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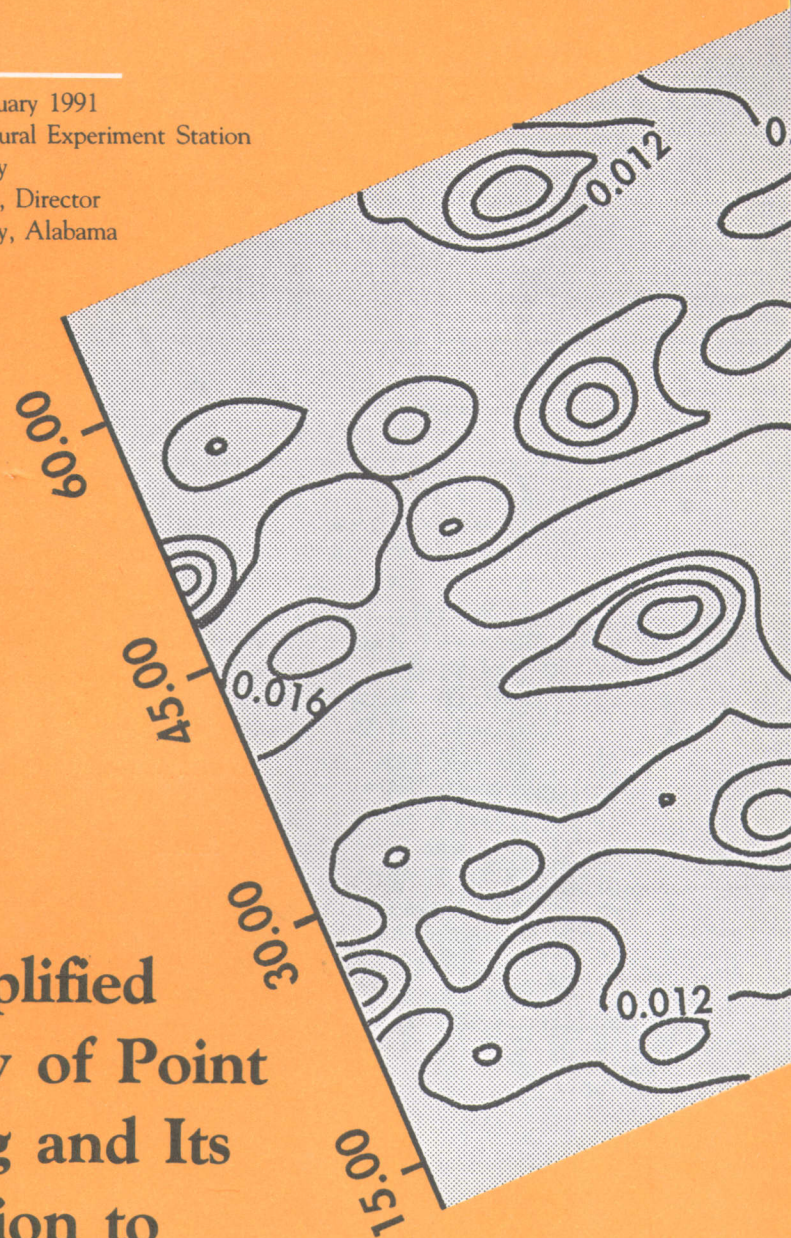

A Simplified Theory of Point Kriging and Its Extension to Co-kriging and Sampling Optimization

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A Simplified Theory Of Point Kriging And Its Extension To Co-Kriging And Sampling Optimization[1]

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INTRODUCTION

A SIMPLIFIED explanation of the linear prediction technique of kriging was derived from a statistical point of view. The kriging technique allows values of a given, spatially dependent, variate to be predicted at points where no measurements were made. It is then possible to construct a contour map for that variate. Based on the theoretically developed equations, computer programs were written to carry out the predictions. Besides assisting the computer user, the aim of this research was also to point out the similarities between kriging and standard least squares, of which it is indeed a special case.

Six computer programs were developed: (1) instead of determining a semi-variogram to specify the spatial interdependency of a given variate, a more general, cross-validation method was developed to determine the range parameter as needed in the kriging equations; (2) the selected model was then more thoroughly examined, e.g., for outliers, by yet another cross validation program; (3) in addition to simple kriging, equations and computer programs were developed for universal kriging, i.e. kriging under a lack of stationarity; (4) these equations and programs were subsequently extended to co-kriging to improve the estimation process by using information on auxiliary variables; (5) a program was written to validate the co-kriged model; (6) a procedure was developed to optimize sampling schemes with the use of kriging and co-kriging, i.e., the best sampling locations in the field and their minimum number according to preset criteria were determined.

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The six developed computer programs were applied to data collected in the following experiment. A 50- by 100-m field was sampled on two occasions at a total of 60 locations and at five to 11 depths to study the spatial variability of pH, Ca, Mg, K, P, organic matter, texture, bulk density, soil water retention, and saturated hydraulic conductivity. The programs were written in such a manner that data sets obtained at two different times could be combined into one for prediction purposes.

The equations developed in the theoretical sections are the same as those used in the computer programs presented in the Appendix, with most of the notation remaining consistent throughout.

KRIGING AS A LEAST SQUARES PROCEDURE

The Kriging Equations

Let $\underline{Z}$ denote a vector of n random variables with mean $\underline{\mu}$ (column vector with n elements) and variance-covariance matrix V (size n x n). This can be written as

$$\underline{Z} \sim (\underline{\mu}, V).$$

It should be noted that $\underline{Z}$ denotes a vector with n observations if only one random variable is considered, as is often done with kriging. Now consider $\underline{Z}$ in partitioned form with vector $\underline{Z}_1$ of dimension (n-1) and vector Z_2 of dimension 1. Then

$$\begin{bmatrix} \underline{Z}_1 \\ Z_2 \end{bmatrix} \sim \begin{bmatrix} \underline{\mu}_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} V_{11} & \underline{v}'_{12} \\ \underline{v}_{12} & V_{22} \end{bmatrix},$$

where $\underline{v}'_{12}$ is a covariance row and $\underline{v}_{12}$ a covariance column vector. The prediction problem is to predict Z_2, denoted as $\hat{Z}_2$, given a set of observations $Z_1 = z_1$. Assuming a linear model relationship among the means, the conditional mean of Z_2, given $Z_1 = z_1$, is:

$$E(Z_2 \mid \underline{Z}_1 = \underline{z}_1) = \mu_2 + \underline{v}'_{12} V_{11}^{-1} (\underline{z}_1 - \underline{\mu}_1), \qquad (1)$$

where $\underline{z}_1$ is a column vector containing the observed values and $E(Z_2 \mid \underline{Z}_1 = \underline{z}_1)$ required **B**est **L**inear **U**nbiased **E**stimate (BLUE).

Now suppose $\underline{\mu} = D\underline{\beta}$ and $\begin{bmatrix} \underline{\mu}_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} D_1 \\ \underline{d}'_2 \end{bmatrix} \beta$, (2)

where the elements of the n x m matrix D are known and $\underline{\beta}$ is a m- dimensional parameter vector. The matrix D is called the design matrix. For example, a particular case might be D = $\underline{1}$, a single column of ones, in which case we have stationarity in the mean. Other models for the mean reflect what is called "trend". The row vector, $\underline{d}_2'$, of dimension m, is that row of the design matrix which corresponds to the random variable Z_2, which depends on the location at which an estimate will be made. The submatrix D_1 is that part of the design matrix corresponding to the column vector of the observed values $\underline{z}_1$. It should be borne in mind that any linear mean model can be used.

Assuming V to be known, the BLUE derived from equations 1 and 2 is the least squares estimate, namely:

$$\hat{Z}_2 = \underline{d}_2' \hat{\underline{\beta}} + \underline{v}_{12}' V_{11}^{-1} (\underline{z}_1 - D_1 \hat{\underline{\beta}}) \quad , \quad (3A)$$

where:

$$\hat{\underline{\beta}} = (D_1' V_{11}^{-1} D_1)^{-1} D_1' V_{11}^{-1} \underline{z}_1 \qquad (3B)$$

is the estimate for $\underline{\beta}$. Equations 3A and 3B are the kriging equations. When the mean model is not stationary, a drift or trend needs to be taken into account. The process is now called "universal kriging." Note that, if a prediction, $\hat{z}_2$, is made at some point which coincides exactly with an existing observation, z_j, then, the vectors of covariances for Z_2 and Z_j are equal. In other words, the column vector $\underline{v}_{12}$ belongs to the column space of V_{11}. Consequently:

$$v_{12}' V_{11}^{-1} = \underline{e}_j$$

is a vector of zeros except for 1 in place j, and

$$\hat{z}_2 = \underline{d}_2' \hat{\underline{\beta}} + (z_j - \underline{d}_2' \hat{\underline{\beta}}) = z_j$$

The above state of affairs, usually referred to as the prediction "honoring" the observation may not always be considered desirable. For example, it may produce rough looking contour maps. This can be avoided by postulating that $\underline{v}_{12}$ does not belong to V_{11}, which is equivalent to defining a non-zero variance, called the "nugget variance," for the difference between two observations on Z made at the same site.

The classic reference to kriging is the book by Journel and Huijbregts,[4] where it is explained in a geological setting. The basis of their derivation of the kriging equations is to find a function of the observations which is unbiased in estimating the conditional mean and has

[4]Journel, A. and C. Huijbregts. 1978. Mining Geostatistics. Academic Press, New York.

minimum variance. For that reason, their "kriging equations" may appear at first sight to differ from equation 3, but it is easy to prove their equivalence.

Extension To Co-kriging

Let $$\underline{Z} = \begin{bmatrix} \underline{Z}_A \\ \underline{Z}_B \end{bmatrix} ,$$

where $\underline{Z}_A$, of dimension n_A, denotes a vector of variates of primary interest and $\underline{Z}_B$, of dimension n_B, a vector of co-variates. Now suppose:

$$\begin{bmatrix} \underline{Z}_A \\ \underline{Z}_B \end{bmatrix} \sim \underline{\mu} = \begin{bmatrix} \underline{\mu}_A \\ \underline{\mu}_B \end{bmatrix} , \; V = \begin{bmatrix} V_{AA} & V_{AB} \\ V'_{AB} & V_{BB} \end{bmatrix} \qquad (4)$$

It is apparent, that by proceeding exactly as for kriging, but with the vector $\underline{\mu}$ and matrix V defined as in equation 4, there is no extra difficulty in finding the least squares estimate of the conditional mean of any element of Z_A, using equation 3. In the simplest case, where there is stationarity of the mean, D will have two columns with each element 0 or 1 depending on whether that observed value of Z is a primary variate or a co-variate.

It is worth mentioning that the formulation given in equation 4 allows observations to be made at any place on either the primary variate or the co-variate; they need not be measured together or equally frequently. It also can be seen that an extension to any number of co-variables is simple in theory.

ESTIMATION AND VALIDATION

Moving Neighborhood Kriging and Cross-validation

In practice, when prediction is required at some point P, only those observations within a given distance of P are used in the prediction. This so-called "moving neighborhood," therefore, contains a specified subset of all the observations. It can be defined by requiring a minimum number of observations (Dubrule[5] recommends about 15) or by spanning a given distance from P. The first advantage of such a strategy is that solution of the kriging equations involves a matrix of reasonably small dimensions. The second advantage is that pragmatic and sensible models can be fitted to the data. For example, it is often perfectly reasonable to fit a simple stationary mean model

[5]Dubrule, O. 1983. Two Methods with Different Objectives: Splines and Kriging. Mathematical Geology Vol. 15(2):245-257.

knowing that this in no way implies stationarity over the whole region.

Perhaps one of the most important aspects of any analysis is the validation of the model used. We recommend cross-validation, which is a sequential procedure whereby each datum point in turn is removed from the set of observations and its value is then predicted by the model based on those observations remaining. A number of criteria can now be used to decide on the "goodness of fit" between predicted and observed values. However, the special spatial nature of the problem should not be ignored and it is often useful to portray the deviations graphically. This may, e.g., illustrate poor predictions on the edges of the map.

Another useful aspect of cross-validation is its ability as an estimation technique in its own right. This matter is pursued in the next section.

Estimation of the Covariance Structure

The basic assumption usually made at this stage is that v_{ij}, the covariance between Z_i and Z_j, depends only on their distance apart, d_{ij}, and possibly on their orientation with respect to each other (e.g., Clark[6]; Journel and Huijbregts). A very simple model, and the only one pursued here, is the spherical model which specifies that the correlation between Z_i and Z_j is

$$\rho_{ij} = 1 - \frac{3}{2}(d_{ij}/\alpha) + \frac{1}{2}(d_{ij}/\alpha)^3 \quad , \quad d_{ij} \leq \alpha$$

$$\rho_{ij} = 0 \quad , \quad d_{ij} > \alpha$$

where the parameter α is called the "range." Points farther apart than the range are uncorrelated.

The literature on spatial statistics invariably recommends that the nature of the spatial correlation should be investigated by means of a "semi-variogram." Suppose observations z_i and z_j have been made at points a distance d_{ij} apart. Then, if all pairs of observations that are a distance d_{ij} apart are collected, and if there are n_{ij} such pairs, it follows that:

$$\hat{\gamma}_{ij} = \frac{1}{2n_{ij}} \sum (z_i - z_j)^2$$

where the summation is only over those pairs that are a distance d_{ij} apart. Now, if a value $\hat{\gamma}_{ij}$ is calculated for every possible distance d_{ij} in the data and $\hat{\gamma}_{ij}$ is plotted versus d_{ij}, such a plot is called a semivariogram. Various models may be fitted through the generated data points and their parameters estimated.

[6]Clark, I. 1979. Practical Geostatistics. Academic Science Publishers, London.

The authors' experience with chemical and physical measurements on soil samples suggests that typically the semi-variogram exhibits poor structure. In addition, any effects of "drift" must be accounted for. These considerations have motivated the authors to first consider only the simplest model, namely, the spherical model, and second to investigate alternative methods for the estimation of the single covariance parameter α.

Consider now the dual problem of estimating α in each given moving neighborhood and then combining these estimates to form one global value. Initially there is the additional problem of defining the collection of moving neighborhoods for the entire procedure. One elementary definition, and the only one pursued in this publication, is to have one moving neighborhood centered on each observation. Given an assumed value for α and a specific neighborhood with n_1 observations z, possible cross-validation estimators will be considered.

Let

z_j = observed value of Z_j at site j

and

$\hat{z}_j$ = predicted value of Z at site j for a given value of α.

Note that this predicted value must be determined from the data set which excludes the actual observation at site j, so it is a cross-validation estimate. For a given value of α

$E_j = Z_j - \hat{Z}_j$ for j = 1 to n.

can be defined. The choice of an estimator for α, based on the cross-validated residuals, is difficult to justify on the grounds of a single criterion in all situations. Among the desirable criteria to consider are the following:

(1) minimum $\sum E_j^2$,
(2) minimum inter-quartile range (E_j),
(3) minimum inter-decile range (E_j), and
(4) minimum rank mean (E_j).

For example, to define (4), suppose that for each site j E_j is evaluated for L values of α ($\alpha = a_1, a_2, \ldots\ldots, a_L$), i.e., $E_j(a_1), \ldots\ldots, E_j(a_L)$. Rank the absolute values of the $E_j(a_i)$ and then calculate the means of these ranks.

DISCUSSION AND CONCLUSIONS

There has been a considerable upsurge of interest in spatial statistics in soil science over the past decade. This reflects a growing need by the scientific community to take into account the non-random

nature of the distributions of variables measured at different locations. One tool which can meet many of these needs is kriging. It is imperative, however, that the entire process of model building should be seen as a whole. One aspect of the statistical model is the mean structure and the other the covariance structure. In the opinion of the authors there has been an over-emphasis on estimation of the latter. This has led to a number of studies which dealt solely with semi-variograms.

In this bulletin an attempt has been made to focus attention on the predictive part of the process. How to fit a model, how to validate it, and how to portray the results. Another aspect of the publication deals with the theoretical explanation from a least-squares point of view, because this is familiar to the authors.

APPENDIX I
DEFINITIONS AND NOTATION

DRIFT MODEL

The mean value of a spatial variate Z at some location identifed by coordinates (x,y) may be written as mean(Z) = $\mu(x,y)$. This is the drift model. Typical examples are:

Mean(Z) = β_0 (stationary model),

Mean(Z) = $\beta_0 + \beta_1 x + \beta_2 y$ (linear drift model),

Mean(Z) = $\beta_0 + \beta_1 x + \beta_2 y + \beta_{11} x^2 + \beta_{22} y^2 + \beta_{12} xy$,
(quadratic drift model)

where β_0, β_1, β_2, ...are unknown parameters, denoted by the vector $\underline{\beta}$.

DESIGN MATRIX

This matrix, denoted by D, contains the coefficients of the drift model for all sample points. If the drift model is stationary, D consists of a single column of ones (m = 1). If the drift model is linear, the i^{th} row of D would contain the following 3 (m = 3) elements:
$\{1, x_i, y_i\}$.

If the drift model is quadratic, the i^{th} row of D would contain the following 6 (m = 6) elements:
$\{1, x_i, y_i, x_i^2, y_i^2, x_i\, y_i\}$.

The mean vector of Z is thus denoted as $\underline{\mu} = D\underline{\beta}$.

MOVING NEIGHBORHOOD

In the kriging procedure, when a prediction is required at coordinates (x*,y*), this prediction is made (using kriging or co-kriging), based on the nearest ng sample points to the given point. This subset of ng points defines the neighborhood of the given point. As kriging pro-

ceeds to predict from one point to another, the neighborhood "moves." This procedure is analogous to the "windows" used in calculating moving averages in one dimensional time series.

NEIGHBORHOOD SIZE

Given some point with coordinates (x*,y*) we define a "neighborhood" of that point as the smallest subset of all observations $Z_i, i = 1$ to n, such that:

(1) it contains at least the closest ng observations, and

(2) the distance from (x*,y*) to the most distant member is at least dg.

In most applications it is safe to set dg = 0, so that neighborhoods depend on numbers of members only. A reasonable value for ng is 12 to 15.

PREDICTED VALUE

The BLUE of Z, namely the "kriged" estimate is given in equation 3 (page 5) which is repeated here:

$$\hat{Z}_2 = \underline{d}_2' \hat{\underline{\beta}} + \underline{v}_{12}' V_{11}^{-1} (\underline{z}_1 - D_1 \hat{\underline{\beta}})$$

$$\hat{\underline{\beta}} = (D_1' V_{11}^{-1} D_1)^{-1} D_1' V_{11}^{-1} \underline{z}_1$$

PREDICTION STANDARD ERROR

If $\hat{Z}_i$ denotes the predicted values of Z at location i (either predicted by kriging or co-kriging), and if Z_i is the true unknown value of Z at this point, then the prediction SE is our estimate of:

$(\text{Variance } (Z_i - \hat{Z}_i))^{1/2}$.

The prediction standard error is a measure of the reliability of the prediction and can be used in tests of significance and probability statements. It is estimated by the following procedure: Since $\hat{Z}_i$ is a linear function of the observations $\underline{z}$, we may write it as:

$$\hat{Z}_i = \underline{c}'\underline{z} ,$$

and it may be verified that

$$\underline{c}' = ((\underline{d}_2' - \underline{v}_{12}' V_{11}^{-1} D_1) H D_1' + \underline{v}_{12}') V_{11}^{-1} ,$$

where

$$H = (D_1' V_{11}^{-1} D_1)^{-1}.$$

Hence it follows that:

$$\text{Var } (Z_i - \hat{Z}_i) = \sigma^2 (1 - 2\underline{v}_{12}' \underline{c} + \underline{c}' V_{11} \underline{c}).$$

To get the prediction SE, σ^2 must be estimated and the best quadratic estimate is given by:

$$\sigma^2 = \underline{e}' V_{11}^{-1} \underline{e} / (ng - m)$$

where: $\underline{e} = \underline{Z} - D\underline{\beta}$.

NEIGHBORHOOD VARIANCE

This quantity, referred to as σ^2 above, measures the conditional variance at any point about the local mean. Within a given neighborhood we expect it to be constant at all points. However, variation from one neighborhood to another is expected.

LOCAL MEAN AND LOCAL SD

In a given neighborhood, the mean value of Z at the point (x*,y*), as defined by the drift model, is called the local mean. Within the entire given neighborhood, a constant conditional variance is assumed, being that variance of the variate Z about its local mean. The local SD is the square root of this variance. Naturally, the local mean and local SD may vary from one moving neighborhood to another. In other words, at any point (x*,y*) there is a corresponding row $d^{*\prime}$ of the design matrix. For example, if (x*,y*) = (4,5) and we fit a linear drift model, then: $\underline{d}^{*\prime} = \{1\ 4\ 5\}$ and the local mean at this point is given by $\mu = \underline{d}^{*\prime} \beta$. Thus, e.g., if the mean model exhibits linear drift, all means in the neighborhood lie on the same plane. In the absence of spatial correlation, the local mean estimate and the kriged estimate coincide.

COVARIANCE MODEL

Given a random variable Z_i at location (x_i,y_i) and another Z_j, at location (x_j,y_j), and if d_{ij} is the Euclidean distance between these two locations, we might propose a model to describe the covariance of Z_i and Z_j as a function of d_{ij} only. This is a simple covariance model (said to be anisotropic).

SPHERICAL COVARIANCE MODEL

If $\text{cov}(Z_i,Z_j) = 1 - 0.5(d_{ij}/\alpha) + 1.5(d_{ij}/\alpha)^3$ for $d_{ij} \leq \alpha$ and zero otherwise, this is the spherical covariance model and the parameter α is called the "range."

PROBABILITY STATEMENTS

On the assumption of normality, the probability that a value of Z at (x*,y*) should exceed some given quantity G, may be estimated by:

$$\Phi\ ((G - \hat{\mu}) / \hat{\sigma})\ ,$$

where Φ denotes the cumulative standardized normal distribution.

$\underline{x}$ $\underline{y}$ $\underline{z}$
The three columns of (x,y)-coordinates and observed values z of the variable of primary interest (each of length n).

n
The number of observed points for the variable of primary interest.

d
The design matrix for the variable of primary interest (of dimension n x m).

m
The number of columns of the design matrix D.

ng
The number of points in each moving neighborhood.

k
The smoothing parameter for kriging. When $k = 0$ the predictions exactly honor the observations. When $k = 1$, maximum smoothing takes place and a predicted value equals the local mean. Note $0 \leq k \leq 1$.

a
The value of the range parameter in the spherical covariance model.

$\underline{x}^*$ $\underline{y}^*$
The (x,y) coordinates for the prediction points, $\underline{\hat{z}}$.

z
The column of kriged or co-kriged predicted values with i^{th} member $\hat{z}_i$.

D*
The design matrix for the prediction points.

as,ad,an
When running program AX, as = starting value for the range parameter, ad = increment by which the value of the range parameter is increased in the sequence; an = total number of values of the range parameter to be tried in sequence.

$\underline{\hat{z}}_c$
The column of cross-validated predicted values. Thus $\hat{z}_{ci}$ is the predicted value at location i when the observed value z_i is itself deleted from the observations.

E
The n x an matrix of cross-validated residuals from program AX. Thus if the current trial value of the range parameter is a_j and this results in a predicted value $\underline{\hat{z}}_{ci}$ for location i during cross-validations, then $e_{ij} = z_{ij} - \underline{\hat{z}}_{ci}$.

$\underline{e}$
The single column of cross-validated residuals produced by fitting a

single specified model by kriging or co-kriging. Note that if program AX was used to fit a single value of the range parameter only, then the matrix E reduces to this single column vector.

$\underline{x}_b\underline{y}_b\underline{z}_b$
The (x,y)-coordinates and observed values of the covariate used in co-kriging.

$\mathbf{d}_b$
The design matrix for the covariate points.

$\mathbf{a}_b$
The value of the range parameter for the covariate.

$\mathbf{m}_b$
The number of columns in the covariate design matrix.

$\mathbf{ng}_b$
The number of points in each moving neighborhood for the covariate.

σ^2
The average local variance for the primary variate.

σ_b^2
The average local variance for the covariate.

ρ
The correlation between primary variate and covariate.

APPENDIX II
COMPUTER PROGRAMS[7]
INTRODUCTION AND GENERAL DESCRIPTION

The suite of computer programs presented in this APPENDIX has been written to carry out point kriging, incorporating non-stationary means (universal kriging), and co-kriging. In addition, there is a program SAM, which searches for the optimal locations of sample sites. The language used is GAUSS. All programs, and files as used in the examples, are stored on the diskette. Model fitting is done by cross-validation.

The programs are not intended to be used as prescriptions, but require interaction and understanding from the user. It is to be expected that a user will interface analyses available here with software from other sources. For example, to use the kriging program KRIG, the user must supply details of his/her chosen drift model and covariance parameter. Although these details can be found using program AX, some people might prefer to use a more conventional procedure based on variograms.

[7]Copies of the computer programs and the data sets as used in this bulletin will be provided on a floppy disk upon request from J.H. Dane, Department of Agronomy and Soils, Auburn University, Auburn, Ala. 36849-5412.

Likewise, once the program KRIG has produced a grid of predicted values, the graphing of contours can be accomplished with any of the user's favorite graphical packages. No graphics procedures are given here. Perhaps a user may be interested in testing a model produced from some other source. The program CROSSK can be used to validate such a model.

Although users of these programs need not have knowledge of GAUSS, such knowledge makes the file manipulation and rearrangement of data infinitely easier and is strongly recommended.

MODEL LIMITATIONS

Any drift model which is linear in its unknown parameters can be fitted. Examples are quadratic drift and multiple regression on any co-variates whose values are known at the prediction points. Where the covariate values have themselves to be estimated at the prediction points, it becomes a co-kriging problem. The only covariance model which is fitted is the spherical model. This model is expanded to handle co-kriging without introducing extra parameters.

PROGRAM DESCRIPTIONS

There are six main programs, which together with supporting procedures, are stored in a library called SPATIAL. Descriptions of each program are given in Appendix tables 1 and 2.

The programs all require input to have been stored previously in files with designated names and output is placed in named files.

Example

Water and clay content were recorded at 60 locations in a rectangular field of 50 m X 100 m. Appendix figure 1 shows the layout of the sample points and Appendix table 3 gives the raw data with their (x,y)-coordinates. The purpose of the analysis is to produce a contour map of predicted water content values. Both kriging and co-kriging will be used. The sequence of analytic steps is shown in Appendix figure 2. A detailed description now follows. Note that all the input files needed to run the examples are stored on diskette. Appendix table 4 lists their file names.

Developing and Using a Kriging Model for Water Content

Using Program AX to Find the Best Water Model

When fitting a model to spatial data there are two aspects to consider jointly. First, what model fits the drift or mean and second, what model fits the covariance structure. We adopted the simplifying stand

Appendix Table 1. Description of computer programs for kriging.

Name:	AX	KRIG	CROSSK
Purpose:	To evaluate a sequence of values for the range parameter, a, given a specific drift model. Cross-validation is used to define various "goodness-of-fit" statistics for each value of α.	To calculate predicted values by universal kriging, given the range parameter α and a specific drift model. Moving neighborhoods may be used.	To produce cross-validated predicted values based on universal kriging.
Preparatory steps:	1. Store as, ad, an, ng, m in the file TEMP__PAR. 2. Store [x y z D] in the file TEMP__AIN.	1. STORE a, ng, m, k in the file TEMP__PAR. 2. Store [x y z D] in the file TEMP__AIN. 3. Store [x* y* D*] in the file TEMP__COR.	1. Store a, ng, m, k in the file TEMP__PAR. 2. Store [x y z D] in the file TEMP__AIN.
Execution:	Run AX.	Run KRIG.	Run CROSSK.
Output:	On the file TEMP__OUT: 1. The matrix E = $\{e_{ij}\}$, i = 1, n and j = 1, an, consists of cross-validation residuals. 2. The "goodness-of-fit" statistics: rank means, mean sum of squared deviations, mean absolute deviations, inter-quartile range, inter-decile range.	On the file TEMP__OUT: For each prediction point (x*, y*), the predicted value, $\hat{Z}$, the prediction SE, the local conditional SD, and the local mean.	On the file TEMP—OUT: For each observation point (x,y), the cross-validation predicted value Z_{CA}, the prediction SE, the local SD, the local mean.

Appendix Table 2. Description of computer program for co-kriging and optimal sampling.

Name:	COK	CROSSC	SAM
Purpose:	To calculate predicted values by co-kriging. Any form of drift models may be specified for the primary and co-variates. The two variates need not have the same drift or co-variance models.	To produce cross-validated predicted values based on co-kriging.	To find an optimal subset of the sample points from a given larger set of potential sample points. A co-kriging model is used and therefore a set of covariates is required.
Preparatory steps:	1. Store a, a_b, ρ,σ^2, σ_b^2,m,m_b,ng,ng_b, k in the file TEMP__PAR.	1. Store a, a_b,ρ ,σ^2, σ_b^2,m,m_b,ng,ng_b, k in the file TEMP__PAR.	1. STORE a, a_b,ρ,σ^2, σ_b^2,m,m_b,ng,ng_b, maxout, in the file TEMP__PAR.
	2. Store [$\underline{x}$ $\underline{y}$ $\underline{z}$ D] in the file TEMP__AIN.	2. Store [$\underline{x}$ $\underline{y}$ $\underline{z}$ D] in the file TEMP__AIN.	2. Store [$\underline{x}$ $\underline{y}$ D] where, these entries refer to potential sample points, TEMP__AIN.
	3. Store [$\underline{x}_b$ $\underline{y}_b$ $\underline{z}_b$ D_b] in the file TEMP-BIN.	3. Store [$\underline{x}_b$ $\underline{y}_b$ $\underline{z}_b$ D_b] in the file TEMP__BIN.	3. Store [$\underline{x}_b$ $\underline{y}_b$ $\underline{z}_b$ D_b] in the file TEMP__BIN.
	4. Store [$\underline{x}$* $\underline{y}$* D*] in the file TEMP__COR.		Store [$\underline{x}$* $\underline{y}$* D*], where the entries refer to the prediction points in file TEMP__COR.
Execution:	Run COK.	Run CROSSC.	Run SAM. Note that this puts the program into an inter-active mode and you will now have to respond to the question asking for a value for parameter ns.
Output:	On the file TEMP__OUT: For each prediction point (x*, y*), the predicted value (co-kriged), z, the prediction SE, the local conditional SD (for the primary variate), the local mean (for the primary variate).	On the file TEMP__OUT: For each observation point (x,y), the cross-validation predicted value z_c, the prediction SE, the local conditional SD, the local mean.	The sequence of points added to and subtracted from the optimal subset. The coordinates of the best subset with their average prediction SE's and those points discarded and also the prediction SE's for the prediction points.

Appendix Table 3. Water and clay content at 80 cm depth at 60 locations.

x m	y m	Water content cm^3/cm^3	Clay content %
0.00	0.00	0.220	15.4
6.25	0.00	0.235	19.2
12.50	0.00	0.243	17.6
18.75	0.00	0.225	17.7
25.00	0.00	0.243	17.4
37.50	0.00	0.241	17.7
10.93	3.12	0.203	13.4
17.18	3.12	0.232	18.4
23.43	3.12	0.229	17.3
29.68	3.12	0.240	17.1
6.25	6.25	0.230	18.1
34.37	6.25	0.258	19.4
17.18	9.37	0.246	21.5
12.50	12.50	0.249	20.7
25.00	12.50	0.262	25.0
7.81	15.62	0.243	19.5
3.12	18.75	0.243	21.5
4.60	21.87	0.265	19.4
0.00	25.00	0.255	19.2
12.50	25.00	0.270	22.0
18.75	25.00	0.274	24.0
25.00	25.00	**	29.0
31.25	25.00	0.261	23.0
37.50	25.00	0.256	22.5
4.68	28.12	0.236	15.3
10.93	28.12	0.276	21.4
3.12	31.25	0.280	26.6
9.37	37.50	0.301	29.9
12.50	27.50	0.295	28.0
25.00	37.50	0.278	24.8
3.12	43.75	0.296	28.9
31.25	43.75	0.242	**
7.81	46.87	0.294	24.7
14.06	46.87	0.287	27.0
20.31	46.87	0.290	27.6
0.00	50.00	0.266	24.2
12.50	50.00	0.306	32.0
25.00	50.00	0.268	26.0
31.25	50.00	0.274	20.7
37.50	50.00	0.238	24.4
7.81	53.12	0.302	25.5
14.06	53.12	0.313	26.8
3.12	56.25	0.299	26.0
18.75	56.25	0.269	23.6
21.87	56.25	0.307	32.9
12.50	62.50	0.291	22.8
15.62	62.50	0.293	24.3
10.93	65.62	0.267	22.0
3.12	68.75	0.292	28.2
18.75	68.75	0.302	25.6
21.87	68.75	0.289	22.7
34.37	68.75	0.234	16.0
1.56	71.87	0.286	20.7
7.81	71.87	0.303	23.5
14.06	71.87	0.299	26.5
29.68	71.87	0.285	29.5
0.00	75.00	0.295	26.9
12.50	5.00	0.305	25.7
25.00	75.00	0.280	20.1
37.50	75.00	0.255	19.8

**missing data

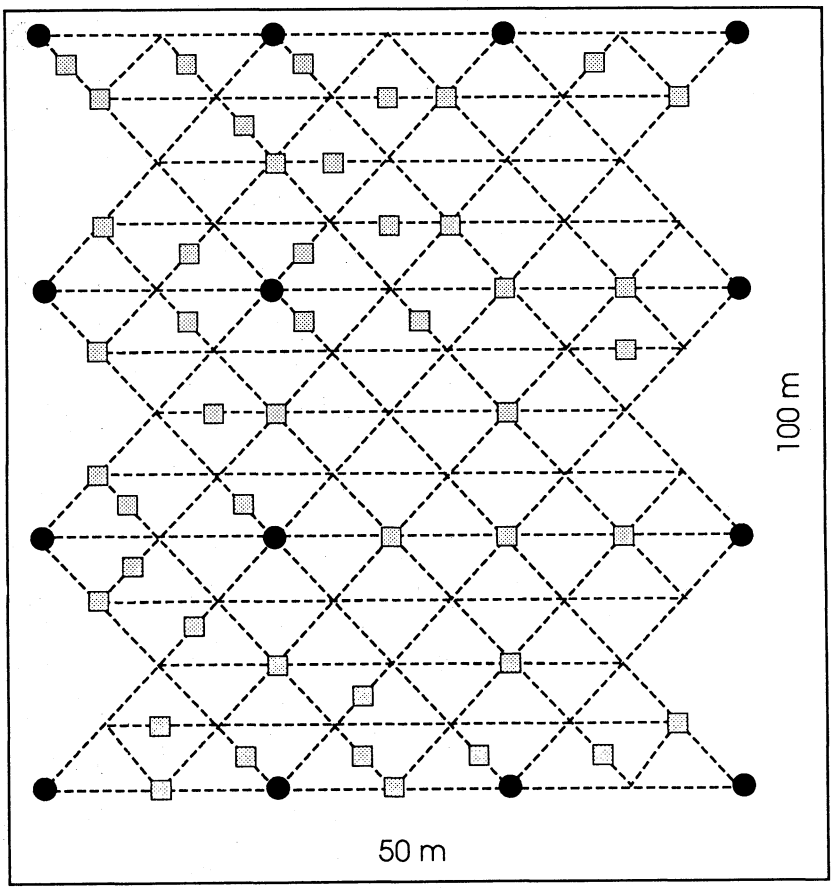
that the spatial correlations may be modelled by the spherical model with a single parameter, α, the range.

Program AX will be executed three times; first for a stationary drift, then for a linear drift and finally for a quadratic drift model. In each case, a range of values for α between 4 m and 13 m will be used, because this represents slightly more than the minimum distance between sample sites and the distance needed to ensure spanning a neighborhood of 20 points respectively.

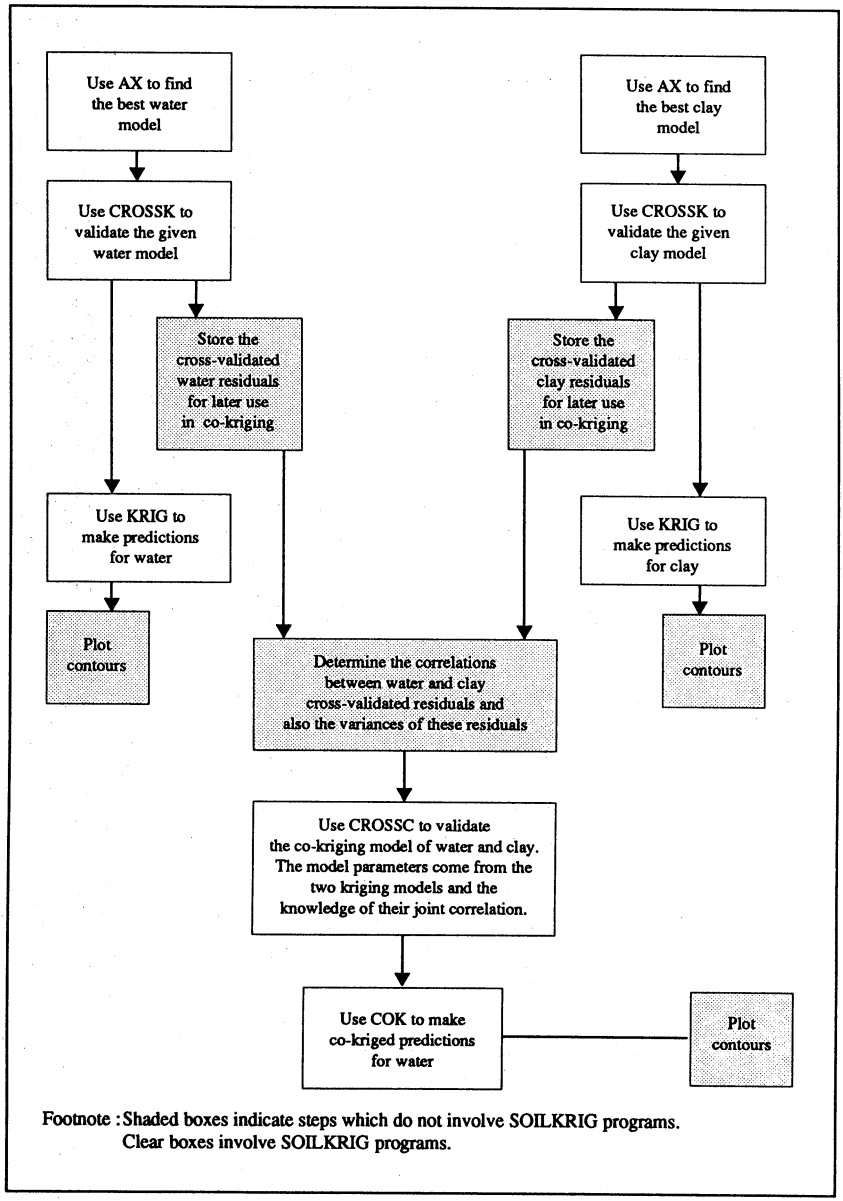
Fitting the Stationary Model

(1) Store 4 .5 19 20 0 on file TEMP_PAR.

Note that the first 3 numbers, as = 4, ad = .5, and an = 19,



APPENDIX FIGURE 1. Distribution of sample locations in the field. The circles and squares distinguish the two times that the field was sampled.



APPENDIX FIGURE 2. A schematic diagram to illustrate the steps in kriging water content and clay content, respectively, and co-kriging water with clay. Shaded boxes indicate steps which do not involive SOILKRIG programs. Clear boxes involve SOILKRIG programs.

Appendix Table 4. The location of input and output computer files used in or produced by the example.

Page	Type of Analysis	Input files TEMP_PAR	TEMP_AIN	TEMP_COR	Output files TEMP_OUT
		Location of Files on Diskette			
18	Using AX to fit a stationary drift model through the water content data.	WAT_PAR.1	WAT_AIN.1		WAT_OUT.1
21	Using AX to fit a linear drift model through the water content data.	WAT_PAR.2	WAT_AIN.2		WAT_OUT.2
21	Using AX to fit a quadratic drift model through the water content data.	WAT_PAR.3	WAT_AIN.3		WAT_OUT.3
24	Using Crossk to validate the linear drift model for the water data.	WAT_PAR.4	WAT_AIN.2		WAT_OUT.4
25	Using KRIG to predict water content.	WAT_PAR.4	WAT_AIN.2	WAT_COR.1	WAT_OUT.5
28	Using AX to fit a stationary model through the clay content data.	WAT_PAR.1	CLA_AIN.1		CLA_OUT.1
28	Using AX to fit a linear drift model through the clay content data.	WAT_PAR.2	CLA_AIN.2		CLA_OUT.2
28	Using AX to fit a quadratic drift model through the clay content data.	WAT_PAR.3	CLA_AIN.3		CLA_OUT.3
32	Using CROSSK to validate the linear drift model for the clay data.	CLA_PAR.4	CLA_AIN.2		CLA_OUT.4
32	Using KRIG to predict clay content.	CLA_PAR.4	CLA_AIN.2	WAT_COR.1	CLA_OUT.5
		Required input files	Location		
33	Using COK to predict water content.	TEMP_COR	WAT_COR.1		WC_OUT.2
35	Using CROSSC to validate the co-kriging model.	TEMP_PAR	WC_PAR.1		WC_OUT.1
		TEMP_AIN	WAT_AIN.2		
		TEMP_BIN	CLA_AIN.2		
35	Using SAM to optimize sampling.	TEMP_PAR	SAM_PAR.1		SAM_OUT.1
		TEMP_AIN	SAM_AIN.1		
		TEMP_BIN	CLA_AIN.2		
		TEMP_COR	SAM_COR.1		

define the range of values for α, and the next two numbers, ng = 20 and m = 0, specify the neighborhood size (a good default value) and a stationary model, respectively.

(2) Store the matrix of values [x y z], where z represents water content, on file TEMP__AIN. There is no need to include a design matrix since the model is stationary.

(3) Run the program by entering: RUN AX. When the execution is complete, examine the output on file TEMP__OUT. We postpone discussion of the output until all three drift models have been fitted.

Fitting the Linear Drift Model

(1) Amend the parameter values in file TEMP__PAR by changing the value of m from 0 to 3, because the design matrix will now contain 3 columns.

(2) Store the array [x y z D] on file TEMP__AIN. Appendix table 5 contains a partial listing of this required input. Note that in the GAUSS language we would simply calculate.

$$S = x\sim y\sim z\sim \text{ones}(n,1)\sim x\sim y$$

and store S in TEMP__AIN.

(3) Run the program by entering: RUN AX. The output is filed on the data file TEMP__OUT.

Fitting the Quadratic Drift Model

(1) Change the value of m to 6 in TEMP__PAR.

(2) Calculate the elements of the quadratic design matrix D and store [x y z D] on file TEMP__AIN. Note that the GAUSS language command is

$$S=S\sim(x.*x)\sim(y.*y)\sim(x.*y)$$

assuming the old array S is retrieved first. This is now stored on TEMP__AIN.

(3) Run the program by entering: RUN AX. The output is filed on data file TEMP__OUT.

Interpreting the Output

There are two parts to the output from program AX. The first part comprises the matrix of cross-validated residuals

$$E = \{e_{ij}\},\ i = 1 \text{ to } 59\ ,\ j = 1 \text{ to } 19$$

where e_{ij} = the residual value for location i using the jth α-value.

This matrix may be useful for extra analysis; for example in graphical representation.

The second part gives measures of spread for the residual values, calculated separately for each α-value. The program AX calculates the following specific measures of goodness of fit for each of the 19 values for α considered:

(1) Rank means.

For each row of E, allocate a rank to each column element, thereby generating a n x p matrix R of ranks. Calculate the column means.

Appendix Table 5. The input file TEMP__AIN required for fitting a linear drift model to water data.

x m	y m	water content cm^3/cm^3		x m	y m
0.000	0.000	0.221	1.000	000.000	000.000
6.250	0.000	0.235	1.000	12.500	000.000
12.500	0.000	0.243	1.000	12.500	000.000
18.750	0.000	0.225	1.000	18.750	000.000
25.000	0.000	0.244	1.000	25.000	000.000
37.500	0.000	0.241	1.000	37.500	000.000
10.938	2.125	0.204	1.000	10.938	3.125
17.188	3.125	0.233	1.000	17.188	3.125
23.438	3.125	0.229	1.000	23.438	3.125
29.688	3.125	0.240	1.000	29.688	3.125
6.250	6.250	0.230	1.000	6.250	6.250
34.375	6.250	0.259	1.000	34.375	6.250
17.188	9.375	0.246	1.000	17.188	9.375
12.500	12.500	0.250	1.000	12.500	12.500
25.000	12.500	0.262	1.000	25.000	12.500
7.813	15.625	0.243	1.000	7.813	15.625
3.125	18.750	0.243	1.000	3.120	18.750
4.688	21.875	0.266	1.000	4.688	21.875
0.000	25.000	0.256	1.000	0.000	25.000
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
14.063	53.125	0.314	1.000	14.063	53.125
3.125	56.250	0.299	1.000	3.125	56.250
18.750	56.250	0.269	1.000	18.750	56.250
21.875	56.250	0.308	1.000	21.875	56.250
12.500	62.500	0.291	1.000	12.500	62.500
15.625	62.500	0.294	1.000	15.625	62.500
10.938	65.625	0.267	1.000	10.938	65.625
3.125	68.750	0.292	1.000	3.125	68.750
18.750	68.750	0.302	1.000	18.750	68.750
21.875	68.750	0.289	1.000	21.875	68.750
34.375	68.750	0.234	1.000	34.375	68.750
1.563	71.875	0.287	1.000	1.563	71.875
7.813	71.785	0.303	1.000	7.813	71.875
14.063	71.875	0.300	1.000	14.063	71.875
29.688	71.875	0.286	1.000	29.688	71.875
0.000	75.000	0.296	1.000	0.000	75.000
12.500	75.000	0.305	1.000	12.500	75.000
25.000	75.000	0.280	1.000	25.000	75.000
37.500	75.000	0.255	1.000	37.500	75.000

The remaining measures are standard, and each is calculated on every column of E separately:

(2) Mean sum of squares.

(3) Mean absolute value.

(4) Inter-quartile range (IQR).

This is the difference between the 25th and 75th percentile.

(5) Inter-decile range (IDR).

This is the difference between the 90th and 10th percentile.

Output data for the different measures of goodness of fit (second part of program AX) are presented in Appendix table 6 when fitting a linear model. Observe from this table that an α-value between 6

Appendix Table 6. Output of program AX when fitting a linear drift model to water content.

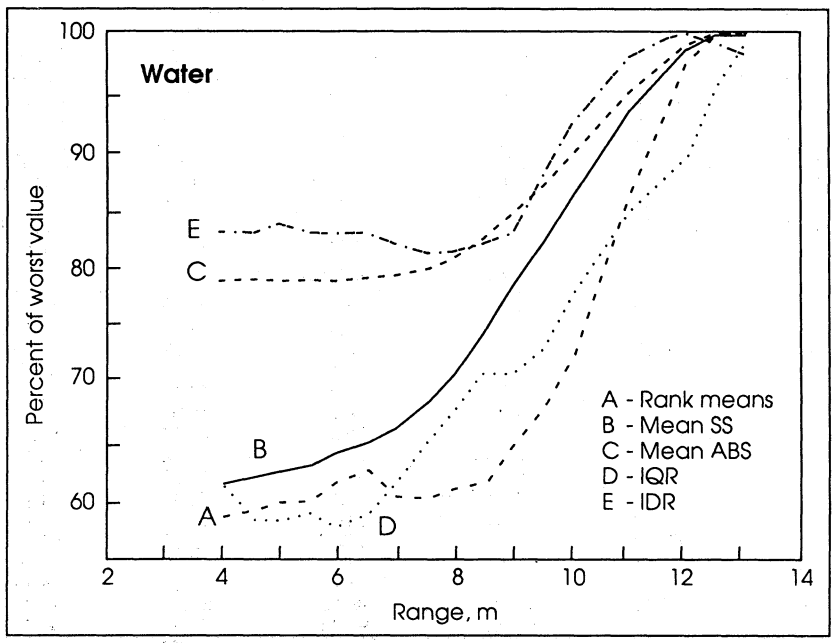
α m	Rank means	Mean SS(resid) $(cm^3/cm^3)^2$	Mean Abs(resid) cm^3/cm^3	I.Q.R. cm^3/cm^3	I.D.R. cm^3/cm^3
4.0	8.20339	0.00020	0.01163	0.01514	0.03749
4.5	8.25424	0.00020	0.01160	0.01439	0.03741
5.0	8.37288	0.00021	0.01161	0.01436	0.03779
5.5	8.37288	0.00021	0.01164	0.01450	0.03747
6.0	8.57627	0.00021	0.01165	0.01415	0.03748
6.5	8.71186	0.00021	0.01166	0.01439	0.03739
7.0	8.44068	0.00022	0.01169	0.01504	0.03697
7.5	8.40678	0.00022	0.01178	0.01597	0.03666
8.0	8.50847	0.00023	0.01192	0.01665	0.03670
8.5	8.57627	0.00024	0.01215	0.01729	0.03698
9.0	8.98305	0.00026	0.01249	0.01732	0.3760
9.5	9.42373	0.00027	0.01286	0.01783	0.03972
10.0	10.11864	0.00028	0.01325	0.01891	0.04163
10.5	10.98305	0.00029	0.01362	0.01992	0.04312
11.0	11.91525	0.00031	0.01401	0.02076	0.04420
11.5	12.79661	0.00032	0.01438	0.02125	0.04491
12.0	13.52542	0.00032	0.01464	0.02182	0.04527
12.5	13.89831	0.00033	0.01477	0.02320	0.04484
13.0	13.93220	0.00033	0.01480	0.02454	0.04421
		Percentage of worst value			
4.0	58.88	61.63	78.57	61.69	82.81
4.5	59.25	61.91	78.41	58.63	82.63
5.0	60.10	62.40	78.47	58.52	83.49
5.5	60.10	63.07	78.62	59.11	82.76
6.0	61.56	63.89	78.73	57.66	82.80
6.5	62.53	64.94	78.82	58.65	82.59
7.0	60.58	66.35	79.02	61.29	81.66
7.5	60.34	68.24	79.60	65.08	80.98
8.0	61.07	70.76	80.56	67.87	81.07
8.5	61.56	74.00	82.11	70.46	81.69
9.0	64.84	77.86	84.36	70.59	83.06
9.5	67.64	81.91	86.87	72.67	87.75
10.0	72.63	85.85	89.53	77.07	91.96
10.5	78.83	89.53	92.05	81.19	95.26
11.0	85.52	93.01	94.70	84.62	97.63
11.5	91.85	96.26	97.18	86.61	99.21
12.0	97.08	98.61	98.91	88.84	100.00
12.5	99.76	99.85	99.82	94.54	99.05
13.0	100.00	100.00	100.00	100.00	97.66

and 8.5 will optimize the IQR and IDR, which are preferred measures of spread, since they are relatively robust to outliers.

In order to compare all three drift models simultaneously, the three outputs from program AX must be examined. Appendix table 7 summarizes the results for the mean sum of squared deviations and interquartile range. The linear drift model is clearly superior to the other two. Given the linear drift model, a reasonable compromise value for α is 6.0. Appendix figure 3 gives a graphical description of variations in measures of spread for different α-values. This confirms a value for α of 6.0 as being reasonable. It is noteworthy that no single choice of parameter values is best by every criterion.

Using Program CROSSK to Validate the Given Water Model

When a tentative model to describe spatial interdependency has been adopted (e.g. by using the program AX), it can be more thoroughly examined by the use of cross-validation. The process of cross-validation for validating any given model is no different from the procedure used by program AX in the search for a best model. The only real advantage from running program CROSSK in this example is to obtain a more detailed output. Program CROSSK uses a specified model and



APPENDIX FIGURE 3. Measures of deviation (as % of worst value) of cross-validated residuals using a linear drift model on soil water content.

Appendix Table 7. Measures of deviation of cross-validated residuals for three different drift models on water content.

α	Sum of squared deviations			Inter-quartile range		
m	$(cm^3/cm^3)^2$			(cm^3/cm^3)		
	S	L	Q	S	L	Q
4.0	0.0176	0.0120	0.0132	0.0219	0.0151	0.0182
4.5	0.0175	0.0120	0.0135	0.0207	0.0144	0.0183
5.0	0.0173	0.0121	0.0137	0.0203	0.0144	0.0184
5.5	0.0172	0.0122	0.0141	0.0207	0.0145	0.0185
6.0	0.0171	0.0124	0.0145	0.0211	0.0141	0.0184
6.5	0.0169	0.0126	0.0149	0.0220	0.0144	0.0181
7.0	0.0169	0.0129	0.0155	0.0215	0.0150	0.0175
7.5	0.0169	0.0132	0.0160	0.0197	0.0160	0.0178
8.0	0.0171	0.0137	0.0167	0.0192	0.0167	0.0192
8.5	0.0175	0.0143	0.0175	0.0191	0.0173	0.0199
9.0	0.0181	0.0151	0.0184	0.0192	0.0173	0.0206
9.5	0.0187	0.0159	0.0194	0.0189	0.0178	0.0217
10.0	0.0194	0.0166	0.0202	0.0195	0.0189	0.0226
10.5	0.0199	0.0173	0.0210	0.0201	0.0199	0.0233
11.0	0.0205	0.0181	0.0218	0.0211	0.0208	0.0236
11.5	0.0211	0.0186	0.0225	0.0227	0.0212	0.0241
12.0	0.0214	0.0191	0.0230	0.0242	0.0218	0.0245
12.5	0.0216	0.0194	0.0232	0.0251	0.0232	0.0247
13.0	0.0215	0.0194	0.0231	0.0256	0.0245	0.0242

S = stationary drift model, L = linear drift model, Q = quadratic drift model.

makes cross-validation predictions at each observed point. Output of the observed values (Z), the predicted values ($\hat{Z}$), the prediction standard errors, the local means and the local standard deviations may be useful in the following ways:

(1) To test for suitability of the model and detection of outliers. The ratio of $(Z - \hat{Z})$ /(prediction SE), at any point, should follow the t-distribution. Any values in excess of about 3 can be seriously considered as outliers.

(2) To find an estimate of the average local variances (actually conditional variances) to be used in a subsequent co-kriging program.

Assuming a linear drift model with $\alpha = 6$, we proceed as follows:

(1) Store 6 20 3 0 in file TEMP_PAR. Note that this sequence of values assigns $\alpha = 6$, ng = 20 (the neighborhood size adopted in all previous analyses), m = 3 (because we are fitting a linear drift model), and k = 0 (because we require predictions to "honor" the observations).

(2) Store [x y z D] in TEMP_AIN. Note that these are exactly the same values as those used in program AX with the linear drift model.

(3) Run program CROSSK and examine file TEMP_OUT for the output. Part of this output is shown in Appendix table 8. The cross-validated residuals should be stored for later use in co-kriging.

Using Program KRIG to Predict Water Content Values

Given a set of spatially oriented data, categorized by coordinates

Appendix Table 8. Output for cross-validation of linear drift model for water content, with parameter values $\alpha = 6$, ng = 20, m = 3, and k = 0.

x	y	z	$\hat{z}$	prediction SE	local SD	local mean
m	m			cm^3/cm^3		
0.000	0.000	0.221	0.216	0.0155	0.0128	0.216
6.250	0.000	0.235	0.220	0.0137	0.0123	0.220
12.500	0.000	0.243	0.219	0.0094	0.0093	0.224
18.750	000	0.225	0.232	0.0117	0.0115	0.232
25.000	00	0.244	0.232	0.0120	0.0118	0.234
37.500	00	0.241	0.239	0.0144	0.0122	0.239
10.938	3.125	0.204	0.236	0.0076	0.0076	0.233
17.188	3.125	0.233	0.234	0.0109	0.0109	0.235
23.438	3.125	0.229	0.241	0.0117	0.0117	0.239
29.688	3.125	0.240	0.242	0.0129	0.0121	0.242
6.250	6.250	0.230	0.232	0.0136	0.0128	0.232
34.375	6.250	0.259	0.243	0.0129	0.0117	0.243
17.188	9.375	0.246	0.245	0.0121	0.0118	0.245
12.500	12.500	0.250	0.245	0.0131	0.0128	0.245
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
14.063	53.125	0.314	0.294	0.0149	0.0150	0.290
3.125	56.250	0.299	0.290	0.0150	0.0141	0.290
18.750	56.250	0.269	0.293	0.0144	0.0148	0.286
21.875	56.250	0.308	0.273	0.0149	0.0153	0.277
12.500	62.500	0.291	0.288	0.0133	0.0142	0.293
15.625	62.500	0.294	0.293	0.0138	0.0142	0.292
10.938	65.625	0.267	0.294	0.0134	0.0135	0.294
3.125	68.750	0.292	0.290	0.0154	0.0149	0.292
18.750	68.750	0.302	0.286	0.0162	0.0166	0.283
21.875	68.750	0.289	0.285	0.0166	0.0170	0.280
34.375	68.750	0.234	0.263	0.0176	0.0159	0.263
1.563	71.875	0.287	0.293	0.0147	0.0149	0.293
7.813	71.875	0.303	0.290	0.0158	0.0147	0.290
14.063	71.875	0.300	0.291	0.0166	0.0166	0.287
29.688	71.875	0.286	0.264	0.0180	0.0166	0.264
0.000	75.000	0.296	0.289	0.0167	0.0149	0.290
12.500	75.000	0.305	0.289	0.0168	0.0163	0.286
25.000	75.000	0.280	0.274	0.0184	0.0170	0.274
37.500	75.000	0.255	0.256	0.0220	0.0179	0.256

$\underline{x}$, $\underline{y}$ and variate values $\underline{z}$, values of Z will be predicted at points not necessarily covered by the original data. Best linear unbiased estimates are obtained by the procedure known as kriging.

The background to the theory is given in an earlier section (page 4,5). The program implements this theory for any given mean model and co-variance parameter α. In addition, it requires specification of neighborhood size. Note the following necessary inequalities.

$$n \geq ng \geq m + 1.$$

The program works by choosing a subset of the data, namely points in the neighborhood of the prediction point (x*,y*), and then making predictions from this neighborhood. Each time the prediction point changes, a new neighborhood is defined and the process repeated. It may happen that two neighborhoods coincide, but the program does not take advantage of this possibility.

It should be noted that, when a prediction point coincides with an observed point, the kriged prediction value equals the observed value. If smoother plots are required, which can be justified on the grounds of the presence of a "nugget" variance, the smoothing parameter, k, can be set non-zero, but now the kriged and observed values differ.

Assume that prediction of water content values at 400 regularly spaced points on a grid covering the entire field is desired. This can be accomplished as follows:

(1) Store 6 20 3 0 in file TEMP__PAR. Note that a = 6, ng = 20, m = 3, and k = 0 are exactly the same values as those used in the earlier program CROSSK.

(2) Store [$\underline{x}$ $\underline{y}$ $\underline{z}$ D] in file TEMP__AIN. Note that these also are exactly the same values as those stored in this file for both earlier programs.

(3) Store the array [$\underline{x}$* $\underline{y}$* D*], made up of the 400 prediction coordinates and corresponding design matrix, on the file TEMP__COR.

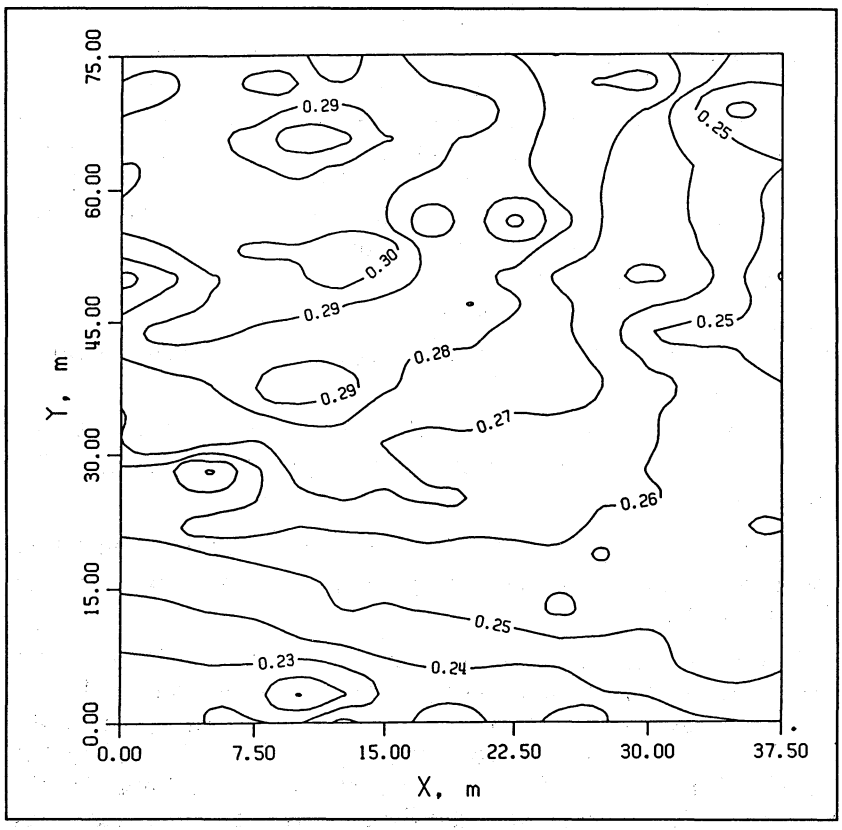
4) Run the program KRIG and examine the file TEMP__OUT for the output. Appendix table 9 lists part of this output. One would normally use this output to create a contour plot, for example by using a package such as PLOT88 (Plotworks, Inc., La Jolla, CA 92037-0635). Appendix figure 4 gives such a graphical display for the predicted values, while Appendix figure 5 gives a similar display of the prediction standard errors.

Developing and Using a Kriging Model for Clay Content

The reason for developing a kriging model for clay is that such a model is needed later in the co-kriging of water content. The percentage clay at 80 cm was chosen as the variable of interest since it is closely correlated with water content and is a physical property of the soil which hardly changes over time.

Using Program AX to Find the Best Clay Model

The sequence of models, namely the stationary, linear and quadratic drift model, with α varying in value from 4 m to 13 m, was fitted to determine the best value for α. Appendix table 10 shows part of the output from the fitting of a linear drift model. The same results are depicted graphically in Appendix figure 6. From these results, depending heavily on the inter-quartile range, we chose a value for



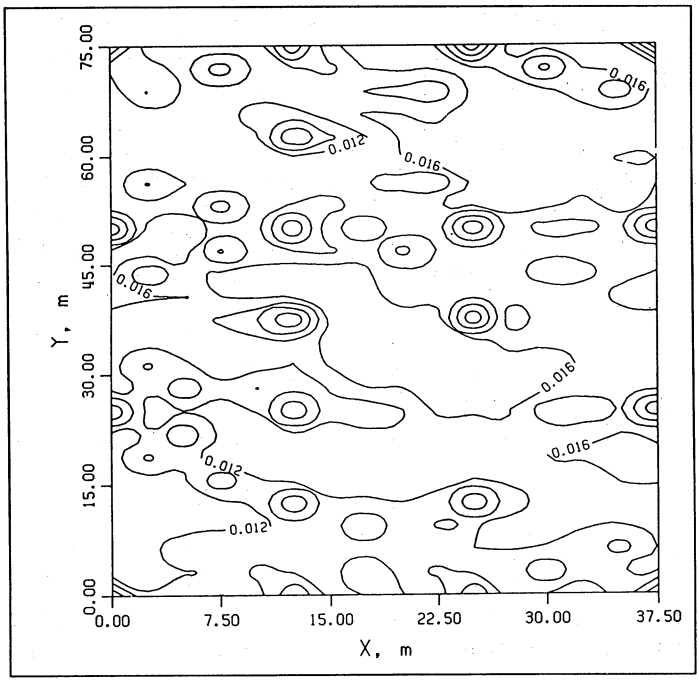
APPENDIX FIGURE 4. Kriging estimates of soil water content using a linear drift model.

Appendix Table 9. Kriging estimates of water content using a linear drift model, with parameter values $\alpha = 6$, ng = 20, m = 3, and k = 0.

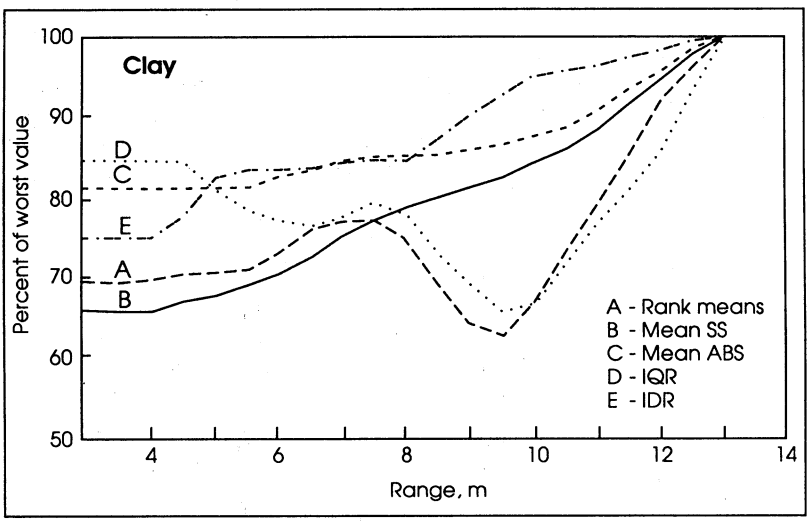
x	y	$\hat{z}$	prediction SE	local conditional SD	local mean
m	m			cm^3/cm^3	
0.000	0.000	0.221	0.00000	0.01271	0.219
0.000	3.215	0.223	0.01404	0.01366	0.222
0.000	6.250	0.227	0.01528	0.01366	0.227
0.000	9.375	0.232	0.01478	0.01346	0.232
0.000	12.500	0.237	0.01466	0.01346	0.237
0.000	15.625	0.242	0.01482	0.01370	0.242
0.000	18.750	0.245	0.01389	0.01365	0.248
0.000	21.875	0.252	0.01349	0.01365	0.253
0.000	25.000	0.256	0.00000	0.01452	0.253
0.000	28.125	0.258	0.01269	0.01281	0.256
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
37.500	15.625	0.252	0.01696	0.01549	0.252
37.500	18.750	0.255	0.01697	0.01549	0.255
37.500	21.875	0.249	0.01480	0.01481	0.247
37.500	25.000	0.256	0.00000	0.01363	0.248
37.500	28.125	0.251	0.01403	0.01405	0.249
37.500	31.250	0.251	0.01537	0.01412	0.251
37.500	34.375	0.251	0.01569	0.01433	0.251
37.500	37.500	0.250	0.01549	0.01402	0.250
37.500	40.625	0.247	0.01719	0.01566	0.247
37.500	43.750	0.247	0.01608	0.01469	0.247
37.500	46.875	0.245	0.01466	0.01463	0.248
37.500	50.000	0.239	0.00000	0.01488	0.249
37.500	53.125	0.246	0.01493	0.01488	0.249
37.500	56.250	0.247	0.01605	0.01453	0.247
37.500	59.375	0.247	0.01601	0.01453	0.247
37.500	62.500	0.250	0.01885	0.01706	0.250
37.500	65.625	0.248	0.01849	0.01699	0.250
37.500	68.750	0.245	0.01759	0.01706	0.252
37.500	71.875	0.251	0.01723	0.01706	0.253
37.500	75.000	0.255	0.00000	0.01706	0.253

Appendix Table 10. Output program AX when fitting a linear drift model to clay content.

α m	Rank means	Mean SS(resid) (pct.)²	Mean Abs(resid) pct.	I.Q.R. pct.	I.D.R. pct.
4.0	9.12	10.92	2.43	3.43	8.19
4.5	9.17	11.04	2.43	3.41	8.50
5.0	9.20	11.22	2.43	3.26	9.01
5.5	9.25	11.44	2.44	3.17	9.12
6.0	9.56	11.72	2.47	3.11	9.14
6.5	9.92	12.07	2.50	3.08	9.16
7.0	10.10	12.42	2.53	3.13	9.20
7.5	9.98	12.74	2.55	3.20	9.22
8.0	9.53	13.00	2.56	3.12	9.28
8.5	9.05	13.22	2.56	3.92	9.58
9.0	8.44	13.43	2.57	2.79	9.88
9.5	8.22	13.66	2.59	2.64	10.15
10.0	8.76	13.92	2.63	2.69	10.40
10.5	9.61	14.25	2.67	2.90	10.45
11.0	10.39	14.66	2.72	3.08	10.51
11.5	11.22	15.17	2.80	3.26	10.66
12.0	12.24	15.68	2.88	3.46	10.76
12.5	12.85	16.15	2.95	3.77	10.87
13.0	13.39	16.59	3.00	4.40	10.96
		Percentage of worst value			
4.0	68.10	65.83	80.93	84.77	74.77
4.5	68.48	66.55	80.93	84.44	77.60
5.0	68.73	67.62	80.95	80.68	82.80
5.5	69.11	68.96	82.34	78.40	83.27
6.0	71.39	70.62	82.17	77.05	83.41
6.5	74.05	72.74	83.33	76.08	83.57
7.0	75.44	74.86	84.30	77.39	83.95
7.5	74.56	76.77	84.93	79.16	84.16
8.0	71.14	78.35	85.20	77.23	84.70
8.5	67.59	79.71	85.22	72.26	87.41
9.0	63.04	80.98	85.53	68.92	90.16
9.5	61.39	82.31	86.24	65.26	92.64
10.0	65.44	83.89	87.45	66.47	94.92
10.5	71.77	85.88	88.90	71.70	95.36
11.0	77.59	88.38	90.73	76.18	95.91
11.5	83.80	91.45	93.21	80.65	97.28
12.0	91.39	94.50	95.80	85.49	98.22
12.5	95.95	97.36	98.06	93.31	99.15
13.0	100.00	100.00	100.00	100.00	100.00



APPENDIX FIGURE 5. Prediction standard errors of soil water content values based on a linear drift kriging model.



APPENDIX FIGURE 6. Measures of deviation (as % of worst value) of cross-validated residuals using a linear drift model on clay content.

α of 9. Analysis of all three models reveals that the linear drift model is to be preferred to either a stationary or quadratic model. Appendix table 11 summarizes some of these results.

Using Program CROSSK to Validate the Given Clay Model

The given model is that of linear drift with $\alpha = 9$. The procedure of validation is an exact repetition of that for the water model. Part of the output is shown in Appendix table 12. It is important to store the cross-validated residuals as these are needed in the co-kriging analysis to come.

Using Program KRIG to Predict Clay Values

The input requirements reflect an exact repetition of those for the water model. Part of the output is shown in Appendix table 13.

Co-kriging Water with Clay

To run the co-kriging program, the best kriging models for clay and water individually must be known. These models were determined in sections "Developing and Using a Kriging Model for Water Content" and "Development and Using a Kriging Model for Clay Content." In addition, the variances of the cross-validated residuals for clay and for water and the correlations between these two sets of residuals are required. Appendix table 14 lists these residuals for the 58

Appendix Table 11. Measures of deviation of cross-validated residuals for three different drift models on clay content.

α	Sum of squared deviations			Inter-quartile range		
m	(pct.)^2			pct.		
	S	L	Q	S	L	Q
4.0	695.01	644.31	722.67	3.64	3.43	3.88
4.5	695.38	651.37	736.38	3.56	3.41	3.94
5.0	698.57	661.89	753.65	3.61	3.26	4.06
5.5	704.55	674.96	772.92	3.63	3.17	4.07
6.0	713.39	691.20	795.31	3.58	3.11	4.18
6.5	724.80	711.97	823.15	3.60	3.08	4.24
7.0	734.85	732.74	850.63	3.38	3.13	4.08
7.5	742.81	751.81	876.29	3.04	3.20	4.06
8.0	748.43	766.91	899.74	2.87	3.12	3.98
8.5	753.00	780.21	921.54	2.78	2.92	3.85
9.0	758.83	792.65	942.50	2.87	2.79	3.83
9.5	767.98	805.65	963.53	3.00	2.64	3.87
10.0	781.32	821.13	986.58	3.04	2.69	3.89
10.5	799.33	840.61	1013.37	3.01	2.90	4.00
11.0	822.97	865.11	1045.05	2.99	3.08	4.13
11.5	852.65	895.14	1082.17	3.14	3.26	4.31
12.0	882.10	924.99	1118.31	3.36	3.46	4.52
12.5	909.47	952.97	1151.79	3.59	3.77	4.75
13.0	934.47	978.80	1182.76	3.76	4.40	4.96

S = stationary model, L = linear drift model, and Q = quadratic drift model.

locations where both water and clay were recorded. An analysis reveals the following:

variance(water residuals) = σ^2 = 0.0002116,
variance(clay residuals) = σ_b^2 = 13.36, and the
correlation coefficient = ρ = 0.6273.

Using Program COK to Predict Water Values by Co-Kriging

We will make predictions at the same 400 regularly spaced grid points used earlier in kriging.

(1) Store the following parameter values on file TEMP_PAR:

6.0 9.0 0.6273 0.0002116 13.36 3 3 20 20 0.0.

Appendix Table 12. Output for cross-validation of linear drift model for clay content, with parameter values α = 9, ng = 20, m = 3, and k = 0.

x	y	z	$\hat{z}$	prediction SE	local SD	local mean
m	m			pct.		
0.000	0.000	15.4	16.66	3.097	2.549	16.29
6.250	0.000	19.2	15.72	2.479	2.425	16.12
12.500	0.000	17.6	15.26	1.898	2.201	16.81
18.750	0.000	17.7	17.71	2.139	2.389	17.30
25.000	0.000	17.4	16.92	2.198	2.422	17.61
37.500	0.000	17.7	18.49	2.932	2.420	18.51
10.938	3.125	13.4	18.25	1.484	1.707	17.94
17.188	3.125	18.4	17.97	2.081	2.386	18.03
23.438	3.125	17.3	18.33	2.077	2.340	18.55
29.688	3.125	17.1	18.65	2.401	2.396	18.89
6.250	6.250	18.1	16.81	2.611	2.543	17.47
34.375	6.250	19.4	19.45	2.581	2.548	19.81
17.188	9.375	21.5	20.13	2.390	2.401	19.86
12.500	12.500	20.7	20.02	2.595	2.644	19.89
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
14.063	53.125	26.8	27.59	3.110	3.570	26.01
3.125	56.250	26.0	25.29	3.962	3.842	25.76
18.750	56.250	23.6	28.83	2.758	3.273	25.79
21.875	56.250	32.9	23.99	3.155	3.625	24.24
12.500	62.500	22.8	23.78	2.870	3.640	24.85
15.625	62.500	24.3	24.01	3.318	3.826	25.56
10.938	65.625	22.0	23.95	3.575	3.966	25.06
3.125	68.750	28.2	21.76	3.292	3.614	23.78
18.750	68.750	25.6	24.10	3.879	4.589	23.95
21.875	68.750	22.7	23.79	3.968	4.558	23.18
34.275	68.750	16.0	24.09	4.407	3.828	22.88
1.563	71.875	20.7	27.03	2.781	3.503	24.92
7.813	71.875	23.5	24.81	4.089	4.119	24.55
14.063	71.875	26.5	25.12	4.009	4.597	23.89
29.688	71.875	29.5	19.42	3.441	3.414	20.23
0.000	75.000	26.9	19.26	3.780	3.710	20.61
12.500	75.000	25.7	24.33	4.230	4.599	23.35
25.000	75.000	20.1	24.39	4.664	4.446	23.00
37.500	75.000	19.8	18.68	5.139	4.181	19.08

Appendix Table 13 Kriging estimates of clay content using a linear drift model, with parameter values $\alpha=9$, ng=20, m=3, and k=0.

x	y	$\hat{z}$	prediction SE	local conditional SD	local mean
m	m		pct		
0.000	0.000	15.4	0.00	2.51	16.19
0.000	3.125	16.2	2.86	3.18	16.25
0.000	6.250	17.0	3.42	3.18	16.91
0.000	9.375	17.6	3.51	3.17	17.48
0.000	12.500	18.3	3.48	3.17	18.14
0.000	15.625	19.9	3.28	3.22	19.32
0.000	18.750	20.8	2.91	3.25	20.37
0.000	21.875	20.3	2.74	3.34	20.69
0.000	25.000	19.2	0.00	3.40	20.37
0.000	28.125	20.9	2.79	3.39	21.15
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
37.500	15.625	22.3	2.65	2.37	22.26
37.500	18.750	22.8	2.58	2.37	22.97
37.500	21.875	21.6	2.30	2.57	21.24
37.500	25.000	22.5	0.00	2.55	21.67
37.500	28.125	22.4	2.37	2.65	21.93
37.500	31.250	22.7	2.97	2.78	22.60
37.500	34.375	23.1	3.95	3.55	23.10
37.500	37.500	24.1	4.10	3.64	24.14
37.500	40.625	22.4	4.61	4.14	22.40
37.500	43.750	22.5	4.45	4.11	22.10
37.500	46.875	23.2	3.59	4.00	21.95
37.500	50.000	24.4	0.00	4.23	21.66
37.500	53.125	22.8	3.79	4.23	21.47
37.500	56.250	22.4	4.65	4.25	22.15
37.500	59.375	21.8	4.79	4.25	21.81
37.500	62.500	20.8	4.64	4.18	21.34
37.500	65.625	18.9	4.34	4.22	21.20
37.500	68.750	17.3	3.76	4.17	20.72
37.500	71.875	18.4	3.46	4.17	20.18
37.500	75.000	19.8	0.00	4.08	19.98

The meaning of each component of this parameter vector is explained in Appendix table 2 (under program COK on page 16).

(2) Store the array [x y z (water) D] on file TEMP_AIN.

(3) Store the array [x y z (clay) D] on file TEMP_BIN. Note that these file contents are exactly the same as those originally stored on file TEMP_AIN for the earlier kriging analyses.

(4) Store the array [x y* D*], made up of the 400 prediction coordinates and corresponding design matrix on file TEMP_COR. Note that this is identical to the contents stored in the same file earlier when using program KRIG.

(5) Run the program COK and examine the output on file TEMP_OUT. Appendix table 15 lists part of this output. Appendix figures 7 and 8 give the contour plots for predicted

Appendix Table 14. Cross-validated residuals from the kriging models on water and clay respectively.

water cm^3/cm^3	clay pct.	water cm^3/cm^3	clay pct.
0.0041	-1.2574	0.0170	5.5313
0.0157	3.4809	0.0090	-2.3833
0.0245	2.3384	-0.0015	-1.8158
-0.0065	-0.0069	0.0125	2.3710
0.0112	0.4754	-0.0199	0.0764
0.0023	-0.7857	0.0116	5.1165
-0.0325	-4.8478	-0.0035	0.2382
-0.0013	0.4267	0.0149	-3.5636
-0.0119	-1.0305	-0.0117	3.5411
-0.0019	-1.5540	0.0105	-1.7545
-0.0015	1.2948	0.0201	-0.7928
0.0153	-0.0457	0.0089	0.7074
0.0014	1.3742	-0.0246	-5.2342
0.0047	0.6846	0.0348	8.9130
0.0117	4.5687	0.0034	-0.9759
-0.0059	-0.9914	0.0008	0.2948
-0.0094	1.8468	-0.0265	-1.9522
0.0104	-1.1814	0.0018	6.4434
0.0031	0.0068	0.0162	1.4985
0.0047	-0.5285	0.0038	-1.0939
0.0102	-0.0624	-0.0291	-8.0895
0.0079	-0.1707	-0.0066	-6.3272
0.0089	0.9369	0.0128	-1.3082
-0.0321	-8.0718	0.0086	1.3795
0.0064	-0.4702	0.0213	10.0780
0.0210	7.3490	0.0069	7.6365
0.0186	3.8222	0.0163	1.3736
0.0127	0.4496	0.0060	-4.2853
0.0113	0.0092	-0.0002	1.1182

The 58 observations relate to those 58 places where both variables were recorded.

water and prediction standard errors, respectively, produced by the package PLOTT88.

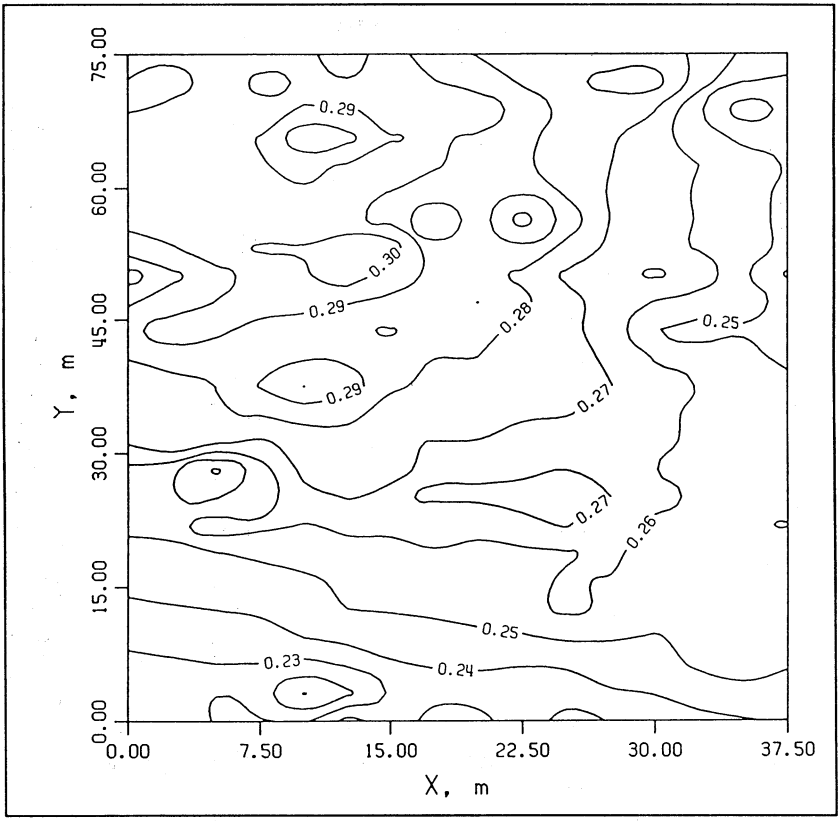
Using Program CROSSC to Validate The CO—KRIGED Model.

(1) The contents of files TEMP_PAR , TEMP_AIN and TEMP_BIN remain exactly the same as those used in the previous program, COK.

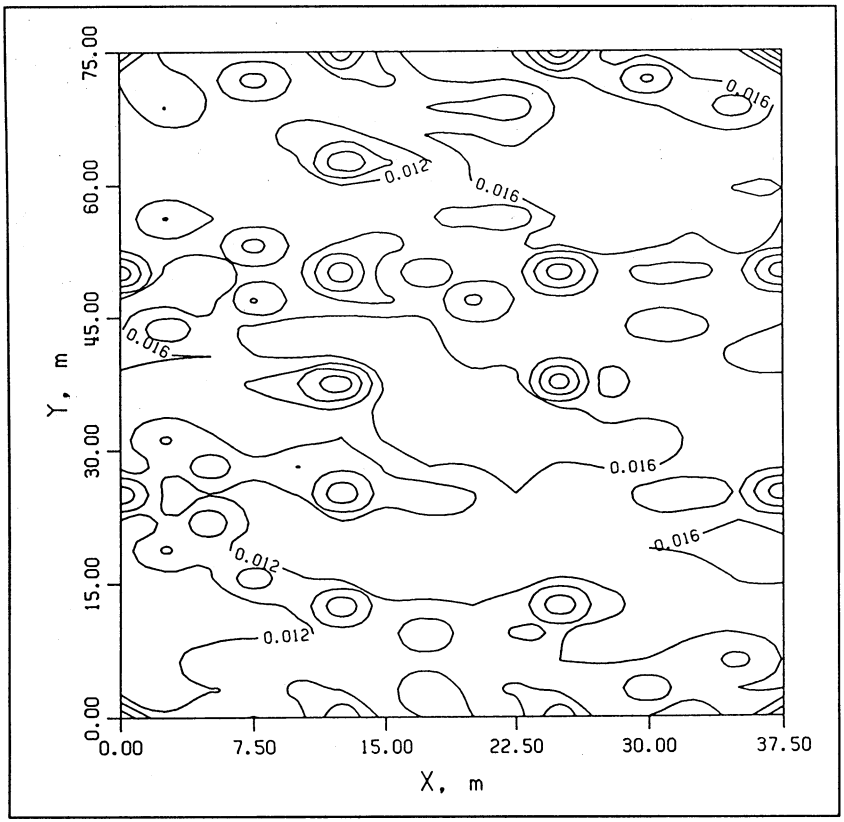
(2) Run program CROSSC and examine file TEMP_OUT for the output. Appendix table 16 lists part of that output. It is immediately apparent, both from the smaller residuals and smaller prediction standard errors, that the co-kriged predictions are considerably more precise than those based on kriging alone.

Finding an Optimal Sampling Strategy

The program SAM is used to answer the following question. Requiring minimal loss of information, which locations should be selected to measure water content values at only 16 sites in the future? There are 60 locations that were used in the past; call these the future potential sample points. Now define 18 prediction points, none of which should coincide with the potential sample points. The idea is to choose a subset



APPENDIX FIGURE 7. Co-kriging estimates of soil water content using linear drift models for water and clay content.



APPENDIX FIGURE 8. Prediction standard errors of soil water content values based on the co-kriging model.

of 16 points from the full set of 60 potential sample points in such a way that the maximum prediction standard error of all 18 prediction points is minimized. The actual technique used in the program is to calculate the prediction SE's for the closest 6 prediction points to any potential sample point and hence the average of these 6 points. This average SE is used as the criterion for retaining a potential sample point; those 16 points having largest average SE's are retained. Appendix figure 9 shows the layout of the potential sample points, the prediction points, and the finally selected optimal 16 points. In using program SAM we make use of our knowledge of the best co-kriging model for water and clay.

Appendix Table 15. Output of co-kriging water and clay with linear drift models. Parameter values are α (water) = 6.0, α (clay) = 9.0, ρ = 0.63, σ^2(water) = 0.0002116, σ^2(clay) = 13.40, m(water) = 3, m(clay) = 3, ng (water) = 20, ng(clay) = 20, and k = 0.0

x	y	$\hat{z}$ water	prediction SE water	local conditional SD water	local mean water
m	m		cm^3/cm^3		
0.0000	0.0000	0.2205	0.0000	0.0127	0.2189
0.0000	3.1250	0.2230	0.0140	0.0137	0.2225
0.0000	6.2500	0.2273	0.0153	0.0037	0.2273
0.0000	9.3750	0.2323	0.0148	0.0135	0.2323
0.0000	12.5000	0.2373	0.0147	0.0135	0.2373
0.0000	15.6250	0.2434	0.0148	0.0137	0.2427
0.0000	18.7500	0.2471	0.0138	0.0136	0.2481
0.0000	21.8750	0.2517	0.0135	0.0137	0.2522
0.0000	25.0000	0.2558	0.0000	0.0146	0.2518
0.0000	28.1250	0.2573	0.0127	0.0128	0.2557
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
37.5000	15.6250	0.2536	0.0170	0.0156	0.2536
37.5000	18.7500	0.2564	0.0170	0.0156	0.2564
37.5000	21.8750	0.2496	0.0148	0.0148	0.2476
37.5000	25.0000	0.2560	0.0000	0.0137	0.2490
37.5000	28.1250	0.2522	0.0140	0.0141	0.2498
37.5000	31.2500	0.2523	0.0153	0.0142	0.2523
37.5000	34.3750	0.2520	0.0157	0.0144	0.2520
37.5000	37.5000	0.2518	0.0155	0.0141	0.2518
37.5000	40.6250	0.2485	0.0172	0.0157	0.2485
37.5000	43.7500	0.2480	0.0161	0.0147	0.2480
37.5000	46.8750	0.2477	0.0146	0.0146	0.2484
37.5000	50.0000	0.2389	0.0000	0.0149	0.2480
37.5000	53.1250	0.2480	0.0149	0.0149	0.2485
37.5000	56.2500	0.2473	0.0161	0.0146	0.2473
37.5000	59.3750	0.2481	0.0160	0.0146	0.2481
37.5000	62.5000	0.2491	0.0189	0.0171	0.2491
37.5000	65.6250	0.2473	0.0185	0.0170	0.2507
37.5000	68.7500	0.2423	0.0176	0.0171	0.2504
37.5000	71.8750	0.2485	0.0172	0.0171	0.2507
37.5000	75.0000	0.2554	0.0000	0.0171	0.2524

Appendix Table 16. Output of cross-validation of co-kriged model of water and clay. Parameter values are α (water) = 6.0, α (clay) = 9.0, ρ = 0.63, σ^2 (water) = 0.0002116, σ^2 (clay) = 13.40, m (water) = 3, m (clay) = 3, ng (water) = 20, ng (clay) = 20, and k = 0.0

x	y	z water	$\hat{z}$ water	prediction SE water	local conditional SD water	local mean water
m	m			cm^3/cm^3		
0.0000	0.0000	0.2205	0.2139	0.0123	0.0128	0.2157
6.2500	0.0000	0.2352	0.2308	0.0102	0.0124	0.2219
12.5000	0.0000	0.2430	0.2243	0.0070	0.0093	0.2248
18.7500	0.0000	0.2251	0.2340	0.0089	0.0116	0.2323
25.0000	0.0000	0.2436	0.2323	0.0092	0.0119	0.2341
37.5000	0.0000	0.2410	0.2383	0.0115	0.0123	0.2387
10.9375	3.1250	0.2038	0.2219	0.0057	0.0076	0.2323
17.1875	3.1250	0.2328	0.2330	0.0081	0.0109	0.2352
23.4375	3.1250	0.2290	0.2375	0.0090	0.0118	0.2393
29.6875	3.1250	0.2400	0.2394	0.0099	0.0121	0.2417
6.2500	6.2500	0.2301	0.2326	0.0105	0.0128	0.2319
34.3750	6.2500	0.2580	0.2450	0.0100	0.0118	0.2443
17.1875	9.3750	0.2462	0.2500	0.0094	0.0118	0.2457
12.5000	12.5000	0.2499	0.2477	0.0101	0.0128	0.2454
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
.	.	.	.	.	.	.
14.0625	53.1250	0.3136	0.2912	0.0110	0.0150	0.2894
3.1250	56.2500	0.2991	0.2917	0.0114	0.0141	0.2906
18.7500	56.2500	0.2691	0.2828	0.0106	0.0148	0.2853
21.8750	56.2500	0.3077	0.2957	0.0114	0.0153	0.2776
12.5000	62.5000	0.2912	0.2840	0.0101	0.0142	0.2926
15.6250	62.5000	0.2936	0.2907	0.0104	0.0142	0.2915
10.9375	65.6250	0.2672	0.2878	0.0103	0.0135	0.2941
3.1250	68.7500	0.2922	0.3082	0.0117	0.0150	0.2949
18.7500	68.7500	0.3023	0.2915	0.0120	0.0166	0.2836
21.8750	68.7500	0.2893	0.2839	0.0126	0.0170	0.2800
34.3750	68.7500	0.2341	0.2413	0.0134	0.0160	0.2588
1.5625	71.8750	0.2868	0.2749	0.0110	0.0149	0.2909
7.8125	71.8750	0.3033	0.2882	0.0116	0.0147	0.2906
14.0625	71.8750	0.2999	0.2979	0.0123	0.0166	0.2879
29.6875	71.8750	0.2856	0.2923	0.0135	0.0167	0.2686
0.0000	75.0000	0.2957	0.3054	0.0129	0.0150	0.2952
12.5000	75.0000	0.3053	0.2944	0.0128	0.0163	0.2869
25.0000	75.0000	0.2800	0.2639	0.0141	0.0170	0.2725
37.5000	75.0000	0.2554	0.2554	0.0172	0.0179	0.2554

(1) Store the following parameter vector (as a row vector) in file TEMP_PAR:

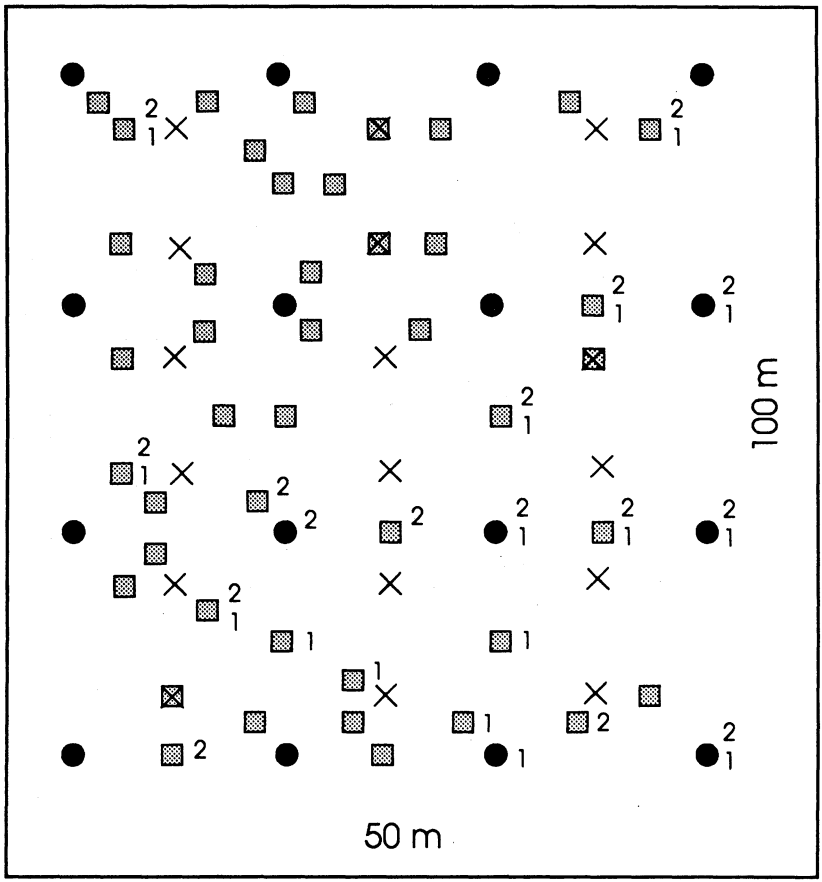
α(water)	6.0
α(clay)	9.0
ρ	0.6273
σ^2(water)	0.0002116
σ^2(clay)	13.36
m (water)	3
m(clay)	3

ng(water)	12 (must be less than 18)
ng(clay)	20
maxout	20 (maximum number of iterations)

(2) Store [x y D], the coordinates and design matrix for the potential sample points, in file TEMP__AIN. Note that the design matrix D corresponds to the linear drift model. Also note that no knowledge of the observed values for water content at these sites is needed.

(3) Store [x y z(clay) D] in the file TEMP__BIN. Note that these stored values are identical to those used in the earlier co-kriging analysis of water with clay.

(4) Store [x* y* D*], the coordinates and design matrix for the 18



APPENDIX FIGURE 9. Lay-out of the potential sample points (solid circles and squares), the prediction points (crosses), the selected optimal 16 points after one run (1), and after a second run (2).

prediction points, in file TEMP_COR. These values are shown in Appendix table 17.

(5) Run the program by entering: RUN SAM. We are now in an interactive mode and the command "Enter the required sample size, ns. Note ns = 0 stops the program," will be displayed on the screen. By entering 16, the program will begin the optimization process, searching for an optimal 16 points. It starts by simply taking the first 16 potential sample points and then runs through 20 iterative cycles (20 being the specified value of the parameter "maxout"), in each cycle replacing one of the 16 points by a better point from the remaining 44. At the end of each cycle it prints out the details of the points added and dropped. When the 20 cycles are complete (or earlier if no improvement can be found), the earlier question is repeated on the screen. If a non-zero value for ns is entered the whole procedure is repeated but with the important difference that it starts with the 16 points from the final stage of the earlier run.

Appendix tables 18, 19, and 20 give the output, while Appendix figure 9 illustrates the positions of the best 16 points. Note that after cycle number 14 the program keeps repeating the same exchange between points (34.375, 68.75) and (3.125, 43.75). At this stage the current run is unable to effect any improvement. The final arrangement arrived at can never be guaranteed to be best and a good idea in practice is to run an extra sequence of cycles with a larger ns value and then revert to the real target sample size. This is easily

Appendix Table 17. The input file TEMP_COR required by program SAM to optimize water sampling

x m	y m		x m	y m
6.250	6.250	1.000	6.250	6.250
18.750	6.250	1.000	18.750	6.250
31.250	6.250	1.000	31.250	6.250
6.250	18.750	1.000	6.250	18.750
18.750	18.750	1.000	18.750	18.750
31.250	18.750	1.000	31.250	18.750
6.250	31.250	1.000	6.250	31.250
18.750	31.250	1.000	18.750	31.250
31.250	31.250	1.000	31.250	31.250
6.250	43.750	1.000	6.250	43.750
18.750	43.750	1.000	18.750	43.750
31.250	43.750	1.000	31.250	43.750
6.250	56.250	1.000	6.250	56.250
18.750	56.250	1.000	18.750	56.250
31.250	56.250	1.000	31.250	56.250
6.250	68.750	1.000	6.250	68.750
18.750	68.750	1.000	18.750	68.750
31.250	68.750	1.000	31.250	68.750

achieved by entering the required non-zero ns value at each stage when the computer screen requests such input. In fact, Apendix figure 9 shows two sets of "best" 16 points. The program was run once as previously reported and then re-run with inproved starting values to eventually yield an even better set of points. Note also that the program is very computer-intensive and it is more efficent to run several sequences of cycles than one long sequence with a high value of the parameter maxout. Finally, note that a different set of prediction points will yield a different (often markedly so) set of optimal sampling sites.

Appendix Table 18. Optimization of sample locations for water content determination. Output from program SAM - part 1. Parameter values are α (water) = 6.0, α (clay) = 9.0, ρ = 0.63, σ^2 (water) = 0.0002116, σ^2(clay) = 13.36, m (water) = 3, m (clay) = 3, ng (water) = 12, ng (clay) = 20, maxout = 20.

Cycle number	sample site added		sample site dropped	
	x m	y m	x m	y m
1	34.3750	68.7500	6.2500	0.0000
2	31.2500	25.0000	10.9380	3.1250
3	3.1250	68.7500	0.0000	0.0000
4	3.1250	31.2500	12.5000	0.0000
5	37.5000	25.0000	6.2500	6.2500
6	25.0000	37.5000	17.1880	3.1250
7	31.2500	43.7500	29.6880	3.1250
8	3.1250	43.7500	31.2500	43.7500
9	37.5000	50.0000	18.7500	0.0000
10	25.0000	25.0000	3.1250	43.7500
11	3.1250	43.7500	34.3750	6.2500
12	31.2500	50.0000	3.1250	43.7500
13	3.1250	43.7500	34.3750	68.7500
14	34.3750	68.7500	3.1250	43.7500
15	3.1250	43.7500	34.3750	68.7500
16	34.3750	68.7500	3.1250	43.7500
17	3.1250	43.7500	34.3750	68.7500
18	34.3750	68.7500	3.1250	43.7500
19	3.1250	43.7500	34.3750	68.7500
20	34.3750	68.7500	3.1250	43.7500

Appendix Table 19. Optimization of sample locations for water content determination. Output from program SAM - part 2.

x m	y m	Average SE cm^3/cm^3
	The best subset of sample points with their average SE's	
3.1250	68.7500	0.0150
34.3750	68.7500	0.0163
3.1250	31.2500	0.0146
37.5000	50.0000	0.0157
25.0000	0.0000	0.0147
37.5000	0.0000	0.0149
31.2500	25.0000	0.0154
25.0000	37.5000	0.0153
23.4380	3.1250	0.0147
25.0000	25.0000	0.0152
37.5000	25.0000	0.0154
31.2500	50.0000	0.0157
17.1880	9.3750	0.0146
12.5000	12.5000	0.0146
25.0000	12.5000	0.0148
7.8130	15.6250	0.0145
	The subset of unused sample points with their average SE's	
3.1250	18.7500	0.0145
4.6880	21.8750	0.0146
0.0000	25.0000	0.0145
12.5000	25.0000	0.0148
18.7500	25.0000	0.0151
34.3750	6.2500	0.0149
10.9380	3.1250	0.0145
6.2500	6.2500	0.0145
4.6880	28.1250	0.0146
10.9380	28.1250	0.0147
12.5000	0.0000	0.0146
9.3750	37.5000	0.0147
12.5000	37.5000	0.0147
17.1880	3.1250	0.0146
31.2500	43.7500	0.0153
29.6880	3.1250	0.0148
7.8130	46.8750	0.0145
14.0630	46.8750	0.0147
20.3130	46.8750	0.0149
0.0000	50.0000	0.0146
12.5000	50.0000	0.0146
25.0000	50.0000	0.0152
3.1250	43.7500	0.0145
18.7500	0.0000	0.0146
7.8130	53.1250	0.0148
14.0630	53.1250	0.0145
3.1250	56.2500	0.0149
18.7500	56.2500	0.0150
21.8750	56.2500	0.0146
12.5000	62.5000	0.0149
15.6250	62.5000	0.0148
10.9380	65.6250	0.0150
0.0000	0.0000	0.0144
18.7500	68.7500	0.0151
21.8750	68.7500	0.0150
6.2500	0.0000	0.0145
1.5630	71.8750	0.0149
7.8130	71.8750	0.0151
14.0630	71.8750	0.0150

Continued

Appendix Table 19 (continued). Optimization of sample locations for water content determination. Output from program SAM - part 2.

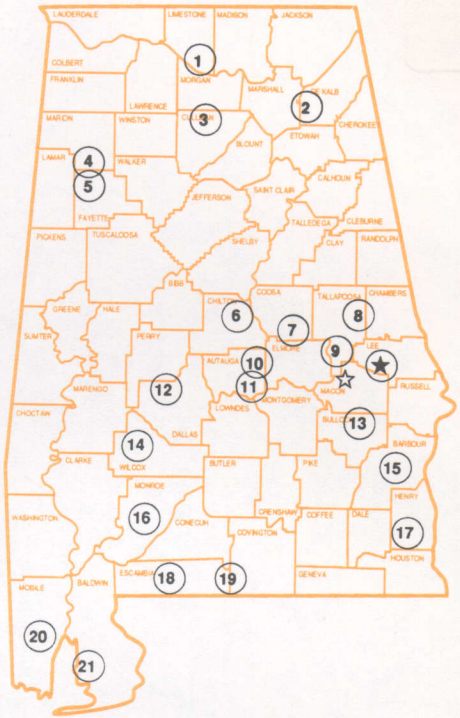
x m	y m	Average SE cm^3/cm^3
	The best subset of sample points with their average SE's	
29.6880	71.8750	0.0161
0.0000	75.0000	0.0149
12.5000	75.0000	0.0151
25.0000	75.0000	0.0154
37.5000	75.0000	0.0158

Appendix Table 20. Optimization of sample locations for water content determination. Output from program SAM - part 3. The prediction SE's.

x m	y m	Initial SE cm^3/cm^3	Final SE cm^3/cm^3
6.2500	6.2500	0.0000	0.0140
18.7500	6.2500	0.0139	0.0144
31.2500	6.2500	0.0139	0.0148
6.2500	18.7500	0.0163	0.0145
18.7500	18.7500	0.0177	0.0151
31.2500	18.7500	0.0195	0.0155
6.2500	31.2500	0.0244	0.0144
18.7500	31.2500	0.0262	0.0151
31.2500	31.2500	0.0295	0.0154
6.2500	43.7500	0.0348	0.0142
18.7500	43.7500	0.0375	0.0149
31.2500	43.7500	0.0424	0.0158
6.2500	56.2500	0.0456	0.0155
18.7500	56.2500	0.0475	0.0131
31.2500	56.2500	0.0540	0.0166
6.2500	68.7500	0.0556	0.0151
18.7500	68.7500	0.0588	0.0143
31.2500	68.7500	0.0675	0.0173

Alabama's Agricultural Experiment Station System
AUBURN UNIVERSITY

With an agricultural research unit in every major soil area, Auburn University serves the needs of field crop, livestock, forestry, and horticultural producers in each region in Alabama. Every citizen of the State has a stake in this research program, since any advantage from new and more economical ways of producing and handling farm products directly benefits the consuming public.



Research Unit Identification

★ Main Agricultural Experiment Station, Auburn.
☆ E. V. Smith Research Center, Shorter.

1. Tennessee Valley Substation, Belle Mina.
2. Sand Mountain Substation, Crossville.
3. North Alabama Horticulture Substation, Cullman.
4. Upper Coastal Plain Substation, Winfield.
5. Forestry Unit, Fayette County.
6. Chilton Area Horticulture Substation, Clanton.
7. Forestry Unit, Coosa County.
8. Piedmont Substation, Camp Hill.
9. Plant Breeding Unit, Tallassee.
10. Forestry Unit, Autauga County.
11. Prattville Experiment Field, Prattville.
12. Black Belt Substation, Marion Junction.
13. The Turnipseed-Ikenberry Place, Union Springs.
14. Lower Coastal Plain Substation, Camden.
15. Forestry Unit, Barbour County.
16. Monroeville Experiment Field, Monroeville.
17. Wiregrass Substation, Headland.
18. Brewton Experiment Field, Brewton.
19. Solon Dixon Forestry Education Center, Covington and Escambia counties.
20. Ornamental Horticulture Substation, Spring Hill.
21. Gulf Coast Substation, Fairhope.