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Landmark Papers

Optimal interpolation and isarithmic mapping of soil properties: I The semi-variogram and punctual kriging

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Summary

Kriging is a means of spatial prediction that can be used for soil properties. It is a form of weighted local averaging. It is optimal in the sense that it provides estimates of values at unrecorded places without bias and with minimum and known variance. Isarithmic maps made by kriging are alternatives to conventional soil maps where properties can be measured at close spacings.

Kriging depends on first computing an accurate semi-variogram, which measures the nature of spatial dependence for the property. Estimates of semi-variance are then used to determine the weights applied to the data when computing the averages, and are presented in the kriging equations.

The method is applied to three sets of data from detailed soil surveys in Central Wales and Norfolk. Sodium content at Plas Gogerddan was shown to vary isotropically with a linear semi-variogram. Ordinary punctual kriging produced a map with intricate isarithms and fairly large estimation variance, attributed to a large nugget effect. Stoniness on the same land varied anisotropically with a linear semi-variogram, and again the estimation error of punctual kriging was fairly large. At Hole Farm, Norfolk, the thickness of cover loam varied isotropically, but with a spherical semi-variogram. Its parameters were estimated and used to krige point values and produce a map showing substantial short-range variation.

Introduction

For many years now the standard product from almost any soil survey has been a map of classes of soil, together with a record of observations and measurements made from pits or boreholes. The latter obviously refer specifically to the points at which the pits or boreholes were sunk, but there is always the hope, expressed or implied, that all places mapped as any particular class will have values of soil properties similar to those recorded for that class, and different from those of at least some of the other classes. The distribution of a single property may be displayed by assigning to each parcel on the map the typical value of that property within its class. Likewise the value at any one place not actually recorded, and this applies to the vast majority, is predicted. Of course, it is realized that the actual value there will differ somewhat from the predicted value.

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The rationale may be expressed in terms of classical statistics by assuming that the value of a property, z_{ij}, at any place i in class j is the sum of three terms:

$$Z_{ij} = \mu + \alpha_j + \varepsilon_{ij}, \quad (1)$$

where μ is the general mean of the property for the whole area, α_j is the difference between the general mean and the mean of class j, and ε_{ij} is a random component distributed normally with zero mean and variance σ_w^2. This is the model underlying the sampling studies by Thornburn & Larsen (1959) and Morse & Thornburn (1961), and the work on prediction and map evaluation (e.g. Webster and Beckett, 1968; Beckett & Webster, 1971). The parameters μ, α_j and σ_w^2 can all be estimated from data as say $\bar{z}$, a_j and s_w^2 respectively by the usual least squares analysis and analysis of variance. The predicted value for an unrecorded point in class j is $\bar{z} + a_j$, and confidence limits are determined from s_w^2, the sample within-class variance. The smaller is σ_w^2 the more precise will any prediction be, and the more valuable the map.

Where measured data are sparse, as they often are, this approach to prediction and mapping is the only feasible one. It obviously

depends on there being an association between the property of interest and the classification, even though the classes are recognized independently. In terms of the model, $|\alpha_j|$ must on average be substantially greater than zero, otherwise the classification does not help to predict the property. However, the procedure takes no account of the spatial arrangement of the data points and their relations to predicted points, nor of any gradation in values across boundaries. These can only be of consequence when data are dense, specifically when they are spatially dependent, and in that event a means of prediction and mapping that uses the spatial information is obviously to be preferred.

In such circumstances interpolation provides an alternative to classification for predicting values of a property at unvisited points. Mapping can be achieved by envisaging such values as forming a continuous statistical surface over the map plane, which can be represented by isarithms. Isarithmic mapping is often known as 'contouring', by analogy with the mapping of topographic height. But caution is needed. Topographic contours are usually drawn to join points of equal *measured* height, whereas soil isarithms join points of *inferred* equal value. In practice topographic contours can be followed continuously, either on the ground or on a pair of air photographs, and this means that they can be drawn as accurately as the surveying equipment allows. Soil isarithms on the other hand must be derived from a finite set of more or less widely spaced points and are therefore subject to sampling variation. As with prediction from classifications, there is an error associated with interpolation.

Several interpolation methods have been proposed, and they have been incorporated into many programs for automatic contouring (Rhind, 1975). The principal ones, reviewed briefly by Webster (1977), have been: linear interpolation across a triangulation, inverse distance and inverse-square distance weighted averaging, least-square polynomials, and Thieissen polygons. They are empirical, and their implementations often represent compromises between the mathematically desirable and the computationally feasible. Though these methods may seem reasonable for many applications they are theoretically unsatisfactory. They may give biased interpolation, they provide no estimate of the error of interpolation, nor do they attempt to minimize that error.

Recently a method known as 'kriging' has become available. It is based on the theory of regionalized variables developed mainly by Matheron (1963, 1965, 1971) and Krige (1966) for the estimation of ore reserves in mining, in which it is being used increasingly. It predicts values without bias and with minimum variance. In this sense it is optimal, just as the best classification of soil in a region is that for which the within-class variance is least (Webster & Beckett, 1968; Webster, 1971). Since kriging possesses these properties it has considerable promise in intensive survey. Also, since the variance of the estimates can itself be estimated the interpolated values can be used with known confidence.

The purpose of this paper is to draw the attention of soil scientists to kriging as a means of spatial prediction, to describe the essential steps of the procedure, as it applies to soil mapping, and to illustrate them with results for areas where detailed surveys had been carried out. Readers who wish to study the procedure in depth should read the source texts by Matheron, though the recent book by Journel and Huijbregts (1978) at an intermediate level is highly recommended. The first stage in kriging is the measurement of spatial variation in the soil property of interest. This not only provides the quantities necessary for optimal interpolation, but can guide the scientist in his choice of technique and sampling strategy. Therefore in Part I of the paper we deal with this stage at some length before showing how the measurements are applied to estimate values at points. In Part II we consider some of the shortcomings of punctual kriging for soil survey and extend the technique to estimate values of soil properties over areas (block kriging), and draw general conclusions.

Spatial Dependence and the Semi-Variogram

Webster (1973) and Webster & Cuanalo (1975) first measured spatial dependence among soil measurements by applying methods of time series. They computed correlograms from data along transects. As it happens regionalized variable theory builds on a complementary function known as the 'semi-variogram', for which a brief explanation is needed.

Consider a transect along which observations have been made at regular intervals to give values $z(i)$, $i = 1, 2, \ldots, n$. Then the relation between pairs of points h intervals apart, the lag, can be expressed as the variance of the differences between all such pairs. The per-observation variance between pairs (Yates, 1948) is half this value thus:

$$\gamma(h) = \frac{1}{2}\mathrm{var}\left[z(i) - z(i+h)\right] \tag{2}$$

It is called the semi-variance, and is a measure of the similarity, on average, between points a given distance, h, apart. The more alike are the points the smaller is $\gamma(h)$, and *vice versa*. The quantity $\gamma(h)$ can be estimated for integer values of h from the data. If the mean of the observations remains constant over distances d, then provided h is less than d the semi-variance is half the expected squared difference between values at that lag:

$$\gamma(h) = \frac{1}{2}\mathrm{E}\left[\{z(i) - z(i+h)\}^2\right]. \tag{3}$$

The graph of $\gamma(h)$ against h is the semi-variogram. It is related to the correlogram by

$$\gamma(h) = \sigma^2\{1 - \rho(h)\}, \tag{4}$$

where σ^2 is the variance and $\rho(h)$ the autocorrelation at lag h. Conversely

$$\rho(h) = 1 - \frac{\gamma(h)}{\sigma^2}. \tag{5}$$

The autocorrelation coefficient thus depends on the variance, which must be finite for the relation in Equation (5) to make sense. The semi-variance is free of this restriction, and is therefore

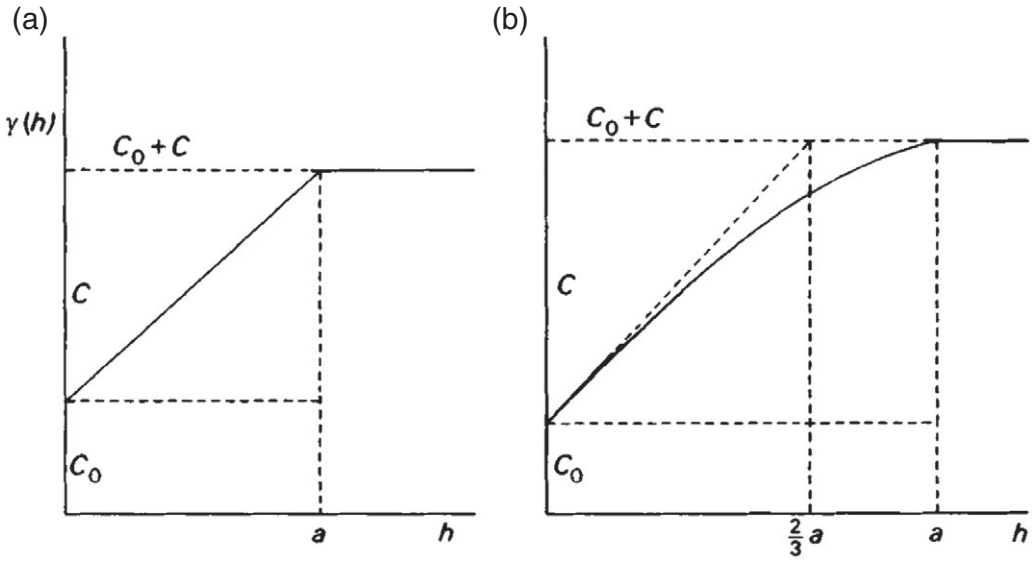

Figure 1 Theoretical semi-variograms for (a) a linear model and (b) a spherical model, illustrating the range, a, the sill, $c_0 + c$, and the nugget variance, c_0. The tangent to the curve at $h + 0$ in (b) meets the horizontal for the total variance at $\frac{2}{3}\ a$.

preferred. A second advantage of working with the semi-variance is that it is easier to take account of local trends in the property of interest. In regionalized variable theory such trend is known as 'drift', and we shall deal with this in a later paper (Webster & Burgess, 1980).

The semi-variogram has certain important characteristics which (a) reveal the nature of the geographic variation in the property of interest, and (b) are needed to provide kriged estimates at previously unrecorded points. These are described with reference to Figure 1. In most instances it is found that $\gamma(h)$ increases with increasing h to a maximum, approximately the variance of the data, at a moderate value of h, say a. The distance a is known as the *range*. If $\gamma(h)$ approaches the maximum asymptotically then a may be chosen where $\gamma(h)$ becomes sufficiently close to the total variance for practical purposes. Points closer together than the range are spatially dependent; points further apart bear no relation to one another, unless there is periodic variation in the soil. Experience to date suggests that in practical soil survey the range will usually be a few hundred metres, and exceptionally up to two or three kilometres. It does, however, depend on the size of area sampled. When interpolating we shall aim to use only those points closer than the range to the predicted point.

By definition $\gamma(h) = 0$ when $h = 0$. However, as can be seen from Figures 2 and 4, any smooth curve that approximates the values of the semi-variance is unlikely to pass through the origin. Instead there appears to be a positive finite value to which $\gamma(h)$ approaches as h approaches 0. This intercept is the nugget variance, c_0 in Figure 1, and the phenomenon in general is known as the nugget effect. The terms derive from gold mining in which the inclusion of a gold nugget in a narrow core sample is a somewhat chance event. Most semi-variograms of soil properties show distinct nugget effects (see also the correlograms in Webster & Cuanalo (1975),

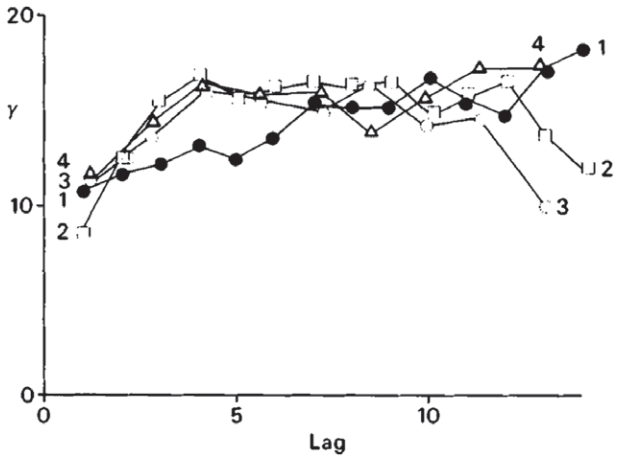

Figure 2 Semi-variograms of sodium content in Cae Ruel, Plas Gogerddan, for the four principal directions of the grid, γ is in units of $(\text{meq}/10\,\text{kg})^2$.

Figures 6.1 and 6.2 in Webster (1977), and Campbell's (1978) semi-variograms). The nugget variance embraces fluctuation in the soil that occurs over distances much shorter than the sampling interval, and limits the precision of interpolation, as we shall show later.

The value at which $\gamma(h)$ levels out is known as the *sill*. It consists of the nugget variance plus a component c (Figure 1) that represents the range of variance due to spatial dependence in the data.

There is no general mathematical formula to describe the shape of soil semi-variograms. A linear model, $\gamma(h) = c_0 + mh$, is simplest, and will often describe $\gamma(h)$ well within the range, *i.e.* for $h = 0$ to $h = a$, Figure 1(a). It would fit several of the correlograms in Webster & Cuanalo (1975) and Webster (1978). Where there is no

Table 1 Slopes of semi-variograms of stone content at Plas Gogerddan estimated for each direction separately, m_i and from pooled semi-variances after fitting a sinusoidal curve, $w(\Theta_i)$

Direction	θ_i	m_i	$w(\theta_i)$
1	$\pi/2$	3.14	3.57
2	0	5.51	5.94
3	$\pi/4$	2.13	1.70
4	$3\pi/4$	8.23	7.80

clear sill, or even where a sill exists, the distance, d, over which $\gamma(h)$ is of interest or can actually be computed may be less than the range. Again for $h=0$ to $h=d$ the linear model may be an adequate description of the graph. This seems to be so for the semi-variograms in Figure 6, for which values for c_0 and m are given on p. 328, and Table 1, and in Figure 2 up to lag 5.

An alternative proposed by Matheron to account for geological deposition and found to fit well in mineral prospecting is the spherical model, see Figure 1(b). It is given by

$$\begin{cases} \gamma(h) = c_0 + c\left\{\frac{3}{2}\frac{h}{a} - \frac{1}{2}\left(\frac{h}{a}\right)^3\right\} & \text{for } 0 < h \leqslant a \\ \gamma(h) = c_0 + c & \text{for } h > a \end{cases}. \quad (6)$$

Royle & Hosgit (1974) used this model to describe the spatial variation in gravel deposits near Doncaster, Yorkshire, and we have found it suitable in a number of instances for soil properties with a distinct sill and range. Figure 4 is an example, in which the spherical model has been fitted to the experimental semi-variances. The values of c_0, c and a are given on p. 325.

Punctual kriging

Consider a survey in which some soil property, Z, has been measured at n points each with location specified by a pair of coordinates x_i, y_i, $i=1,2, \ldots, n$, and for which we shall use the vector notation $\mathbf{x}_i$, where $\mathbf{x}_i=[x_i, y_i]$. We shall thus have a set of values $z(\mathbf{x}_1), z(\mathbf{x}_2), \ldots, z(\mathbf{x}_n)$. Suppose now that we wish to estimate the value $z(\mathbf{x}_0)$ of Z at a point $\mathbf{x}_0$. Let our estimate be $\hat{z}_0$, where $\hat{z}_0$ is a linear sum, or weighted average of the observed values:

$$\hat{z}_0 = \lambda_1 z(\mathbf{x}_1) + \lambda_2 z(\mathbf{x}_2) + \cdots + \lambda_n z(\mathbf{x}_n), \quad (7)$$

where the λ_i are coefficients or weights associated with the data points. The concept of such an average is familiar enough whether in the form of simple moving averages, the more complex averages with weights proportional to inverse functions of distance as in the SYMAP contouring algorithm (Shepard, 1968) or even trend surface interpolation. In kriging, however, the weights are so chosen that the error associated with the estimate is less than that for any other linear sum. The weights take account of the known spatial dependences expressed in the semi-variogram and the geometric relationships among the observed points. In general, near points carry more weight than distant points, points that occur in clusters carry less weight than lone points, and points lying between the point to be interpolated and more distant points screen the distant points so that the latter have less weight than they would otherwise.

The model for simple kriging, analogous to Equation (1) for usual soil survey practice, is

$$z(\mathbf{x}) = \mu_v + \varepsilon(\mathbf{x}), \quad (8)$$

where $z(\mathbf{x})$ is the value of the property at $\mathbf{x}$ within a neighbourhood V, μ_v is the mean value in that neighbourhood and $\varepsilon(\mathbf{x})$ is a spatially dependent random component with zero mean and variation defined by

$$\text{var}[\varepsilon(\mathbf{x}) - \varepsilon(\mathbf{x}-\mathbf{h})] = \text{E}\left[\{\varepsilon(\mathbf{x}) - \varepsilon(\mathbf{x}+\mathbf{h})\}^2\right] = 2\gamma(\mathbf{h}) \quad (9)$$

and equals $2\gamma(h)$ if variation is isotropic. It is assumed that μ_v is constant for the neighbourhood, though different neighbourhoods may have different means, and that the semi-variogram is the same over the whole area. The last assumption implies that there are no sharp boundaries: it is not sensible to interpolate across 'cliffs', and if a sharp boundary is known to exist then interpolation should be carried out separately on either side of it.

We shall show how the coefficients, λ_i, are calculated for ordinary kriging, *i.e.* for situations where there is no drift, first to estimate values at points (punctual kriging), and in Part II to estimate average values over areas (block kriging).

The first requirement of our interpolation estimate is that it be unbiased; i.e. we want $\hat{z}_0$ to be the same as the expectation $\text{E}[z(\mathbf{x}_0)]$. The weights must therefore sum to 1: $\sum_{i=1}^{n}\lambda_i = 1$. The estimation variance at $\mathbf{x}_0$ is then the expected value of the squared difference between $\hat{z}_0$ and $z(\mathbf{x}_0)$. This can be shown to be

$$\text{E}\left[\{z(\mathbf{x}_0) - \hat{z}_0\}^2\right] = -\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(\mathbf{x}_i,\mathbf{x}_j) + 2\sum_{j=1}^{n}\lambda_j\gamma(\mathbf{x}_0,\mathbf{x}_j), \quad (10)$$

where $\gamma(\mathbf{x}_i,\mathbf{x}_j)$ is the value of the semi-variogram along the line joining $\mathbf{x}_i$ and $\mathbf{x}_j$ at a distance $|\mathbf{x}_i - \mathbf{x}_j|$. When a soil property varies isotropically $\gamma(\mathbf{x}_i,\mathbf{x}_j) = \gamma(|\mathbf{x}_i - \mathbf{x}_j|)$; i.e. the semi-variance depends only on the separating distance.

The second requirement is to minimize the error variance with respect to each λ_i, subject to the constraint that $\sum_{i=1}^{n}\lambda_i = 1$. This involves finding the partial derivatives with respect to each λ_i and introduces a Lagrange parameter μ. The minimum variance is obtained when

$$\sum_{j=1}^{n}\lambda_j\gamma(\mathbf{x}_i,\mathbf{x}_j) + \mu = \gamma(\mathbf{x}_i,\mathbf{x}_0) \text{ for } i = 1, 2, \ldots, n. \quad (11)$$

In matrix notation the coefficients λ_i are given by

$$\begin{bmatrix}\lambda \\ \mu\end{bmatrix} = \mathbf{A}^{-1}\mathbf{b} \quad (12)$$

where

$$\mathbf{A}=\begin{bmatrix}\gamma\left(\mathbf{x}_1,\mathbf{x}_1\right) & \gamma\left(\mathbf{x}_2,\mathbf{x}_1\right) & \cdots & \gamma\left(\mathbf{x}_n,\mathbf{x}_1\right) & 1\\ \gamma\left(\mathbf{x}_1,\mathbf{x}_2\right) & \gamma\left(\mathbf{x}_2,\mathbf{x}_2\right) & \cdots & \gamma\left(\mathbf{x}_n,\mathbf{x}_2\right) & 1\\ \vdots & \vdots & & \vdots & \\ \gamma\left(\mathbf{x}_1,\mathbf{x}_n\right) & \gamma\left(\mathbf{x}_2,\mathbf{x}_n\right) & \cdots & \gamma\left(\mathbf{x}_n,\mathbf{x}_n\right) & 1\\ 1 & 1 & & 1 & 0\end{bmatrix}$$

$$\mathbf{b}=\begin{bmatrix}\gamma\left(\mathbf{x}_1,\mathbf{x}_0\right)\\ \gamma\left(\mathbf{x}_2,\mathbf{x}_0\right)\\ \vdots\\ \gamma\left(\mathbf{x}_n,\mathbf{x}_0\right)\\ 1\end{bmatrix},\text{ and }\begin{bmatrix}\lambda\\ \mu\end{bmatrix}=\begin{bmatrix}\lambda_1\\ \lambda_2\\ \vdots\\ \lambda_n\\ \mu\end{bmatrix} \tag{13}$$

The minimum estimation variance is σ_{E}^2 given by

$$\sigma_{\mathrm{E}}^2=\mathbf{b}^T\begin{bmatrix}\lambda\\ \mu\end{bmatrix}. \tag{14}$$

Thus the vector of coefficients, λ, and the error of the estimate, σ_E^2, can be obtained from the single matrix inversion of **A**. Nevertheless, if n is large this can still be a formidable task, and if inversion has to be repeated for many points for contouring, it may be prohibitive. But since λ_i decreases as the distance between $\mathbf{x}_0$ and $\mathbf{x}_i$ increases, and because of the screen effect, most points far from $\mathbf{x}_0$ can be omitted from the calculation without serious consequences. For irregularly distributed observations Olea (1975) suggests using only the nearest two points in each octant around $\mathbf{x}_0$. For data on a square grid the nearest 16 or 25 points are usually quite sufficient to give an accurate estimate.

The accuracy of kriged estimates depends, of course, on the goodness of the computed semi-variogram. Unfortunately there is no efficient way of calculating confidence intervals for semi-variance, but two precautions can ensure that the values of $\gamma(h)$ used in the kriging equations are satisfactory. First, the spatial analysis should be performed on long runs of data, or numerous shorter runs, so that the semi-variances at short lags will be computed from many pairs of comparisons. Second, a sensible model must be chosen to describe the results, and individual estimates of $\gamma(h)$ can be weighted according to the number of comparisons on which they are based when fitting the model. As above, since only the nearest few points are likely to be used for kriging the semi-variograms need be accurate only over the first few lags.

The nature of the kriging equations has important implications for the design of soil survey. First, there is a big advantage in making observations on a regular grid for the following reason. The vector of coefficients, λ, depends on the semi-variogram and the configuration of the observation points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ in relation to $\mathbf{x}_0$, the point to be interpolated. If the semi-variogram has been computed from a previous sampling then λ does not depend on the values $z_1, z_2, \ldots, z_n$. Suppose the system were shifted by a vector **h**, then since $\gamma(\mathbf{x}_1+\mathbf{h}, \mathbf{x}_2+\mathbf{h})=\gamma(\mathbf{x}_1, \mathbf{x}_2)$ the matrices **A** and **b** remain the same for an equivalent point $\mathbf{x}_0$ in any other square, except near the edges of the grid: the configuration of data points retains the same relation to the point to be estimated. This means that to interpolate a fine grid with interval $1/r$ times that of the original observation grid, we need solve Equation (12) at most r^2 times for the central part of the map. Computation can also be reduced by noting that **A** does not depend on the point $\mathbf{x}_0$. So, to interpolate any other points near to $\mathbf{x}_0$ using the same observations at $\mathbf{x}_1$,$\mathbf{x}_2, \ldots, \mathbf{x}_n$ only **b** changes, and we need not invert **A** again. Further short cuts can be made when the semi-variogram is isotropic. Near the edges of the map the configuration will usually be different, and additional matrix inversions will be necessary.

A second very important feature is that the estimation variance also depends on the semi-variogram and the configuration of data points in relation to $\mathbf{x}_0$, and not on the observed values of Z. This means that if the semi-variances are known then the interpolation errors can be calculated for a particular sampling design *before the survey is made*. Thus, a sampling interval can in principle be chosen to reduce the interpolation error to any desired value. In practice, of course, it might cost too much.

Thirdly we note that when a point $\mathbf{x}_0$ coincides with an observation point **x** all the elements of λ are zero except λ_i, which equals 1. Thus, an interpolation surface passes through the observed values, and the estimation variance at these points is zero. This property is particularly desirable when the nugget variance is small and the observations themselves are made with negligible error. Some other commonly used interpolation techniques, such as trend-surface analysis, lack this property. However, if the nugget variance is large punctual kriging may produce undesirable effects. Delfiner & Delhomme (1975) have shown that a regionalized variable $Z(x)$, in one dimension, can be considered mathematically as the sum of two random terms. These are a term $Y(x)$ with a semi-variogram equivalent to that of $Z(x)$ without the nugget variance plus an uncorrelated random term $\varepsilon(x)$ with zero mean and variance equal to the nugget variance, c_0 in figure 1. When an interpolation point x_0 does not coincide with an observation point the best estimate of $Z(x_0)$ depends on the autocorrelated component $Y(x_0)$. The quantity $\varepsilon(x_0)$ does not influence the estimate itself, but only the estimation variance, which will exceed the variance of $Y(x_0)$ by the amount of the nugget variance. In other words it is impossible to predict random variation that occurs over distances much less than the sampling interval. This feature can result in a discontinuity in a kriged line, or surface in two dimensions, at each observation point. Discontinuity may be avoided by computing kriged averages of the soil property over small areas, and is considered in Part II.

Automatic contouring

The mechanism by which an interpolated surface is displayed is essentially a separate problem from that of interpolation itself, especially if the display is produced on a graph plotter. We deal with it briefly. In most automatic contouring systems a fine grid of values is generated to represent the surface, usually by methods that are not optimal. The contours are threaded through this grid using a procedure similar to that described by Dayhoff (1963). Positions are found where the isarithms intersect the sides of

the grid cells by linear interpolation, and these are then joined across the cells by straight line segments. The procedure can be refined by prior triangulation, and to prevent the resulting isarithms appearing rough the intersections can be joined using splines. Most large scientific computer installations now have library programs that do this. The examples shown below, were obtained using the GHOST system (Calderbank & Prior, 1977) run on the Oxford University ICL 1906A machine from our own interpolation grid.

The accuracy of this stage in mapping can be increased by increasing the fineness of the interpolation grid. If it is fine enough the isarithms will appear as smooth curves even though they consist of straight segments. However, the capacity of the computer to store interpolated values is finite and so is the time available for processing, and some compromise has to be struck betwen use of resources and accuracy. We have found that in most instances a grid with nodes at about 2 mm intervals at the scale of the finished maps is graphically quite acceptable.

Examples of kriging from isotropic data

Sodium content, Plas Gogerddan

A survey had been made of the soil at the Welsh Plant Breeding Station, Plas Gogerddan. The soil in each field was examined at 50 ft (15.2 m) intervals on a square grid and several soil properties including sodium and stone content (see later) measured on bulked samples of 10 cores 2.5 cm diameter and 15 cm deep chosen randomly within the 50 ft × 50 ft squares around the grid nodes. Unfortunately for present purposes the grids in different fields had different origins and orientations, and to minimize the computing we have restricted this study to a single field, Cae Ruel. This is nevertheless the largest, and had 440 observation points in it. Sodium content was determined on an acetic acid extract and expressed in milli equivalents per 10 kg of soil.

Semi-variograms of sodium content were computed for four principal directions, namely along the axes of the grid and along the diagonals, with lag extending to approximately 200 m, Figure 2. They are all linear up to a range of 4 lag intervals (about 50 m), and although the semi-variogram for direction 1 is somewhat different from the other three we have judged them sufficiently alike for sodium content to be spatially isotropic. The following equation for the semi-variance was fitted to the pooled results:

$$\gamma(h) = 8.7 + 1.69\ |h| \text{ for } |h| \leqslant 4,$$

where h is in units of 50 ft.

The semi-variances become increasingly erratic after 13 terms at the right-hand side of figure because there are fewer data points from which to compute them. It would have been reasonable to fit a spherical model to the result, but since the simpler linear model seemed adequate we used it.

Using this model for the semi-variogram we interpolated a grid of values at 25 ft (7.6 m) intervals by punctual kriging using the nearest sixteen data points for each interpolation point. These were then contoured using GHOST to give Figure 3. The estimation variances for the central portion of the field are as follows:

*	•	*	
0	10.68	0	Key
•	•	•	* observation point
10.68	10.72	10.68	• interpolated point
*	•	*	
0	10.68	0	

These are equivalent to a standard error of the estimate of about 3.3 for unobserved points. This is fairly large, bearing in mind that the sodium content lies mainly in the range 15 to 30. It arises largely from the nugget variance, which is large despite the bulk sampling procedure.

Figure 3 is the resulting contour map. It is distinctly 'spotty': there are many small near-circular contours. These represent discontinuities in the surface as a result of the large nugget variance. They can be smoothed out by average kriging (Figure 1, Part II).

Cover loam, Hole Farm

The distribution of cover loam at Hole Farm in Norfolk has already been shown to be associated with the patterns of crop establishment there (Corbett & Tatler, 1974), and Webster (1977) used SYMAP (Laboratory for Computer Graphics, 1968) to map the thickness of the cover loam. Data from the same survey have been re-analysed to produce optimal maps.

Thickness of cover loam (depth to sand and gravel) was measured by auger boring at 20 m intervals over a field of approximately 18 ha, to give some 450 observations. Semi-variograms were computed for four principal directions assuming no drift. As before

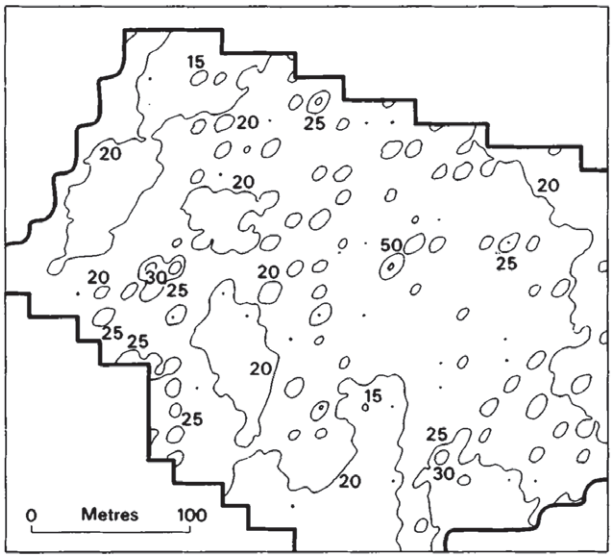

Figure 3 Isarithmic map of sodium content in Cae Ruel, Plas Gogerddan, produced by punctual kriging. Isarithms are at intervals of 5 meq/10 kg.

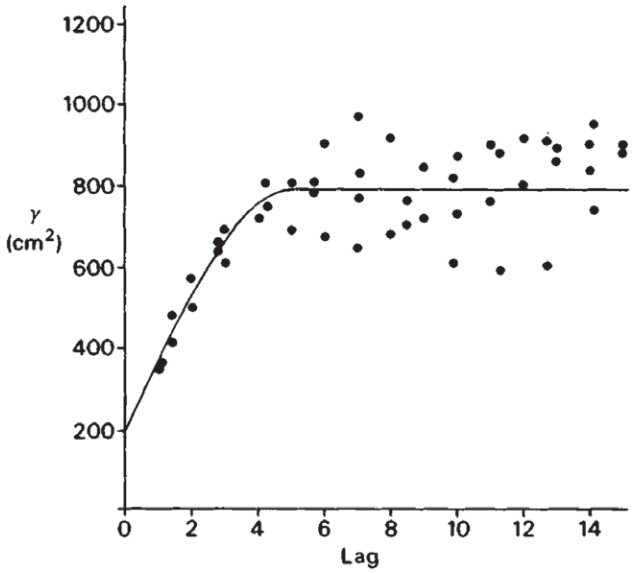

Figure 4 Semi-variances of the depth of cover loam at Hole Farm, Norfolk, with a spherical model fitted.

they were approximately the same as one another: the thickness of cover loam may be regarded as isotropic, and the spatial dependence may be represented by a single semi-variogram. Figure 4 shows the results with a spherical model fitted, equation (6). Its parameters were estimated as follows:

$$\text{nugget variance, } c_0 = 187.0\,\text{cm}^2$$

$$c = 603.8\,\text{cm}^2$$

$$\text{range, } a = 5.06 \text{ sampling intervals.}$$

The nugget variance accounts for about a quarter of the total, and probably arises from deep pockets of loam less than 20 m across that are scattered over the area.

The thickness of cover loam was then kriged at 6.67 m intervals to give a fine grid with nine times as many points as the original observation grid. Twenty-five observations were used to interpolate each point. The estimation-variances in the central portion of the map were:

*	•	•	*	
0	316.4	316.4	0	
•	•	•	•	Key
316.4	324.1	324.1	316.4	* observation point
•	•	•	•	• interpolated point
316.4	324.1	324.1	316.4	
*	•	•	*	
0	316.4	316.4	0	

The estimation variances at the unobserved points correspond to standard errors of about 18 cm. This again may be thought fairly large (loam thickness varies between 0 and 100 cm only), and, as with sodium content at Plas Gogerddan, the nugget variance is the major contributor.

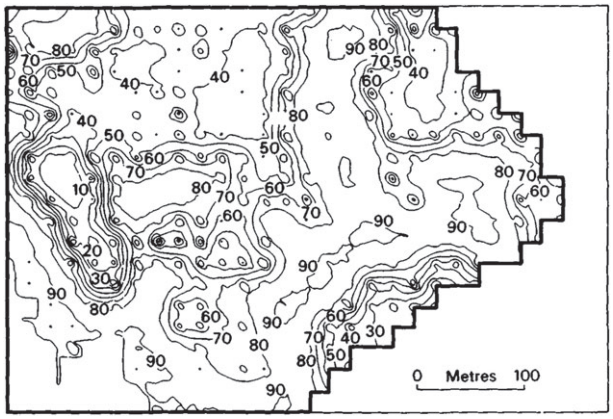

Figure 5 Isarithm map of cover-loam thickness of Hole Farm produced by punctual kriging. Isarithms are at 10 cm intervals.

Figure 5 is a contour map produced from the interpolation grid. As in Figure 3 there are marked discontinuities around the data points.

Kriging from anisotropic data

Soil does not always vary isotropically, even in small areas. On a point-bar deposit or river levee one would expect greater spatial dependence in the direction parallel to the river than at right angles to it. Likewise where the land surface bevels a sequence of sedimentary rocks the soil at points along the strike is more likely to be similar than that at points the same distance away in the direction of the dip. Anisotropy of this sort will be revealed by computing semi-variograms for different directions.

The stone content of the soil at Plas Gogerddan varies anisotropically. Data from the same points in Cae Ruel have been used to compute semi-variances for the four principal directions of the grid up to 10 sampling intervals (152 m). All four semi-variograms (Figure 6) are approximately linear, and have much the same nugget variance. But their slopes are very different as a result of the anisotropy. Each may be approximated by a straight line with slope m_i, where i is the direction and nugget variance of 10.0:

$$\gamma_i(h) \approx 10.0 + m_i h \quad \text{for} \quad h \geq 0 \tag{15}$$

The values of m_i are given in Table 1.

Suppose Θ is the angle for the direction then the four separate semi-variograms can be represented by a single equation:

$$\gamma(h) = 10.0 + w(\Theta)\,h \tag{16}$$

where $w(\Theta_i) = m_i$, when Θ_i is the angle for the ith direction, $i = 1,2,3,4$. Let $w(\Theta)$ be given by

$$w(\Theta) = A\cos^2(\Theta - \Phi) + B\sin^2(\Theta - \Phi) \tag{17}$$

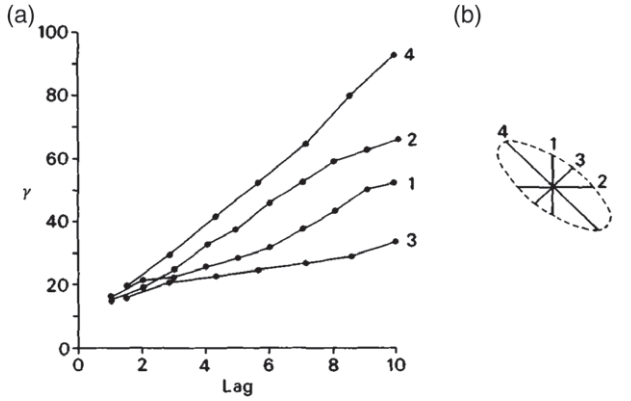

Figure 6 (a) Semi-variograms of stoniness in Cae Ruel, Plas Gogerddan, for the four principal directions. (b) Diagram with the slopes of the semi-variograms represented by vectors and a sinusoidal function, equation (16), fitted.

where Φ is the direction of greatest variation; i.e. the direction in which the semi-variogram is steepest, A is the slope of the semi-variogram in this direction, and B is the slope of the semi-variogram in the direction perpendicular. The quantities of A, B and Φ can be estimated by fitting a sinusoidal curve $w(\Theta)$ to the four slopes of m_i and their known directions Θ_i. This curve was fitted by non-linear least squares, taking direction 2 as $\Theta = 0$ (see Figure 6 for directions), to give the following equation for $w(\Theta)$

$$w(\Theta) = 8.02\cos^2(\Theta - 2.54) + 1.48\sin^2(\Theta - 2.54),$$

where the angles are in radians. Table 1 lists the slopes estimated by $w(\Theta)$ for semi-variograms in the four principal directions, and compares them with the values calculated directly for the individual semi-variograms. The agreement is good.

Using expression (17) for the semi-variogram a grid of values was kriged at 25 ft (7.6 m) intervals using 16 data points for each interpolation. The estimation variances for the central portion of the map were:

*	•	*	
0	13.1	0	Key
•	•	•	* observation point
12.8	12.7	12.8	• interpolated point
*	•	*	
0	13.1	0	

The map of stone content produced from the grid is shown in Figure 7. Notice the orientation of the isarithms reflecting the anisotropy. The soil also becomes increasingly stony from top left to bottom right, and it might be thought that removal of this gradual drift would result in an isotropic semi-variogram. However, a structural analysis taking account of both linear and quadratic drifts over small neighbourhoods by the methods of Olea (1975) showed this not to be so.

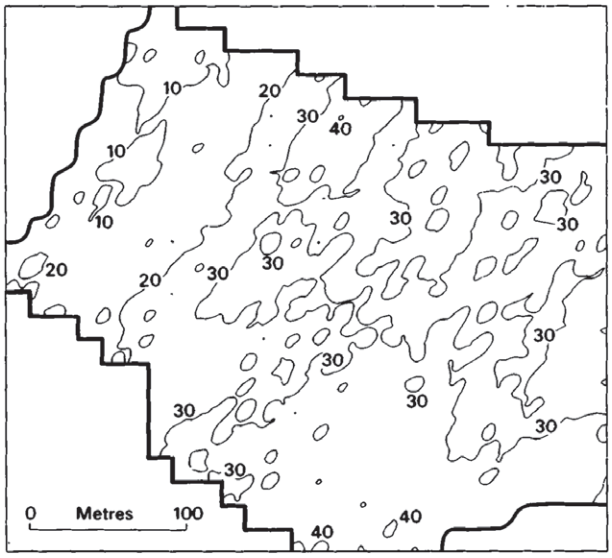

Figure 7 Isarithmic map of stone content in Cae Ruel produced by punctual kriging. Isarithms are at 10 per cent intervals.

Conclusion

The principal steps of kriging are thus seen to be, in order of their execution:

i. spatial analysis to compute a semi-variogram;
ii. choice and fitting of a suitable model to the semi-variogram;
iii. computation of weights in each local average.

Computation of the estimation variances is an optional extra.

This part of the paper also shows results of applying ordinary punctual kriging to typical intensive soil surveys, and in particular how strongly point estimates are influenced by large nugget variances. In Part II we consider whether point estimates are actually desired, and where they are not, how to interpolate soil properties over large blocks of land.

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