

Orthogonal Polynomial Trend Surfaces for Irregularly Spaced Data¹

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The advantages of using orthogonal rather than nonorthogonal polynomials for trend-surface analysis are discussed briefly. A method for calculating orthogonal polynomial trend surfaces of any degree on the basis of irregularly spaced data is described. The method is illustrated with subsurface data for the elevation on top of the Devonian Dundee Limestone, Michigan.

INTRODUCTION

In earth sciences mapping problems, there is commonly one dependent variable value X_j for each sample point, but to define the geographic location two coordinate values (u_j, v_j) are required. It will be assumed that the coordinates are measured along orthogonal axes, although, of course, other coordinate systems could be used. It is necessary to express $X_j = f(u_j, v_j)$. In trend-surface analysis, it has been common to use simple power-series polynomials of the form

$$X_j = \gamma_0 + \gamma_1 u_j + \gamma_2 v_j + \gamma_3 u_j^2 + \gamma_4 u_j v_j + \gamma_5 v_j^2 + \dots + \varepsilon_j \quad (1)$$

The data points (u_j, v_j) either may be equally spaced on a rectangular grid, or irregularly spaced. A regression analysis with uncorrelated γ_i is called orthogonal (Graybill, 1961, p. 172; Kendall and Stuart, 1967, p. 356). One important application of orthogonal polynomials arises if the regressor variables u and v take values at equal intervals, for example, where the data points are equally spaced over a map area. In such situations, the arithmetic involved in solving for the coefficients γ_i is easier and can be completed readily with a desk calculator. As a result, earlier work in the earth sciences used orthogonal polynomials and much of the terminology of trend-surface analysis developed at that time; the definitive paper is that of Grant (1957). Later, with the growing availability of digital computers, nonorthogonal polynomials were used extensively for analyzing many types of irregularly spaced data; the definitive paper is by Krumbein (1959). More recently, several investigators in the petroleum industry and elsewhere have recognized the importance of using orthogonal polynomials for

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trend-surface analysis studies of irregularly spaced data (for example, IBM, 1969a and b, abstracts of which were given by Lea, 1969, p. 83–84). The method used by Grant (1957) requires that values be available at each node of an orthogonal grid. In most earth science applications, the geographical locations of samples are irregularly spaced and it is difficult, if not impossible or prohibitively expensive, to obtain samples at grid nodes. For such irregularly spaced data, polynomial trend surfaces can be developed by one of three methods.

“Orthogonalize” the data. Use is made of one of several available techniques for estimating the value of the dependent variable at the nodes of an arbitrary grid. For example, if the data are manually or machine contoured (Walters, 1969) values can be read at the desired grid points for use with the standard orthogonal system described by Grant (1957). Unfortunately, all available methods of orthogonalizing a data set are subject to severe criticism (Grant, 1957, p. 335) and are not recommended in a majority of situations.

Use nonorthogonal polynomials. This is the most widely used technique but it has several disadvantages that are not associated with orthogonal polynomials. At least three are important in the present context. First, solution of the requisite simultaneous equations to obtain the coefficients γ_i may be a difficult and complex problem, even with a large digital computer (Mandelbaum, 1963; Whitten and others, 1965); this is true particularly for polynomials of degrees five and higher, and the machine time involved tends to be high. Second, unlike the orthogonal polynomial coefficients, the coefficients are not independent. Third, existing methods do not permit identification and separation of the trend as defined by Grant (1957).

Make direct use of orthogonal polynomials. This technique involves simple arithmetic operations that are executed extremely fast by computer; no matrix inversion is necessary. The orthogonal coefficients are independent so that the proportion of the total sum of squares associated with each coefficient is easily computed. Following DeLury's (1950) method, Grant (1957) used the z^2 array as a basis for defining the trend; this array is developed immediately from the orthogonal coefficients. Mapping functions are developed readily from the orthogonal coefficients and permit contoured maps of the trend component and of any part of the residual component to be computed.

An example of the use of orthogonal polynomials for irregularly spaced data does not seem to have been described in the geological literature previously. A simple situation based on subsurface data for the Michigan Basin is presented in this paper.

ORTHOGONAL POLYNOMIALS FOR IRREGULARLY SPACED DATA

Wishart and Metakides (1953), Forsythe (1957), and Robson (1959) showed how orthogonal polynomial coefficients can be calculated for irregularly spaced independent variables in the one-dimensional case. Robson (1959) used a simple recursive technique to build a table of polynomial values analogous to those listed by Beyer (1966), DeLury (1950), Fisher and Yates (1963), and Pearson and Hartley (1958) for grid data. It is impracticable to construct a general set of tables for irregularly spaced

data because the values depend on both the number of points n and the varying interval between each of the (u, v) coordinate points. Price and Simonsen (1963) described the logic for constructing orthogonal polynomials with a single irregularly spaced independent variable and outlined a computer program based on SHARE program RWCF2F. Dempsey (1966) also gave the logic and published an ALGOL computer program for the same general purpose.

Robson (1959) indicated how his method could be extended to the two-dimensional case but his particular technique is of little current application in earth science problems because his data points are required to lie at the nodes of a grid composed of orthogonal lines with unequal spacing.

Spitz (1966) described a more general method for fitting orthogonal polynomials appropriate to genuinely irregularly spaced data. Following Forsythe's (1957) method, he generated orthogonal polynomials:

$$\hat{X} = f(u, v) = \sum_{i=0}^n \sum_{j=0}^m A_{ij} P_i(u) Q_j(v)$$

where $P_i(u)$ was calculated for $\hat{X} = f_1(u)$, and $Q_j(v)$ for $\hat{X} = f_2(v)$. For approximations higher than the first degree, cross-product terms in u and v occur and remove the equation from the general linear model class. Although Spitz showed how cross-product terms can be accommodated, it is more convenient to develop the orthogonal polynomials for $\hat{X} = f(u, v)$ directly.

Suppose that X_{ij} is measured at n irregularly spaced locations (u_i, v_j) . Consider the vectors:

$$\begin{aligned} (1, 1, 1, 1, \dots, 1) &= \mathbf{V}_0 \\ (u_1, u_2, u_3, u_4, \dots, u_n) &= \mathbf{V}_1 \\ (v_1, v_2, v_3, v_4, \dots, v_n) &= \mathbf{V}_2 \\ (u_1^2, u_2^2, u_3^2, u_4^2, \dots, u_n^2) &= \mathbf{V}_3 \\ (u_1 v_1, u_2 v_2, u_3 v_3, u_4 v_4, \dots, u_n v_n) &= \mathbf{V}_4 \\ (v_1^2, v_2^2, v_3^2, v_4^2, \dots, v_n^2) &= \mathbf{V}_5 \end{aligned}$$

and so on, for terms of type $u^3, u^2 v, u v^2, v^3, u^4, u^3 v, \dots$, corresponding to vectors $\mathbf{V}_6, \mathbf{V}_7, \mathbf{V}_8, \dots, \mathbf{V}_k$, respectively.

It now is possible to define a set of polynomials as

$$\phi_0(u_n, v_n) = a_{00} \mathbf{V}_0 \tag{2a}$$

$$\phi_1(u_n, v_n) = a_{01} \mathbf{V}_0 + a_{11} \mathbf{V}_1 \tag{2b}$$

$$\phi_2(u_n, v_n) = a_{02} \mathbf{V}_0 + a_{12} \mathbf{V}_1 + a_{22} \mathbf{V}_2 \tag{2c}$$

$$\begin{aligned} &\vdots \\ &\vdots \\ &\vdots \end{aligned} \tag{2d}$$

$$\phi_k(u_n, v_n) = a_{0k} \mathbf{V}_0 + a_{1k} \mathbf{V}_1 + \dots + a_{kk} \mathbf{V}_k \tag{2k}$$

Now, if

$$\begin{aligned} \mathbf{p} &= p_1, p_2, p_3, \dots \\ \mathbf{q} &= q_1, q_2, q_3, \dots \end{aligned}$$

the dot product is $(p, q) = \sum p_i q_i$, which is called orthogonal if the summation equals zero (Kendall and Stuart, 1967, p. 356). It is required that all of the k polynomials defined above be orthogonal; for this purpose, it is necessary to find values of the coefficients a_{00}, \dots, a_{kk} that establish

$$(\phi_g(u_n, v_n), \phi_h(u_n, v_n)) = \sum_{m=1}^n \phi_g(u_m, v_m) \cdot \phi_h(u_m, v_m) = 0 \quad (3)$$

for $g = 0, 1, 2, \dots, k$ and $h = 0, 1, 2, \dots, k$ and $g \neq h$.

Equation (2a) yields

$$\phi_0(u_n, v_n) = a_{00} \mathbf{V}_0 = (1, 1, 1, \dots)$$

and therefore $a_{00} = 1$. If a vector \mathbf{W}_0 is defined as

$$\mathbf{W}_0 = \frac{\phi_0}{\|\phi_0\|} = \frac{\phi_0}{\sqrt{\sum_{m=1}^n [\phi_0(u_m, v_m)]^2}}$$

where $\|\phi_0\|$ is the length of vector ϕ_0 , then

$$\mathbf{W}_0 = \left(\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots \right)$$

and, using the Gram-Schmidt orthogonalization process (Thomas, 1969, p. 451) it follows that

$$\begin{aligned} \phi_1(u_n, v_n) &= \mathbf{V}_1 - (\mathbf{V}_1, \mathbf{W}_0) \mathbf{W}_0 = (u_1, u_2, u_3, \dots) - n\bar{u} \left(\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \dots \right) \\ &= \sum_{m=1}^n u_m - n\bar{u} \end{aligned} \quad (4)$$

Equation (2b) also gives

$$\phi_1 = a_{01} \mathbf{V}_0 + a_{11} \mathbf{V}_1 = na_{01} + a_{11} \sum_{m=1}^n u_m = \sum_{m=1}^n u_m - n\bar{u} \quad (5)$$

(by equating with the previously derived expression). Using eq (3) we have

$$\begin{aligned} \sum_{m=1}^n \phi_0(u_m, v_m) \cdot \phi_1(u_m, v_m) &= \sum_{m=1}^n a_{00} \mathbf{V}_0 \cdot (a_{01} \mathbf{V}_0 + a_{11} \mathbf{V}_1) \\ &= \sum_{m=1}^n (a_{00} a_{01} \mathbf{V}_0^2 + a_{00} a_{11} \mathbf{V}_0 \mathbf{V}_1) = a_{00} a_{01} n + a_{00} a_{11} \sum_{m=1}^n u_m = 0 \end{aligned}$$

Therefore, by rearranging this last expression, $a_{01} = -a_{11} \bar{u}$, and substitution of this value in eq (5) yields

$$-a_{11} n\bar{u} + a_{11} \sum_{m=1}^n u_m = -n\bar{u} + \sum_{m=1}^n u_m$$

and thus $a_{11} = 1$. Hence, $a_{00} = a_{11} = 1$ and, in general, it can be shown that $a_{kk} = 1$. The general formula for the orthogonal coefficients now can be derived by use of eq (3) with $g = 1$ and $h = 4$ but with the subscripts generalized as follows:

$$\phi_1(u_n, v_n) = \phi_i(u_n, v_n) = a_{i-1, j-3} + a_{i, j-3} V_1$$

and

$$\phi_4(u_n, v_n) = \phi_j(u_n, v_n) = a_{i-1, j} + a_{ij} V_1 + a_{i+1, j} V_2 + a_{i+2, j} V_3 + a_{i+3, j} V_4$$

where $i = j - 3$. Now, the orthogonality condition requires that

$$\{\phi_i(u_n, v_n), \phi_j(u_n, v_n)\} = 0$$

Therefore,

$$\begin{aligned} & a_{i-1, j-3} a_{i-1, j} n + a_{i-1, j-3} a_{ij} \sum_{m=1}^n u_m + a_{i-1, j-3} a_{i+1, j} \sum_{m=1}^n v_m \\ & + a_{i-1, j-3} a_{i+2, j} \sum_{m=1}^n u_m^2 + a_{i-1, j-3} a_{i+3, j} \sum_{m=1}^n u_m v_m + a_{i-1, j} \sum_{m=1}^n u_m \\ & + a_{ij} \sum_{m=1}^n u_m^2 + a_{i+1, j} \sum_{m=1}^n u_m v_m + a_{i+2, j} \sum_{m=1}^n u_m^3 + \sum_{m=1}^n u_m^2 v_m = 0 \end{aligned}$$

but from eq (6)

$$a_{i-1, j-3} = -\bar{u}$$

so

$$\begin{aligned} & (-a_{i-1, j} + a_{i-1, j-3} a_{ij} + a_{i-1, j}) \sum_{m=1}^n u_m + a_{ij} \sum_{m=1}^n u_m^2 \\ & = -a_{i+1, j} \left(a_{i-1, j-3} \sum_{m=1}^n v_m + \sum_{m=1}^n u_m v_m \right) - a_{i+2, j} \left(a_{i-1, j-3} \sum_{m=1}^n u_m^2 + \sum_{m=1}^n u^3 \right) \\ & \quad - a_{i+3, j} \left(a_{i-1, j-3} \sum_{m=1}^n u_m v_m + \sum_{m=1}^n u_m^2 v_m \right) \end{aligned}$$

Therefore,

$$a_{ij} = \left\{ \begin{array}{l} -a_{i+1, j} \sum_{m=1}^n [v_m \cdot (a_{i-1, j-3} + u_m)] \\ -a_{i+2, j} \sum_{m=1}^n [u_m^2 \cdot (a_{i-1, j-3} + u_m)] \\ -a_{i+3, j} \sum_{m=1}^n [u_m v_m \cdot (a_{i-1, j-3} + u_m)] \end{array} \right\} / \sum_{m=1}^n [u_m (a_{i-1, j-3} + u_m)]$$

Hence, $a_{kk} = 1$ and

$$a_{ij} = - \sum_{s=i+1}^j a_{sj} \sum_{m=1}^n [V_s \cdot \phi_i(u_n, v_n)] / \sum_{m=1}^n [V_i \cdot \phi_i(u_n, v_n)] \tag{6}$$

The polynomials $\phi_0, \phi_1, \dots, \phi_k$ are now defined and X_m can be represented as

$$X_m = b_0 \phi_0(u_m, v_m) + b_1 \phi_1(u_m, v_m) + b_2 \phi_2(u_m, v_m) + \dots + b_k \phi_k(u_m, v_m) + \varepsilon_m \tag{7}$$

where ε is the error term. The standard least-squares criterion requires that $\sum_{m=1}^n \varepsilon_m^2$ be minimized; that is, that

$$\sum_{m=1}^n [b_0 \phi_0(u_m, v_m) + b_1 \phi_1(u_m, v_m) + \dots + b_k \phi_k(u_m, v_m) - X_m]^2 = F$$

be minimized. To achieve this, the partial differentials of F with respect to b_0, b_1, \dots, b_k must be equated to zero. For example,

$$\frac{\partial F}{\partial b_k} = \sum_{m=1}^n 2 [b_0 \phi_0(u_m, v_m) + b_1 \phi_1(u_m, v_m) + \dots + b_k \phi_k(u_m, v_m) - X_m] \cdot [-\phi_k(u_m, v_m)] = 0$$

and similarly for the partial differentials with respect to b_0, b_1, \dots, b_{k-1} . Rearranging this equation,

$$\sum_{m=1}^n b_0 \phi_0(u_m, v_m) \cdot \phi_k(u_m, v_m) + \sum_{m=1}^n b_1 \phi_1(u_m, v_m) \cdot \phi_k(u_m, v_m) + \dots + \sum_{m=1}^n b_{k-1} \phi_{k-1}(u_m, v_m) \cdot \phi_k(u_m, v_m) + \sum_{m=1}^n b_k \phi_k^2(u_m, v_m) = \sum_{m=1}^n X_m \phi_k(u_m, v_m)$$

but, because of the orthogonality of the polynomials, this reduces to

$$b_k \sum_{m=1}^n \phi_k^2(u_m, v_m) = \sum_{m=1}^n X_m \phi_k(u_m, v_m) \quad (8)$$

which immediately gives the value of b_k . Thus, the independent coefficients b_0, b_1, \dots, b_k of the orthogonal polynomials are immediately and easily calculated. Following the procedures of DeLury (1950) and Grant (1957), the percentage of the total corrected sum of squares associated with each of the coefficients can be calculated; in turn, this leads immediately to the z^2 array, although only those items of the z^2 array corresponding to the particular b coefficients can be calculated in this manner.

By using the values of a given by eq (6) to evaluate the orthogonal polynomials [eq (2)], the latter are used with the values of b [eq (8)] to express eq (7) as a simple

Table 1. Top of Devonian Dundee Limestone, 900-sq-mi Area of Central Michigan, 487 Wells (Not More than One per Square Mile)

Well number	u coordinate, miles	v coordinate, miles	X , depth below sea level, ft
2	14.50	6.10	-2762
7	10.61	6.61	-2754
11	11.61	6.90	-2753
15	12.52	6.50	-2770
17	13.19	6.56	-2766
31	15.82	7.20	-2718
33	16.86	7.43	-2726
.	.	.	.
.	.	.	.
.	.	.	.

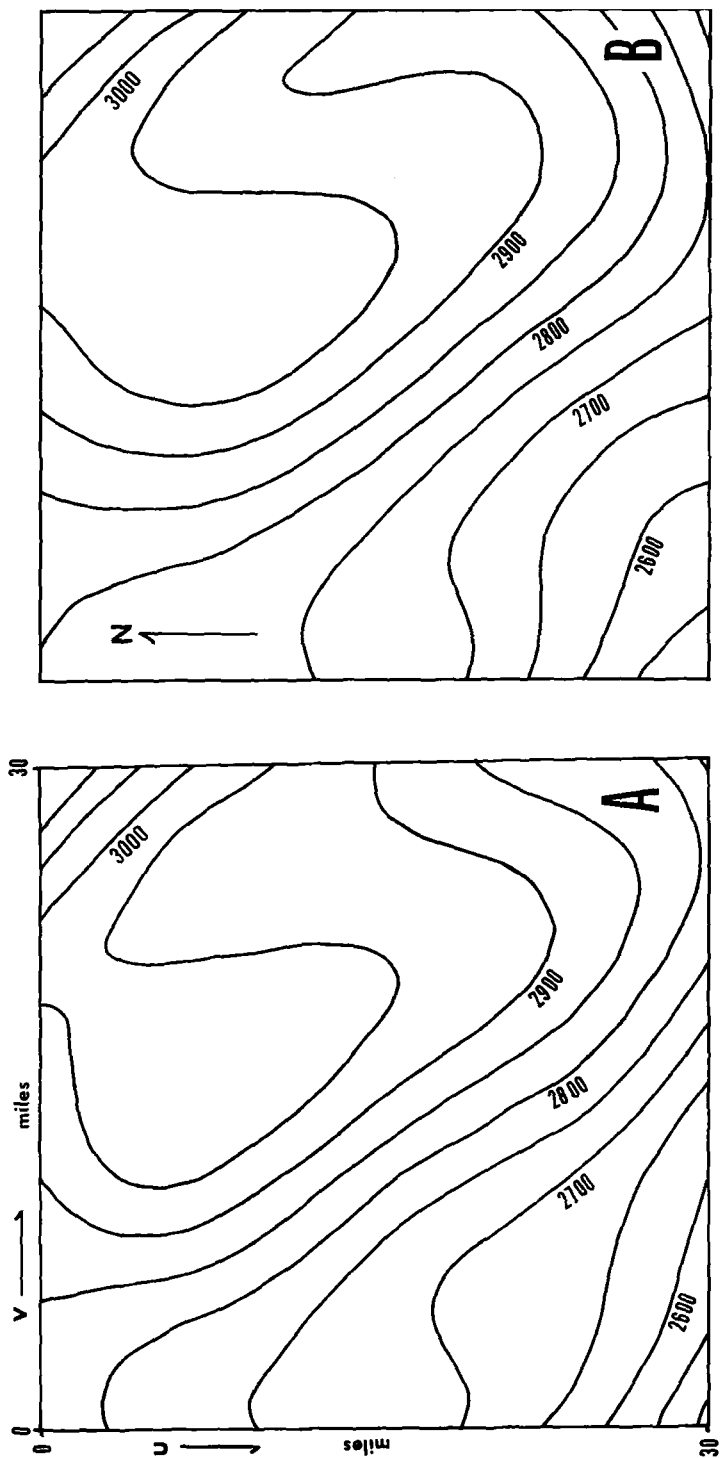


Figure 1. Trend-surface maps for top of Dundee Limestone, central Michigan (contours in ft below sea level). (A) Complete eighth-degree surface based on 45 orthogonal coefficients and accounting for 94.81 percent of total sum of squares; (B) surface based on 18 orthogonal coefficients used to define trend (defined in Table 3); surface accounts for 92.91 percent of total sum of squares.

components. Use of all the eighth-degree orthogonal coefficients (Table 2) permits calculation of the mapping coefficients [c coefficients of eq (9)] listed in Table 5; the coefficients are identical to those computed with a standard program for irregularly spaced data (Whitten and others, 1965). Figure 1A is the trend surface constructed with these coefficients. However, using only those orthogonal coefficients contributing to the trend (as defined in Table 3) results in a different set of mapping coefficients (Table 6) and Figure 1B is the map of the trend.

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