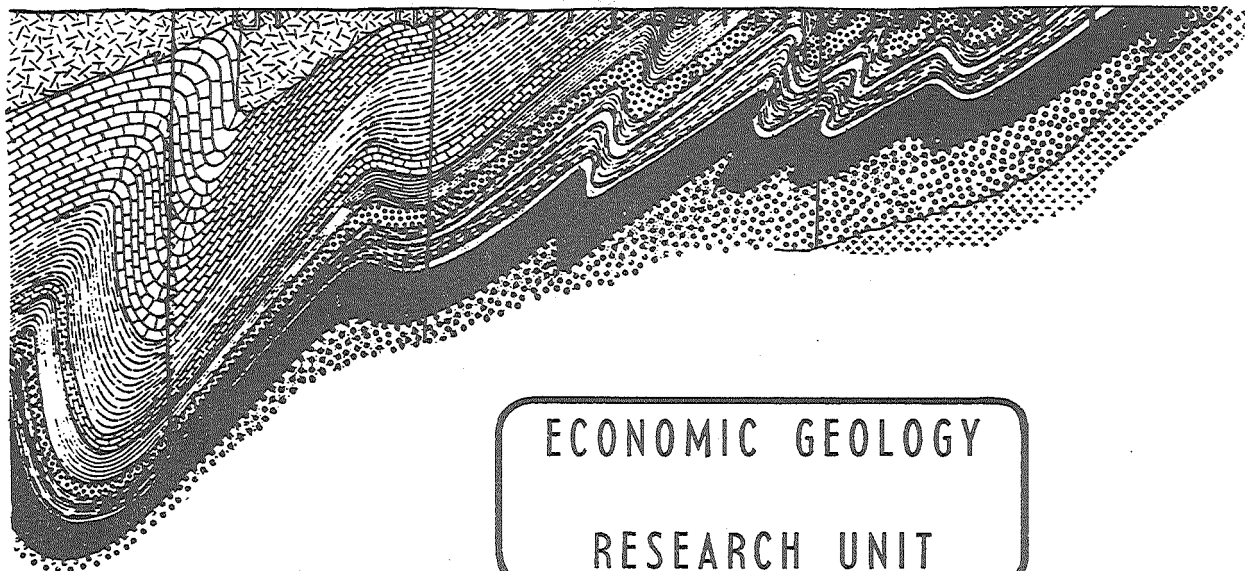




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THE APPLICABILITY OF MATHEMATICAL SURFACES TO CORRELATION  
AND PREDICTION IN WITWATERSRAND GOLD MINES

W. B. HEMP KINS

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AND PREDICTION IN WITWATERSRAND GOLD MINES

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THE APPLICABILITY OF MATHEMATICAL SURFACES TO CORRELATION  
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ABSTRACT

This paper is designed to aid the geologist in utilizing the recently introduced concept of a mathematical surface. Its primary purpose is to outline the general theory of such surfaces in terms of their physical and mathematical meaning. In order to realize the full potential and difficulties of such usage, with particular application in mining geology, the moving average technique is discussed in some detail. No preference for one technique over another is indicated, even though the technique of the moving average occupies the major portion of the paper. All techniques, if properly used, can be powerful tools in geological correlation and prediction.

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# THE APPLICABILITY OF MATHEMATICAL SURFACES TO CORRELATION AND PREDICTION IN WITWATERSRAND GOLD MINES

## INTRODUCTION

The problems of correlation and prediction have long been of importance to the mining industry, not only on the Witwatersrand of South Africa, but throughout the world. In recent years, there have been considerable advances in the use of mathematical surfaces for depiction and prediction of ore-value surfaces in mines (cf. Krige and Ueckermann, 1963; Krige, 1965; Hewlett, 1964; Whitten, 1964).

Since 1955, a vast literature on mathematical surfaces with applications in the earth sciences has appeared. The use of such devices has been primarily to interpolate and simplify the data in such a manner that trends, which were not particularly obvious, have been revealed, and to employ such trends in correlation and interpretation. The more active workers in this field have been Krumbein (1959-1963), Whitten (1959-1964), and Miller (1956-1962). The surfaces produced have been referred to as "trend surfaces", and the approach used has been a fitting of data by the method of least squares or orthogonal polynomials. Krige and Ueckermann (1963) introduced a second type of surface, the two-dimensional moving average. The purpose of such a surface was not primarily one of simplification, but of producing the best representation of ore-value distribution based on a minimum of data, i.e. the extrapolation and interpolation of a complex surface from profiles.

The aims of the geological profession and the mining industry, thus, are slightly different. One is attempting to produce a simplified and systematic representation of the data surface, the other as complicated and complete a surface as can be made to fit the existing data. For both groups, however, it is desirable to correlate these surfaces with those for other parameters. The mining industry wishes to evaluate the grade of ore in a mine from preliminary data obtained in development of the mine; the geologist, on the other hand, desires to find geological parameters which can be correlated with the prediction of ore grade.

Because of the use of similar techniques for two different aims, it is appropriate and desirable to outline the applicability of such mathematical devices, and to point out the problems involved in utilizing the techniques in prediction and correlation. The aim of this paper is to indicate what may be expected from a trend surface analysis, and to acquaint the geologist with the mathematics and physical meaning of such surfaces. Rigorous mathematical treatment will be omitted where possible, as the original papers on the subject should be consulted before using the techniques involved.

\* \* \* \* \*

## CONSIDERATIONS OF A SURFACE

### A. THE MATHEMATICAL CONSIDERATION OF A SURFACE

In order to better understand the meaning and use of a mathematical surface, consider the simple one-dimensional use of the equation

$$y = mx + b \quad (1)$$

the standard and well-known straight-line relationship which may also be written

$$f(x) = mx + b \quad (2)$$

since  $y$  is a function dependent upon the value of  $x$ . Equations (1) and (2) may be considered as profiles in the  $X$ - $Y$  plane of a set of data values plotted against coordinate axes  $X$  and  $Y$ , as illustrated in Figure 1. The general equation (2) represents a family of lines dependent upon three values - the slope of the line ( $m$ ), the value of the independent variable ( $x$ ), and the intercept of the line on the  $Y$ -axis ( $b$ ).

Consider now the extension of this concept into two-dimensional terminology (three-dimensional space) in which the  $Z$ -axis is introduced to represent the value of the dependent variable at any point determined by  $x, y$ . By convention, the  $Z$  axis is vertical, and the  $X$ - $Y$  plane of Figure 1 is now the horizontal plane. There are thus two other planes - the  $X$ - $Z$  and the  $Y$ - $Z$  plane - as in Figure 2. The equation of these planes can be written generally as

$$Ax + By + Cz + D = 0 \quad (3)$$

and it will readily be seen that the following is true :

$x = 0$  is the equation of the  $Y$ - $Z$  plane, and  $x = a$  the equation of any plane parallel to the  $Y$ - $Z$  plane  
 $y = 0$  is the equation of the  $X$ - $Z$  plane, and  $y = a$  the equation of any plane parallel to the  $X$ - $Z$  plane  
 $z = 0$  is the equation of the  $X$ - $Y$  plane, and  $z = a$  the equation of any plane parallel to the  $X$ - $Y$  plane

It is now desired to establish a plane which best represents some set of data having the value  $z$  as a function of  $x, y$  - the horizontal distances. The data may also be described as  $f(x, y)$ . Since the coefficients  $A, B, C$ , and  $D$  may be of any algebraic sign or value, the equation of any plane may be rewritten as

$$f(x, y) = Ax + By + D \quad (4)$$

as illustrated graphically in Figure 3. To evaluate  $z$  at any point  $x, y$ , only the coefficients  $A, B$ , and  $D$  have to be evaluated. Equation (4) is said to be linear, or of the first order.

Another data distribution is given in Figure 4. The linear representation of the data  $f(x) = mx + b$  is shown. Another fit, which is better, is also shown. Because this fit is no longer linear, the equation is given as

$$f(x) = A + Bx + Cx^2 \quad (5)$$

a quadratic, or second-order, equation, in which three coefficients -  $A, B, C$  - must be determined to evaluate  $f(x)$  or the value of  $y$  at a point  $x$ .

As before, this concept may readily be extended into two-dimensions, the equation of the function being

$$f(x, y) = (A + Bx + Cy) + (Dx^2 + Ey^2 + Fxy) \quad (6)$$

Since most geologic data are not readily represented in their entirety by even a quadratic equation, the general representation is

$$f(x,y) = a_0 + a_1x + a_2y + a_3x^2 + a_4y^2 + a_5xy + a_6x^3 + a_7x^2y + a_8xy^2 + a_9y^3 + \dots \quad (7)$$

The fore-going discussion has been limited to the two-dimensional representation of a surface where the three coordinate axes are used to depict the two independent variables x, y and the dependent variable z or f(x, y). It is possible to extend this notation into three-dimensional space where the three independent variables x, y, z represent position, and the value of f(x, y, z) is to be determined. The general equation of such a notation is of the form

$$\begin{aligned} f(x,y,z) = & a_0 + a_1x + a_2y + a_3z + a_4x^2 + a_5xy + a_6xz + a_7y^2 + a_8yz + a_9z^2 + \\ & a_{10}x^3 + a_{11}x^2y + a_{12}x^2z + a_{13}xy^2 + a_{14}xz^2 + a_{15}xyz + a_{16}y^3 + \\ & a_{17}y^2z + a_{18}yz^2 + a_{19}z^3 \dots \dots \dots \end{aligned} \quad (8)$$

as represented graphically in Figure 5, where the contours are interpreted in the usual sense, and are distributed about a surface as a function of x, y, z. The number of coefficients to be evaluated for various orders, p, is given in the following table. The remainder of discussion will be limited to two-dimensional representations, and, generally, to those surfaces of lower order.

Number of Independent Variables	Order of Fitted Surface (p)			
	linear	quadratic	cubic	quartic
2 (x and y)	3	6	10	15
3 (x, y, and z)	4	10	20	35

It will be seen in the above equations that the terms for the linear surface, quadratic surface, and so on, up to the order n, enter into the equations. Should there have been no linear component in equation (6), f(x, y) would have been reduced to the form

$$f(x,y) = A + Dx^2 + Ey^2 + Fxy \quad (9)$$

where the coefficients B and C would be zero, and the surface would be situated on a horizontal plane, as determined by the value of A. Figure 6 illustrates the only possible second-order surface in which there is no linear component. In Figure 6(a) and (b), the fundamental surfaces are illustrated. Figure 6(c) and (d) may be regarded as special cases of 6(a) and (b). Figure 6(a) is produced when coefficients D and E are of the same sign. If these coefficients are negative, the surface is domical in structure; if positive, the surface is a trough. Figure 6(b) is produced when coefficients D and E are of opposite signs. A saddle is formed at the mid-point. Figure 6(c) and (d) are produced when the coefficient E is zero - (c) may be regarded as (a) or (b) infinitely attenuated along the X-axis, while (d) may be regarded as having the centre of the system at infinity.

Figure 6 results from the projection of the z value onto the X-Y plane. Consider now the representation of the z-surface in three-dimensional space, as in the surfaces of Figure 7. For practical



purposes, these may be viewed as representing surfaces of a given percent of a variable,  $z$ , as a function of  $x$  and  $y$ , or as those of the position of a variable,  $w$ , in  $xyz$  space. The relationship between Figures 6 and 7 will be readily visualized by considering a plane of projection at any level through Figure 7.

For geological purposes, the coordinate axes are normally designated as  $U$ ,  $V$ , and  $W$ , for  $X$ ,  $Y$ , and  $Z$ , respectively. It is true that many, but by no means all, geological surfaces are generally of low order. It is also true that, in the more complex geological surfaces, only some of the components of a particular order contribute to the total surface of the data. It is the aim of mathematical surfaces to separate the geologic surface into its lower order components and its residual components (i.e. all components above this lower order) to illustrate the more simple trends revealed by this separation. This will be shown in detail elsewhere in this paper.

## B. THE CONSIDERATION OF A GEOLOGICAL SURFACE

A geological surface may be considered as composed of two components, and may be mathematically stated as

$$f(u, v) = t(u, v) + e \quad (10)$$

where  $t$  is the component designated as the "trend", and  $e$  is that portion of the original surface not represented by  $t$ . Consider the surface of Figure 8. In terms of the mathematical description of a surface, this is quadratic in nature. The left-hand and right-hand surfaces are the same, only their attitude in space is different. Their contour representation is shown in the  $X$ - $Y$  plane. Mathematically, these surfaces possess only two possible components - the linear and the quadratic terms. In the left-hand surface, only the quadratic terms are involved, plus the coefficient  $A$ . In the right-hand surface, both the linear and quadratic components occur. The right-hand surface may be regarded as the left-hand surface added to the linear surface shown in the inset. Since  $f(u, v)$  is completely describable by two components of low order, these together represent the trend, and the residual,  $e$ , is zero.

Now consider that the surfaces are not regular, as shown in Figure 8, but possess slight irregularities, as in Figure 9. The similarity between Figures 8 and 9 will be readily seen, and obviously Figure 9 may be generally represented by the right-hand member of Figure 8. Thus, the trend of Figure 9 may be represented by Figure 8, but it does not indicate the total surface, and the residual,  $e$ , will have some value which may be contoured. Even had the surface of Figure 9 been quite variable, it still could have been represented, in part, by the surface in Figure 8. The degree to which the entire surface is depicted may be represented by the amount of residual surface.

In Figure 10(a), a profile through a surface which can be described by a sine wave is plotted. By adding other sine waves of related frequency, as in Figure 10(b) and (c), a more complex profile can be created. This is further illustrated by another group of sine waves in Figures 11. These profiles may be considered as partial sections through a piece of corrugated metal. In order to describe these surfaces in terms of a "trend", a third component must be added to the description of a geologic surface

$$f(u, v) = t(u, v) + h(u, v) + e \quad (11)$$

where  $h$  is an harmonic term describable by sines and cosines, mathematically represented by a Fourier expansion of the form

$$h(x) = A/2 + A' \cos x + A'' \cos 2x + A''' \cos 3x + \dots + B' \sin x + B'' \sin 2x + B''' \sin 3x + \dots \quad (12)$$

The A's and B's are coefficients to be evaluated. In terms of the profiles of Figure 10, the A coefficients are zero.

### C. THE EFFECT OF THE REMOVAL OF A TREND

If a trend is removed by some mathematical device from a set of data  $f(u, v)$ , the effect of such a removal is important. The original set of data  $f(u, v)$  is describable in terms of

$$f(u, v) = g(u, v) + h(u, v) + e \quad (13)$$

where  $g(u, v)$  represents the  $t(u, v)$  of the previous equations. If  $T$  is now defined as some operation which produces a trend surface from the data, and the operation  $T$  is performed on  $f(u, v)$ , the result may be illustrated as

$$T(f(u, v)) = T(g(u, v)) + T(h(u, v)) + T(e) \quad (14)$$

Removal of this computed trend to illustrate the residual is given by the subtraction of equations (14) and (13) to yield

$$f(u, v) - T(f(u, v)) = [g(u, v) - T(g(u, v))] + h(u, v) - T(h(u, v)) + e - T(e) \quad (15)$$

If the mathematical operation on  $f(u, v)$  is successful, and only the trend is thus described, the terms  $T(h(u, v))$ ,  $T(e)$ , and the bracketed expression are zero. The residual surface described by equation (15) is, then, the true residual. If, however, the trend is "over-fitted", distortion of the residual surface is effected by the terms  $T(h(u, v))$  and  $T(e)$ .

### D. THE CONSIDERATION OF SCALE AND HOMOGENEITY OF DATA

In order to describe any data surface by a sample, the sampling interval must be considered in terms of the extent to which the sampling interval from one portion of the area is useable in another portion. Consider the profile of Figure 12 with a sampling interval of  $d$ . The curve is reasonably well described by the samples taken at interval  $d$  in Section (a), but all detail is lost in Section (b) because the sampling interval was too large. This effect in Section (b) is termed "aliasing". Obviously, if the profile is to be considered as a single unit, a much smaller  $d$  should have been chosen. This is a very important consideration in using some of the techniques which are to follow.

\* \* \* \* \*

## TYPES OF TREND SURFACE ANALYSES

The methods of analysing a set of data by the techniques of least squares and orthogonal polynomials are given by Krumbein (1959). This paper is probably the best summary and discussion of the techniques, from the point of view of the geologist. The methods are summarized, in part by the writer, in order to give the terminology and methodology employed in evaluating the coefficients of equation (7).

### A. THE TECHNIQUES OF PRODUCING MATHEMATICAL SURFACES

Because the term "trend" has been used to describe a portion of a geologic surface, and the term "trend surface" has been used to designate the trend produced by a particular method, the terminology used here will be such that the surface produced by a particular mathematical technique, whether truly representing the trend or not, will be referred to as the "response surface", following the example of Box (1954). The term "trend" will be reserved for the actual trend component of the general equation, while the term "trend surface" will be reserved for the fit produced by the method of least squares and orthogonal polynomials, as given in the literature (Oldham and Sutherland, 1955; Grant, 1957; Krumbein, 1959; Whitten, 1959-1964).

The mathematical methods to be described are ways of fitting data in two dimensions. Two techniques will be discussed in detail, but many others exist. The first of these techniques - the trend surface - is of two types, one of orthogonal polynomials and the other of a least-squares fit. The second technique is the two-dimensional moving average.

Each of the methods is concerned with evaluating the coefficients of equations (7) and (8). In the trend surface analysis, the coefficients are evaluated, and the value estimate of the data is determined. In the method of the moving average, only the value estimate of the data is computed, the intermediate step not being readily obtainable. In the following paragraphs, Y or X will be used as the values in the original and computed data matrix, and  $f(u, v)$  as the response surface. In some cases, the terms observed and computed will be used to refer to the original data matrix and the estimated matrix of order p, respectively.

#### (a) The Method of Least Squares

In the method of least squares, for any order, p, the response surface,  $f(u, v)$ , may be regarded as the computed values, and the expression

$$\sum (X_{n_{ij} \text{ observed}} - X_{n_{ij} \text{ computed}})^2 \quad (16)$$

must be minimized, where n denotes a particular observation at some U, V coordinate, i, j. This expression, by substitution of equation (7), is equivalent to

$$\sum (X_{n_{ij} \text{ observed}} - a_0 - a_1 u - a_2 v - \dots)^2 \quad (17)$$

for order p. The sums of squares, as given by equation (17), are functions only of the coefficients in a,  $F(a_0, a_1, \dots, a_n)$ . To illustrate the minimization in the linear case, Whitten (1963 b, p. 7) has

shown that, since there are three unknowns to be evaluated, there will be three equations, the solution of which is given as

$$\frac{\partial F}{\partial a_0} = \frac{\partial F}{\partial a_1} = \frac{\partial F}{\partial a_2} = 0 \quad (18)$$

When the operation of partial differentiation of the function  $F(a_0, a_1, a_2)$  is carried out, the results reduce to three normal equations

$$\begin{aligned} a_0 N + a_1 \sum U + a_2 \sum V &= \sum X_{n \text{ obs}} \\ a_0 \sum U + a_1 \sum U^2 + a_2 \sum UV &= \sum UX_{n \text{ obs}} \\ a_0 \sum V + a_1 \sum UV + a_2 \sum V^2 &= \sum VX_{n \text{ obs}} \end{aligned} \quad (19)$$

which are readily solved by matrix algebra as

$$\begin{bmatrix} N & \sum U & \sum V \\ \sum U & \sum U^2 & \sum UV \\ \sum V & \sum UV & \sum V^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum X_{\text{obs}} \\ \sum UX_{\text{obs}} \\ \sum VX_{\text{obs}} \end{bmatrix} \quad (20)$$

where  $N$  is the number of observations,  $U$  and  $V$  the distance coordinates,  $X$  the observed data, and  $a$  the coefficients to be evaluated. The matrix solution for the  $a$ 's is then given by multiplying both sides of the equation by the inverse of the  $[UV]$ , indicated by  $[UV]^{-1}$ , to yield

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} U & V \end{bmatrix}^{-1} \begin{bmatrix} \sum X_{\text{obs}} \\ \sum UX_{\text{obs}} \\ \sum VX_{\text{obs}} \end{bmatrix} \quad (21)$$

Thus, only the data values and their  $UV$  coordinates are necessary to evaluate the coefficients.

#### (b) The Method of Orthogonal Polynomials

When the data values are regularly spaced, i.e. when the data matrix is a regular grid, the method of orthogonal polynomials may be used to express the response surface. From the general equation of a surface, as given by equation (7),  $f(u, v)$  may be written as

$$f(u, v) = a_{00} + a_{10}u + a_{01}v + a_{11}uv + a_{20}u^2 + \dots + a_{qp}^q u^q v^p \quad (22)$$

where the  $a$  coefficients may be shown on a diagram, as in Figure 13, and their contribution to the overall surface assessed from this array (cf. Grant, 1957; Krumbein, 1959). It is now required to evaluate the coefficients  $a_{qp}$ . Oldham and Sutherland (1955) have shown that the response surface may be written in terms of the

orthogonal polynomials,  $z_{ij}^*$ , as

$$f(u, v) = b'_{00} z'_0(u) z'_0(v) + b'_{10} z'_1(u) z'_0(v) + b'_{11} z'_1(u) z'_1(v) + \dots b'_{qp} z'_q(u) z'_p(v) \quad (23)$$

where the  $a$  coefficients are now replaced by some coefficient in  $b$  and the orthogonal polynomials,  $z_{ij}$ , which are available in tabulated form (DeLury, 1950) up to  $n = 26$ . In order to estimate  $f(u, v)$  by this new form, the method of least squares is used, and the solution  $Y$ , the approximation of  $f(u, v)$ , given by

$$Y = B_{00} z'_0(u) z'_0(v) + B_{10} z'_1(u) z'_0(v) \dots + B_{qp} z'_q(u) z'_p(v) \quad (24)$$

The  $B$  coefficients may now be solved by

$$\sum_{r=0}^q \sum_{s=0}^p B'_{rs} S [z'^2_r(u)] S [z'^2_s(v)] = S [y z'_r(u) z'_s(v)] = g_{rs} \quad (25)$$

and the parameters of the equation (24) may be expressed by

$$B'_{rs} = \frac{g_{rs}}{S [z'^2_r(u)] S [z'^2_s(v)]} \quad (26)$$

where  $S$  denotes summation over all the data observations,  $y$ , and equation (26) may be expressed in matrix notation as

$$[g] = [z'_q]' [y] [z'_p] \quad (27)$$

where  $(q, p)$ ,  $(q, q)$ ,  $(p, q)$ , and  $(p, p)$  are the respective orders of the matrices, and where  $[z'_q]'$  represents the transform of  $[z'_q]$ .

### (c) The Method of the Two-Dimensional Moving Average

In this method it is desired to find a polynomial of order  $p$  in which different parts of the distribution are represented by different polynomials, such that, over  $m \times n$  terms, the polynomial determines their arithmetic mean. The desired coefficients can, as before, be found by the method of least squares, the solution of which is

\* The letter  $z$  is used here to represent the Greek letter "zeta", the usual representation of the orthogonal polynomials

given by Kendall (1946, p. 372) for the one-dimensional case. The equation describing the technique of establishing such a mean value in two dimensions is given as

$$A\left(r + \frac{n}{2}, s + \frac{m}{2}\right) = \frac{1}{nm} \sum_{i=r}^{n+r} \sum_{j=s}^{m+s} X_{ij}$$

$$r = 1, 2, 3, 4, \dots, N - \frac{n}{2}$$

$$s = 1, 2, 3, 4, \dots, M - \frac{m}{2}$$
(28)

where

- $X_{ij}$  = values to be averaged
- $n$  = spread of averaging function in U direction
- $m$  = spread of averaging function in V direction
- $A$  = computed estimate of  $X_{ij}$ , the data at  $(r + \frac{n}{2}, s + \frac{m}{2})$
- $N, M$  = limits of data matrix

The actual physical process of computing a two-dimensional moving average may be illustrated as in Figure 14. In practice, especially in the mining industry, the value  $X_{ij}$  represents the mean value of a square in which  $X_{ij}$  is positioned at its mid-point, as illustrated by Figure 14(b). For computational purposes by equation (28), the matrix of the squares' centre points is one unit less than that described by such an arrangement of squares. It will be obvious that, regardless of the extent of the moving average over  $M \times N$  terms, the generated estimate of the original matrix must be  $m \times n$  terms less than the size of the original data matrix.

#### (d) Other Techniques of Producing a Mathematical Surface

Many other methods of producing a surface exist. Perhaps, one of greatest potential use, but with few two-dimensional illustrations in geology, is that of the Fourier expansion. As illustrated by equation (12), the harmonic components of a surface may be fitted by a Fourier curve in terms of sines and cosines. A profile fitted by an equation of this form is given in Figure 15. Only the random components of such a curve cannot be fitted by higher order harmonic terms of such a series. Schwartz (1954) has used such a simple, two-dimensional Fourier series to produce combined surfaces in geophysical work (Figure 16). A Fourier expansion could be used to study the harmonic components of a response surface above the surface determined as the trend.

### B. THE EFFECTS OF THE VARIOUS TECHNIQUES

Because the use of a mathematical surface to represent the systematically describable portion of a geological surface is a somewhat artificial device, a few considerations will now be given as to the effect of the surfaces produced by the various techniques when the trend is computed and used as a representation of the

original data surface, or, as recommended by Potter and Pettijohn (1963, p. 271) and by Dawson and Whitten (1962), the trend is removed and the residual surface used for correlation with geological features. An aspect of this problem is being investigated for the Transvaal and Orange Free State Chamber of Mines by E.H.T. Whitten and D.G. Krige in their studies of the use of trend surfaces to represent ore-values. Therefore, most of the discussion will be limited to considerations of the two-dimensional moving average technique, with only an indication being given as to problems involved in other techniques.

(a) The Effect of Scale, Homogeneity, and Shape of the Data Surface in a Moving Average Computation

The moving average, being based on the arithmetic mean of the data, is sensitive to large deviations from the mean. In addition, the shape of the data surface is of extreme importance in such a computation. Figure 17 illustrates a symmetrical surface in which the original data are contoured in 17(a), and the moving average response-surface, over a spread of one-half unit, contoured in 17(b). The residual surface will obviously be symmetrical. Another surface is shown in the same manner in Figure 18(a), (b), and (c). It is readily seen that no distortion of the surface occurs in the symmetrical surface of Figure 17, and little distortion in the asymmetrical surface of Figure 18, when the spread of the moving average is over one-half unit. In both cases, the region of high topographic closure on the original map is illustrated by a broken line or a plus sign. Consider now the effect of increasing the spread of the moving average to two units in order to illustrate the regional nature of the surface. In Figure 19(a) and (b), the data surface of Figure 18(a) is subjected to a moving average, and the response surface plotted. The residual surface appears in Figure 19(b). It is readily seen that considerable distortion of the surface has been introduced, such that the high areas have been off-set by more than one-half unit.

This effect is similar to that of aliasing, because the data spread is such that the higher-order components of the surface are being mis-represented. Figure 20 shows such an effect on a profile, and the residual is plotted to show offset.

An actual example of such a computation can be shown from geophysical data. Figure 21 shows the map of aeromagnetic data for which a moving average over 4 miles was computed. The residual is plotted in Figure 22(a). Because the shape of the surface is not homogenous over the entire surface, differential distortion occurs. The sampling interval for the original data was one mile. In order to correct this distortion, a portion of the area was re-computed, using an average spread of one mile, and the residual surface plotted in Figure 22(b). Distortion again occurs, indicating that, from the available data, the moving average cannot illustrate the trend surface of a local nature.

(b) The Moving Average of a Series of Averaged Terms

Consider the use of a moving average of a series of terms which were produced by averaging all values within a certain area, i.e. the squares represented by X of Figure 14(b). Assume that the component values within a term of the series were such that one value possessed a relationship with its nearest neighbour, but that this relationship decayed rapidly as the distance increased. In other words, the correlation function between variables varied inversely as the distance. Further assume that the terms in any  $X_{ij}$  were un-correlated with any of its neighbouring members of the series.

The value of  $X_{ij}$  may be represented as some average, say

$$X_{ij} = (y_1 + y_2 + y_3 + \dots + y_n)/n$$

and the value of any other neighbouring average value,  $X'_{ij}$ , by

$$X'_{ij} = (z_1 + z_2 + \dots + z_n)/n$$

The values  $X_{ij}$  and  $X'_{ij}$  possess no components which are highly correlated. Designate the moving average values of such a series by  $A_1, A_2, \dots, A_p$ . The first term of such a generated surface or series over a spread of two values is formed by

$$A_1 = (X_{ij} + X'_{ij})$$

and the second term by

$$A_2 = (X'_{ij} + X''_{ij}) \text{ and so on.}$$

Successive terms which may have been uncorrelated are now correlated by the preceding and following terms which have common values involved.

#### (c) The Moving Average of a Moving Average

A further consideration of the moving average is given when the terms involved in the method have been themselves produced by a moving average technique. Following the example of Kendall (1946, p. 375) the extension of his argument into two dimensions can be given as

$$V_{11} = 1/4 (u_{11} + u_{12} + u_{21} + u_{22})$$

$$V_{21} = 1/4 (u_{21} + u_{22} + u_{31} + u_{32})$$

$$V_{22} = 1/4 (u_{32} + u_{33} + u_{23} + u_{22})$$

$$V_{22} = 1/4 (u_{12} + u_{22} + u_{13} + u_{23})$$

for a moving average of extent  $2 \times 2$ , over some set of values  $u$ . Reference to Figure 14 may help to visualize the values being considered in these equations. The first term of a moving average,  $W$ , over the values of the moving average,  $V$ , is

$$W_{11} = 1/4 (V_{11} + V_{21} + V_{12} + V_{22})$$

which may be reduced to the form

$$W_{11} = 1/256 (u_{11} + u_{12} + u_{21} + u_{22} + u_{21} + u_{22} + u_{31} + u_{32} + u_{12} + u_{22} + u_{12} + u_{23} + u_{32} + u_{33} + u_{23} + u_{22})$$

and simplified to

$$W_{11} = 1/256 (u_{11} + u_{13} + 2u_{21} + 2u_{12} + 4u_{22} + 2u_{23} + 2u_{32} + u_{31} + u_{33}).$$



This may be written symbolically as

$$W_{11} = 1/256 (1, 1, 2, 2, 4, 2, 2, 1, 1)$$

where the weights of each term are given within the parenthesis. It can thus be shown that different areas of the polynomial surface described by a moving average are unequally weighted. Obviously, the central portion of the surface will possess the same weights, as this process is continued across the matrix, but the periphery of such a surface will not be as equally weighted as the central portion. In small matrices, such a consideration could be of great importance, especially if such a technique were used in prediction of ore-values.

#### (d) The Use of a Weighting Function in Prediction

It is desirable to utilize some function in the technique of the moving average to raise the overall level of the predicted data surface. The equation of such a technique may be shown as a modification of equation (28)

$$A \left( r + \frac{n}{2}, S + \frac{m}{2} \right) = \frac{1}{nm} \sum \sum (X_{ij}) (F_{ij}) \quad (29)$$

where  $F_{ij}$  is the weighting function. The weighting values are empirically determined and dictated by the needs of the worker. In order to determine the shape of such a function, the autocovariance function may be used, as shown by Krige and Ueckermann (1963). The use of a two-dimensional autocovariance function should yield a correct shape for such a weighting configuration. The computation of a two-dimensional autocovariance function has been shown by Horton, Hempkins, and Hoffman (1964).

#### (e) The Effect of the Moving Average on Harmonic Components

If it is desirable to remove the trend to concentrate study on the oscillatory components of a matrix, Kendall (1946, p. 380) has shown, in one-dimensional cases, that the slow oscillations can be treated as a trend by the moving average, and thus eliminated. In general, the moving average emphasizes the shorter oscillations at the expense of the longer oscillations. A distortion of the harmonic structure can result if the extent of the terms averaged by the technique is slightly longer than the period of the oscillations involved. If the moving average is a weighted one, even greater distortion can occur. The effect of the moving average on harmonic components can be lessened by taking a simple (unweighted) average over components, the extent of which is equal to the wave-length of the oscillations which are to be preserved.

#### (f) The Effect of the Moving Average on Random Components

A moving average on random components can be shown to generate an oscillatory series if the weights involved are such that they give positive correlation between successive members of the generated matrix (cf. Kendall, p. 381). This is the Slutsky-Yule effect, and is always present in a moving average. While the oscillations thus induced are not cyclical, they can produce spurious effects on the truly oscillatory components of the harmonic term. Again, a weighted moving average will enhance this spurious effect, and an unweighted moving average is preferable to a weighted one.

Because each term of the moving average is correlated with the preceding and following terms, if a correlation exists in the original data surface, then the effect can be one of emphasizing the trend. In Figure 23 a surface has been generated by making each row of the matrix conform to a rectangular random series that may take integral values from 0 to 19. The columns do not necessarily possess the characteristic of randomness. The contour representation of this surface shows a pronounced lineation in the northeast-southwest direction and another, less pronounced, east-west structure. In Figure 24, a  $2 \times 2$  unit moving average surface has been contoured. The extent of the moving average is such that several features have completely disappeared, and, because there is a distinct correlation between values in a northeast-southwest direction, the prominent lineation has been accentuated at the expense of the less correlated east-west direction.

### C. THE LIMITATIONS OF THE VARIOUS TECHNIQUES

#### (a) Trend Surface Computation of Higher Orders with Paucity of Data or Poor Data Distribution

It has been shown by Whitten and Krige (unpublished) that, if the data used for trend surface computation are poorly distributed, erroneous response surfaces may be produced for higher orders. Consider the examples in Figures 25 and 26. The data are distributed only along the heavy lines at intervals of five feet. The 7th-order response surface is shown as produced by the method of least squares. The smaller diagrams show the respective areas from regional response surfaces produced by the method of least squares and the moving average. There is a great similarity between these regional diagrams, but little resemblance to the 7th-order surface.

While the cause of this behaviour is not readily obvious, the key to the problem probably lies in the fact that the data actually occupy a very small portion of the area involved. The assumption has been made that a polynomial fitted to this data actually describes the surface over the entire area. It is more likely that it does not. The variance of the data is such that there are extreme deviations from the mean, and in such cases the use of such a polynomial is dangerous in extrapolation and interpolation. It is, further, a property of a third-order surface to extend to infinity beyond the limits of the fitted data. This can be visualized by imagining a fit of the cubic parabola,  $y = ax^3$  to a set of observed values. The two-dimensional analog of this equation is also to be considered. If the extrapolation is allowed to extend beyond the region of data control, it will tend to infinity as a characteristic of the function. That higher-order surfaces might still give a good fit is the result of the interaction of the various orders and their cross-terms. In general, it should be difficult to fit a polynomial of this nature of order higher than two to any set of data distributed as in Figures 25 and 26, without resorting to some form of regional weighting.

Whitten is presently investigating various techniques of stabilizing this polynomial so that extreme distortion of the data will not occur. Preliminary computations show that a third-order fit is not appreciably distorted, but higher-order surfaces are greatly so. If the data are logarithmically transformed, the third-order fit is significantly improved.

In regard to a paucity of data, only lower-order response surfaces may be calculated -- the fewer the points, the lower the order, and the lower the confidence with which a surface of order  $p$  may be fitted. In theory, only three points are required to fit a linear trend, these three points completely describing the plane. This plane is, however, not necessarily the linear component of the complete data set of  $n$  points. It is generally unwise to fit a linear trend with less than nine points, a quadratic fit with less than 21 points, and a cubic with less than 35 points. As a rule of thumb, the amount of data required to describe a surface of order,  $p$ , is 10 times  $p$ .

Mandelbaum (1963) has outlined a method for weighting the values in such a manner that distortion can be overcome with some success. In the case of irregularly distributed points, this method may also be used, i.e. when a paucity of points occurs in some areas and a dense distribution in others.

(b) The Assumptions Made in Fitting a Response Surface to Data

In all the techniques described, several assumptions have been made. Without these assumptions, confidence tests cannot be computed, and, in some cases, the surface may have no validity. These assumptions are outlined below:

- (i) the data are distributed normally
- (ii) a polynomial can be used to describe components of the data
- (iii) the residual surface sums to zero
- (iv) for purposes of extrapolation and interpolation, the polynomial which describes the data also describes the remainder of the surface

In cases where the data are not normal and there are large deviations from the mean, steps must be taken to normalize the values. Krumbein (1959) and Hewlett (1964) have used a log-transform method to normalize values which were highly skewed. Square-root transformations or transformations based on an exponential function may also be used. Krige (1960) and Krige and Ueckermann (1963) have used a transform based on the log of the data value plus a constant. The method employed depends largely upon the data distribution, and should be determined before computation of a response surface.

The validity of the other assumptions remains largely at the discretion of the worker. It is seldom that these can be tested before computation, and only the resulting response surface may be used to form an opinion. Regional response, or residual, surfaces compared with actual surfaces can frequently be used to relate the produced trends to underlying factors.

In regard to confidence levels of response surfaces, Krumbein (1963) has given a method of computing such for low-order trend surfaces. Kendall (1946) and Wold (1949) have discussed the problem for moving averages in one-dimension, but, as yet, no solution to the problem has been found for two-dimensional moving averages. A general method in all cases lies with the amount of residual surface in terms of the ratio of the sums of squares of the computed surface to the sums of squares of the original data – the sums of squares reduction. If the percent reduction produced by a surface of order  $p$  is high, then the fit is obviously good at that level.

(c) The Meaning of a Trend and its Relation to an Analysis of Variance

The trend is a somewhat qualitative term. It is most often used to express the systematic variation in a set of data. Just what the trend is, in the sense of equations (10) and (11), cannot be determined. If it is desired to remove all but the random effects, then the trend will also include all harmonic effects. If the harmonic effects are desired, then the trend may be the original surface minus the random residual and the linear component only. Thus, the trend is dictated only by the worker's needs. Some writers have referred to the fitted trend as the "partial trend surface", in order to indicate that the data have not been completely fitted, and that not all major coefficients of the surface have been evaluated.

In geological use, on data acquired from mines, it is often the case that ore data describe a rather complicated surface, while geological data form a surface of lower-order. The trend in the ore data is that surface which reduces the original ore data to one of similar order to that of the geological surface.

In terms of an analysis of variance, the trend is a regression surface, and the aim of the technique is to partition the total variance of the data into two or more parts : (1) that variance attributable to the regression surface, and (2) that variance not attributable to the regression surface. As such, the method lends itself to statistical tests, as dictated by an analysis of variance. The particular application to geology is well given by Chayes and Suzuki (1963).

#### (d) The Use of Polynomial Surfaces in Correlation

From the fore-going sections, it can be seen that some consideration should be given to the data before undertaking the fitting of a response surface to illustrate trends which are not particularly obvious, or to reduce a set of data to some specified order. The use of such surfaces, especially in the gold mines of South Africa, is becoming widespread. It is a common practice to express the ore data in terms of inch-pennyweights or inch-pounds, and to correlate these surfaces with those of other geological parameters. The use of such expressions as inch-pennyweights and inch-pounds is based on the assumption that the ore-body is rather thin over its entire extent, and that the value is virtually determined by the concentration of the mineral. Values are thus computed by multiplying the thickness of the ore-body at any point by the concentration of the mineral at that point. It is then common to compare trend surfaces with those of ore-body isopachs, pebble-size distributions, etc. Since either factor - ore concentration or ore-body thickness - can cause a change in such values, it is possible to produce spurious correlations by comparisons with parameters which are correlated with either variable. If neither of the factors possesses a high correlation with the variable being compared, then their product may truly show a correlation with such a parameter. If one factor does remain relatively constant, then the correlation produced is virtually a function of the variable parameter. It is misleading to compare an inch-pennyweight map with ore-body isopachs or with pebble-size which is, in turn, usually correlated with ore-body thickness, unless surfaces of mineral concentration and of isopachs of the ore-body are available.

A loss of correlation can be effected by the use of a moving average to describe a surface when compared to one which has not been produced by a similar technique. Consider the two curves of Figure 27. These are plots of ore values in pennyweights, ore values in inch-pennyweights, and reef thickness. The correlations present will be obvious. Had a moving average been used to produce the profile of any of these, some of the effects present in Figure 20 may have been exhibited, and the correlation would have been affected. While it has not been shown, it is thought that this problem would not be very serious if a least-squares or Fourier fit had been used to represent the data.

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### CONCLUSIONS

Based only on preliminary data, it seems that all the techniques of representing a response surface have something to offer. The most dangerous technique for use in correlating geological parameters seems to be the moving average. At the present time, however, it remains one of the best techniques for evaluating an area in which only development profiles are available, especially if some form of weighting function is used in conjunction. Krige (1965) has used the method successfully in depicting the regional nature of the ore distribution in a mine (Figure 28 a). The least-squares technique has been fitted by Whitten to the same data (1964, unpublished data), as shown in Figure 28(b). It is obvious that the two maps reflect the same

features. As a measure of how well they agree, a plot of the deviations in terms of the absolute value of the deviations in contour intervals is given in Figure 28(c). The desirable feature of the moving average in this case is the relative complexity of the surface in relation to that of the eighth-order trend surface. By computing the sums of squares reduction of these surfaces, Krige (1965) found the moving average of Figure 28(a) to be 59% efficient with regard to the original surface, but the trend surface of Figure 28(b) to be only 45% efficient. There is probably little distortion of the data, since the spread of the averaging function was very broad in relation to the smaller oscillations.

The very nature of a moving average forces it to approach the mean of the data matrix as the spread of the average grows larger. Thus, on a regional basis, the average value of any area may be evaluated by the relative area covered by a particular contour interval. The equation of the surface produced in this manner is, however, not readily available. In the case of a trend surface, where the coefficients of the surface are produced as a consequence of fitting the response surface, the equation of the surface is readily available. In such a case, by integration of the equation, the total expected production of a mine may be computed.

The use of any form of surface to describe a trend in the data is necessarily an artificial device. That a surface thus fitted does not give any greater insight into the underlying physical principles of the geological situation does not indicate that the fit is wrong, for a proper fit is completely dictated by the data. It does, perhaps, indicate that the type of technique used is wrong. Consider an example given by Saha (1964) in which he fitted a second-order polynomial surface to data exhibiting a periodicity. He concluded that this fitted surface did not show the periodic nature of the data surface. It has been shown in Figure 6 of this paper, that it is not the nature of a second-order surface to exhibit such periodicity. In the example of Saha, had he used the technique given by Miller (1956), where he divided the surface into areas having only one curve, the second-order surface could have shown the periodic nature of the data. Had a higher-order surface or a Fourier fit been utilized, such periodicity would have been shown. On the other hand, a Fourier technique should not be used if there is not a reasonable supposition that some underlying physical process can produce a periodicity in the data. Although the curve may be fitted by an equation in sines and cosines, and further analysis computed from the resulting terms, it will help little in the eventual analysis, and may lead to completely erroneous conclusions, if such a periodic process were not operative. The assumption that such a polynomial can describe the data is, then, of great importance.

The more relevant points of this paper can be stated as follows :

- (i) the data should be normally or near-normally distributed so that un-equal weight is not given to abnormally large or small values
- (ii) the trend surface should be computed only to describe some systematic variation in the data, and should not be viewed in the same manner as a standard contour map of the values
- (iii) the trend surface is interpretable by an analysis of variance
- (iv) trend surfaces may be subjected to tests of goodness of fit, but no confidence level computation has yet been described for a moving average surface
- (v) a trend surface can effect a distortion if the order of the surface is not considered, or if there is a poor distribution of data values
- (vi) the moving average surface can effect distortion of the data if the scale of the phenomena is not considered
- (vii) the moving average surface and the trend surface, if used properly, produce similar results, the advantage of the trend analysis being the creation of an equation which may be useable in further work, such as integration, to produce the mean value of the surface

- (viii) the method of orthogonal polynomials possesses the advantage that higher-order surfaces can be computed without re-computation of the lower-order coefficients, but orthogonal data are required
- (ix) the moving average surface possesses the advantage that data may be added to the periphery of the matrix and the computed surface extended without re-computation of the previous matrix, and that non-orthogonal data may be used, but surfaces of other orders require re-computation of the matrix
- (x) the least squares technique may be used with non-orthogonal data, but higher-order computation requires re-computation of the data
- (xi) the moving average is the easiest technique to use and understand
- (xii) extrapolation and interpolation of data may be effected by any of the techniques, but generally only for lower-order components and in a regional nature.

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#### LIST OF PUBLICATIONS CONSULTED

The following is a list of publications in geology dealing with the use of mathematical surfaces for various purposes. The list, while by no means complete, includes most of the major works in geology, as well as those in other fields. The symbol \* is used to indicate that the reference deals with the two-dimensional moving average technique, as well as with trend surface methods.

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# KEY TO FIGURES

- Figure 1 : Graph of the function  $f(x) = mx + b$  in the X-Y plane.
- Figure 2 : The relationship of the three coordinate axes, X, Y, and Z, and their respective planes.
- Figure 3 : The relationship of any plane to the three coordinate axes.
- Figure 4 : Diagram of a linear (1) and quadratic (2) fit of data, (from Dawson and Whitten, 1962, p. 5).
- Figure 5 : A mathematical surface in three dimensions. This surface may also be regarded as a two-dimensional fit to data, as represented by dots in the X-Y plane. The actual position, or value, of Z is indicated with respect to the computed or estimated value of Z. (after Miller, 1956, p. 429).
- Figure 6 : Fundamental second-degree surfaces, (a) and (b), and limiting second-degree surfaces, (c) and (d). (from Box, 1954, p. 36).
- Figure 7 : Some possible second-degree surfaces in three dimensions. (from Box, 1954, p. 39).
- Figure 8 : A quadratic surface and its contour representation. The inset shows the linear component plane of (b).
- Figure 9 : A higher-order surface with a prominent quadratic component.
- Figure 10 : Illustration of the addition of odd harmonics to produce the function,  $f(x) = M_1 \sin X + M_3 \sin 3X + M_5 \sin 5X$ . (1) :  $f(x) = M_1 \sin X$ ; (2):  $f(x) = M_3 \sin 3X$ ; (4):  $f(x) = M_5 \sin 5X$   
(b) : (3) = (1) + (2); (c) : (5) = (3) + (4) = (1) + (2) + (4).
- Figure 11 : Illustration of the addition of odd and even harmonics.  
(1) :  $f(x) = A_3 \sin 3X$ ; (2):  $f(x) = A_6 \sin 6x$  = octave of (1); (3) = (1) + (2).
- Figure 12 : The effect of 'aliasing' of data, as illustrated by the dashed profile. The loss of detail in Section (b) is due to an excessively large sampling interval, d.
- Figure 13 : Diagram showing arrangement of polynomial coefficients, or  $Z^2$  terms, in an array. (from Krumbein, 1949, p. 826). (see also Oldham and Sutherland, 1955, and Grant, 1957).
- Figure 14 : (a) Moving average method for orthogonal data.  $A_{11} = 1/4 (X_{11} + X_{12} + X_{21} + X_{22})$ , etc.  
(b) Moving average method for averaged squares.  $X = 1/n \sum_i \sum_j z_{ij}$ ;  $A_{11} = 1/4 \sum_i \sum_j X_{ij}$
- Figure 15 : A curve fitted by the Fourier function,  $f(t) = 24.9 - 8.4 \cos t - 0.7 \cos 3t + 0.4 \cos 4t + 5.0 \sin t + 1.1 \sin 2t + 1.8 \sin 2t - 0.9 \sin 3t$ .
- Figure 16 : Contours of a two-component surface describable as the function  $G = \sin 2\pi x + \sin (2\pi/3)y$ . (after Schwartz, 1954, p. 51).

- Figure 17 : The effect of a moving average computation on a symmetrical surface. (a) contour map of original data (b) the response surface as computed by a two-dimensional moving average, the spread of which is  $\frac{1}{2}$  unit. The original map is six units square.
- Figure 18 : The effect of a moving average computation on an asymmetrical surface. (a) and (b) the same as for Figure 17. (c) is the residual surface. The dashed line indicates the position of the original high marked in (a).
- Figure 19 : The effect of using a moving average spread which is too wide for the harmonic characteristics of the data. Data the same as for Figure 18. (a) is the moving average surface for a spread of  $2 \times 2$  units. (b) is the residual surface.
- Figure 20 : Illustration of the effects of the relationship of harmonic effects and moving average spread. Entire profile is 55 units long. The vertical lines indicate the offset of peaks in the original profile from the highs in the residual graph. (1) - the original data; (2) - moving average over three units; (3) - moving average over 10 units; (4) - residual surface for 3-unit spread; (5) - residual surface for 10-unit spread.
- Figure 21 : Contour representation of geophysical data from South Africa. Contour values are not important, the higher zones being marked by dashed lines. The indicated area is approximately  $10 \times 15$  miles.
- Figure 22 : Two moving average computations for data of Figure 21. The dashed line indicates the high zones of the residual maps. (a) and (b). For further explanation see the text.
- Figure 23 : A contour map of a plot of 64 rectangular-distributed random numbers from 0 to 19. The area measures  $8 \times 8$  units.
- Figure 24 : Moving average computation of the data in Figure 23. The spread of the moving average was  $2 \times 2$  units.
- Figure 25 : Comparisons of response surfaces computed from different data distributions. (a) is the 7th - order trend surface from data appearing only along the straight lines. (b) is the 8th - order trend surface from data distributed over an entire area of which this map is a small portion. (c) the moving average surface - description same as in (b).
- Figure 26 : Same explanation as for Figure 25.
- Figure 27 : Comparative graphs of gold values in pennyweights and inch-pennyweights and of reef thicknesses in inches as a function of distance. Data from Hartebeestfontein Mine, Klerksdorp Goldfield. (1) graph of pennyweights; (2) graph of inch-pennyweights; (3) graph of reef thickness in inches.
- Figure 28 : (a) moving average surface of gold in inch-pennyweights. (b) 8th - order trend surface of gold in inch-pennyweights. (c) correlation map between (a) and (b) - no marking indicates perfect correlation, cross-hatching indicates  $\pm 1$  contour interval; black areas indicate  $\pm 2$  contour intervals.

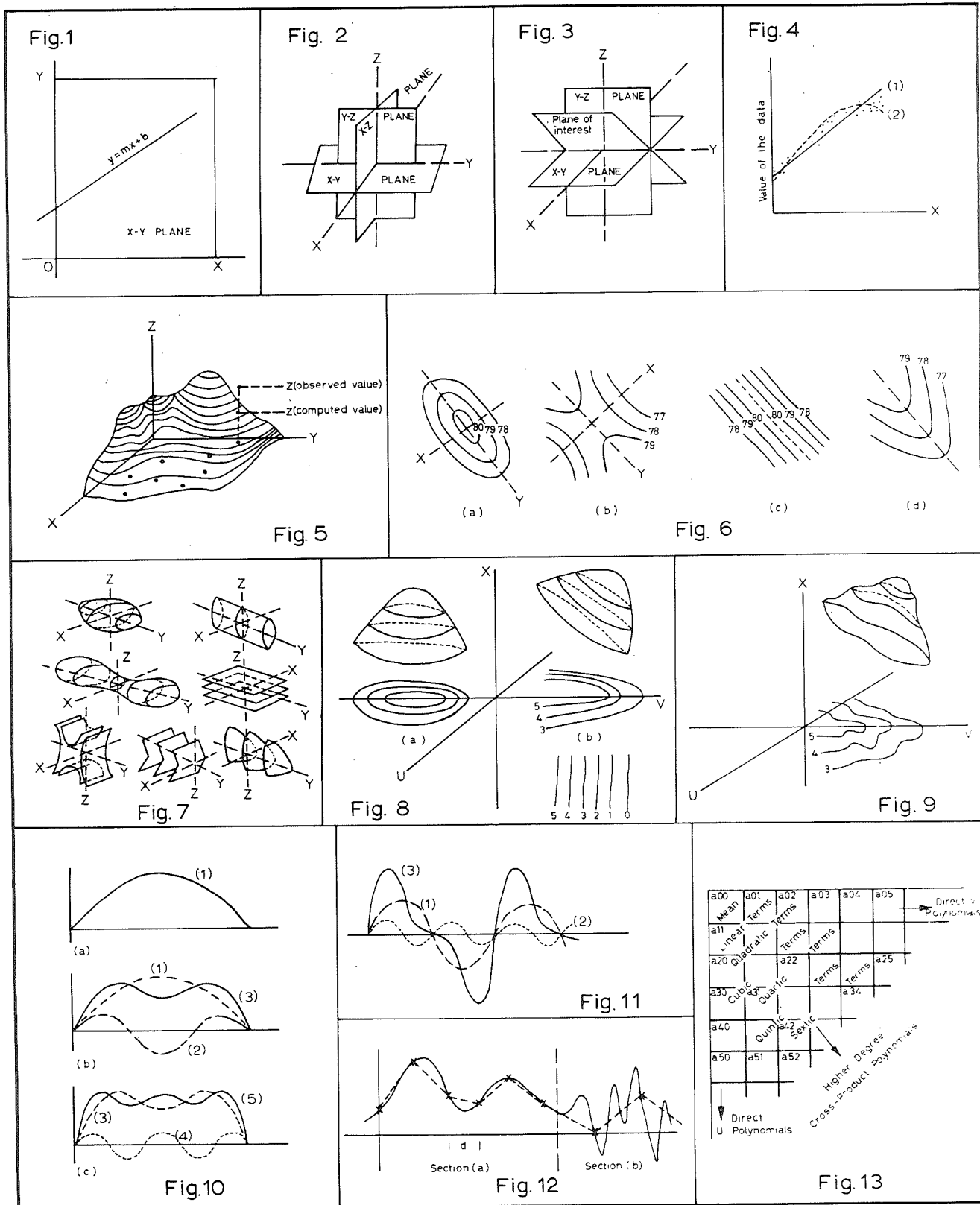


Fig. 14

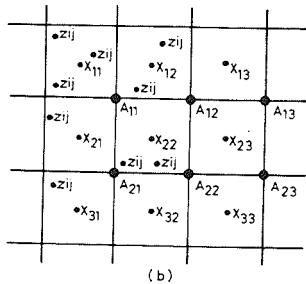
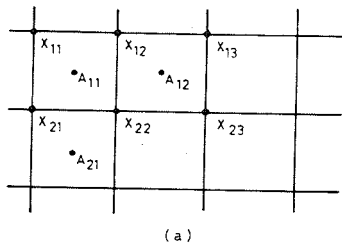


Fig. 15

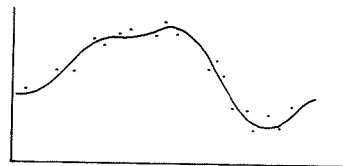


Fig. 16

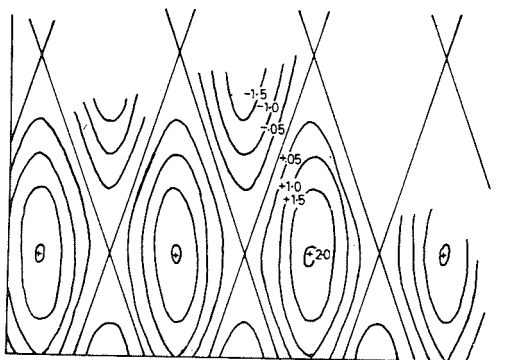


Fig. 17

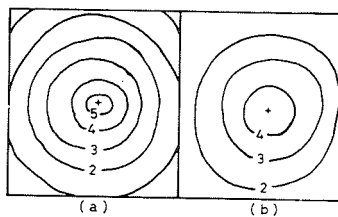


Fig. 19

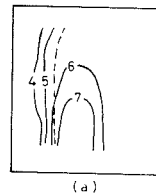


Fig. 18

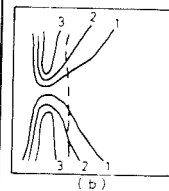
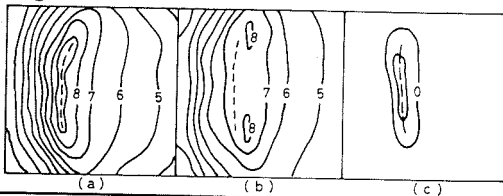


Fig. 20

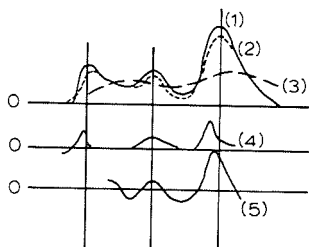


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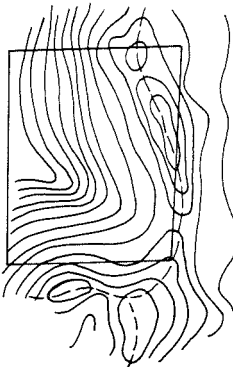


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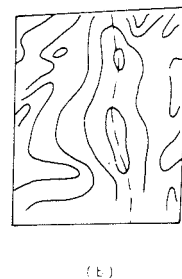
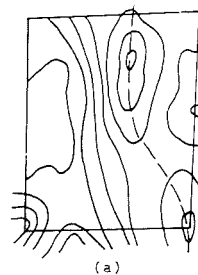


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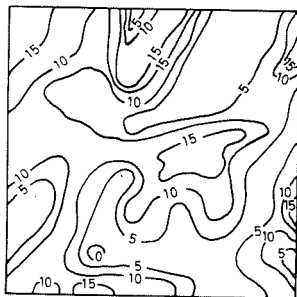


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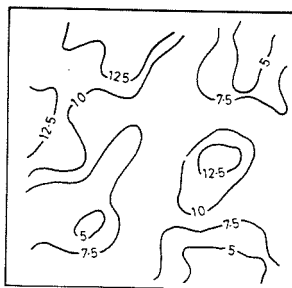


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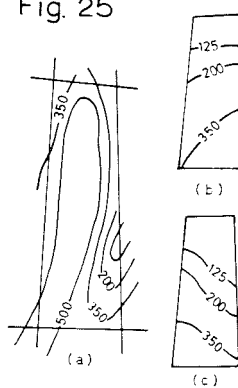
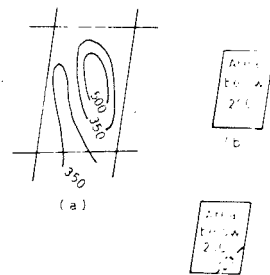


Fig. 26



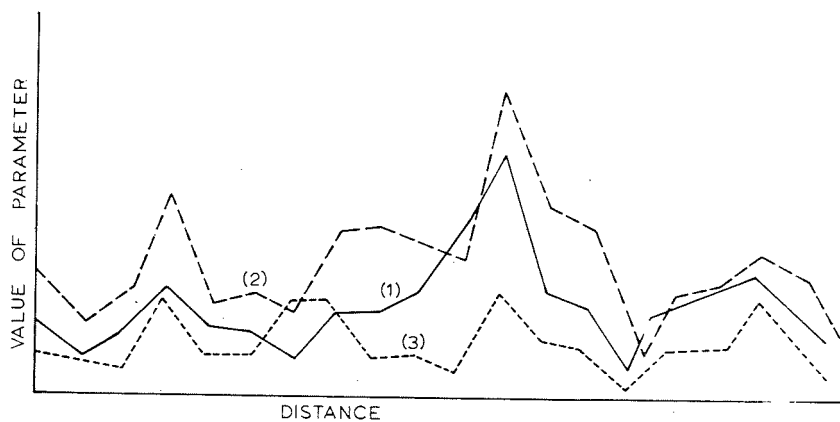
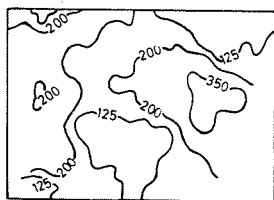
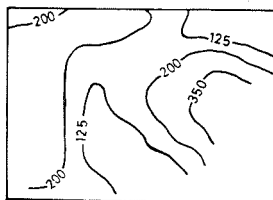


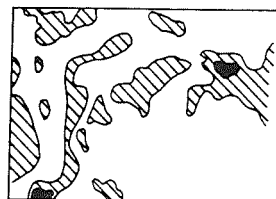
Fig. 27



(a)



(b)



(c)

Fig. 28