>
<tr>
<td>U= 1.000</td>
<td>1.721</td>
<td>2.294</td>
<td>2.258</td>
<td>1.615</td>
<td>0.356</td>
</tr>
<tr>
<td>U= 2.000</td>
<td>1.861</td>
<td>2.463</td>
<td>2.457</td>
<td>1.846</td>
<td>0.622</td>
</tr>
<tr>
<td>U= 3.000</td>
<td>1.963</td>
<td>2.135</td>
<td>2.158</td>
<td>1.574</td>
<td>0.312</td>
</tr>
</tbody>
</table>

CUBIC COMPUTED VALUES

<table>
<thead>
<tr>
<th>U= 0.000</th>
<th>1.005</th>
<th>2.207</th>
<th>1.677</th>
<th>0.475</th>
<th>-0.344</th>
</tr>
</thead>
<tbody>
<tr>
<td>U= 1.000</td>
<td>1.188</td>
<td>2.403</td>
<td>2.130</td>
<td>1.127</td>
<td>0.562</td>
</tr>
<tr>
<td>U= 2.000</td>
<td>1.673</td>
<td>2.951</td>
<td>2.586</td>
<td>1.639</td>
<td>1.155</td>
</tr>
<tr>
<td>U= 3.000</td>
<td>1.456</td>
<td>2.549</td>
<td>2.042</td>
<td>0.991</td>
<td>0.459</td>
</tr>
</tbody>
</table>

VARIABLE X-2  
QUADRATIC COMPUTED VALUES

<table>
<thead>
<tr>
<th>U= 0.000</th>
<th>1.083</th>
<th>1.626</th>
<th>1.562</th>
<th>0.889</th>
<th>-0.391</th>
</tr>
</thead>
</table>
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

\[ UU = \frac{(UB - UA)}{(UN - 1)} \]

and successive columns

\[ VV = \frac{(VD - VC)}{(VN - 1)} \]

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 (1). 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.
REFERENCES CITED


NORTHWESTERN UNIVERSITY GEOLOGY DEPARTMENT

SURFACE-FITTING PROGRAM FOR IRREGULARLY-SPACED MAP DATA
LINEAR, QUADRATIC, CUBIC - DOUBLE PRECISION - EIGHT VARIABLES
1957 Krumbein and Harris Machine Language for Basic IBM 650 - 4 VAR
1960 Krumbein and Faulkner Rewritten in Soap for IBM 650 - 4 VARS
1961 Axelrod and Benson for Krumbein Rewritten in Fortran for
IBM 709 - Four Variables and Single Precision
1962 Whitten Extended to Double Precision Eight Variables and
Card Output for Coefficients for Computing Grid of UV-Values

DIMENSION ZEROU(2), ONE(2)
DIMENSION U(1), V(1)
DIMENSION TIT1(9), TIT2(9), TIT3(9), TIT4(9), VFT1(10)
DIMENSION X(8), T(10), B(10,8)
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), SRES3(8,3), SXXCR(8,3)
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 20 J=1,10
20 P(I,J) = ZERO
DO 904 I = 1,10
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,PCHD
73 FORMAT (A6,A4,Il,F1.0)
READ INPUT TAPE 5,11,VFT
11 FORMAT (10X,10A6)
WRITE OUTPUT TAPE 6,9,(I=1,NX)
9 FORMAT (/20X4HDATA/20X4H-----/5X7HCONTROl,4XLUH,10X1HV,X,8(9X1HX,I1))
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 (5K, 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*V*V
D T(9)=V*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 R(I,J)=X(J)*T(I)+R(I,J)
GO TO 25
C WRITE UV CUBIC MATRIX
31 WRITE OUTPUT TAPE 6,78,
78 FORMAT (////10X8HV 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 (///10X11VECTOR X(S)/)
DO 33 I=1,10
33 WRITE OUTPUT TAPE 6,70,I,(R(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
802 MH=6
803 MH=10
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 FURMAI (/10X,26HINVERTED MATRIX OF DEGREE ,11)
DO 140 I=1,MH
140 WRITE OUTPUT TAPE 6,70,1,(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
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
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 ,11)
DO 703 I=1,MH
703 WRITE OUTPUT TAPE 6,70,1,(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 DU 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
C BEGIN COMPUTING ANSWERS - PHASES FOUR AND FIVE
6 WRITE OUTPUT TAPE 6,75,
75 FORMAT(8H1CONTR0L/3X2HP?,15X5HxDB,14X6HCOMP,13X9HDEVIA?)
KCD = 0
DO 705 L=1,NX
DO 704 K=1,3
SXCP(L,K) = 0.0
SXCPQ(L,K) = 0.0
SRESO(L,K) = 0.0
SUMX(L) = 0.0
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, 11, 6H CARD, 13)
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)
RESO(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
SRES(L,K) = SRES(L,K) + RESO(L,K)**2
715 WRITE OUTPUT TAPE 6, 71, ID, L, X(L), XCP(L,K), RESO(L,K)
71 FORMAT (2XA4, 3H X, 11, 3F20.5)
GO TO (862, 863, 864), K
864 GO TO 25
255 WRITE OUTPUT TAPE 6, 76,
76 FORMAT (1H1, 15H SUMS OF SQUARES / 20X5HX OBS, 14X, 6HX COMP13X9H DEVIAT
11ON//)
C0=KCD
DO 718 K=1,3
WRITE OUTPUT TAPE 6, 903, K
903 FORMAT (8H DEGREE, 11)
DO 718 L=1,NX
SSX(L) = SUMXQ(L) - (SUMX(L)**2/CD)
SSXCP(L,K) = SXCPQ(L,K) - (SXCP(L,K)**2/CD)
SRES(L,K) = SRES(L,K)
SSXCR(L,K) = (SSXCP(L,K)/SSX(L))*100.0
718 WRITE OUTPUT TAPE 6, 77, L, SSX(L), SSXCP(L,K), SRES(L,K)
WRITE OUTPUT TAPE 6, 9078,
9078 FORMAT (1//2X, 55H PERCENT OF SUM OF SQUARES ACCOUNTED FOR BY EACH
9078 1 SURFACE / 20X, 6H LINEAR, 13X, 9H QUADRATIC, 10X, 5H CUBIC)
DO 9718 L=1,NX
9718 WRITE OUTPUT TAPE 6, 77, L, SSXCR(L,K), K = 1, 3
77 FORMAT (6X3H X, 11, 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

GRID OF COMPUTED VALUES FROM COEFFICIENTS OF LQC PROGRAM

PREPARED BY WHITTEN - JANUARY 1962

DIMENSION TITI(12), TIT2(12), TIT3(12), TIT4(12), COE(20,4)

**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)

**READ MASTER CARD

READ INPUT TAPE 5,1, NPROJ,UB,UA,NU,UD,VC,NV,NVAR

1 FORMAT (A6,2F10.3,13,2F10.3,13,11)

**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)

**READ CUBIC COEFFICIENTS

DO 13 I = 1,20
13 READ INPUT TAPE 5,3, (COE (I,J), J = 1,NVAR)
3 FORMAT (10X, 4E15.8)

**COMPUTE UV-MATRIX

UN = NU
VN = NV
UU = (UB - UA)/(UN - 1.0)
VV = (UD - VC)/(VN - 1.0)

DO 14 I = 1, NU
14 UUM(I) = UA + (UU*FLOAT(F(I -1)))
DO 15 J = 1, NV
15 VVM(J) = VC + (VV*FLOAT(F(J-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,44HV-COMPUTED VALUES LISTED BY ROWS ACROSS MAP//5X,
107141IHQUADRATIC ANSWERS FIRST FOLLOWED BY CUBIC)
M = 1
DU 12 K = 1,11,10
DO 12 J = 1, NU
DU 12 I = 1, NU
12 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,'l1HVARABLE X-,11)
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),(COMIX(I,J,K),J=I,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(1,0,0,0,0,0,0,1,0,0,0,0,0)
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