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SITE CHARACTERIZATION: A SPATIAL
ESTIMATION APPROACH

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PREFACE

In this report we discuss the application of spatial estimation techniques or kriging to representative groundwater and geological data sets. This work was funded under the Nuclear Regulatory Commission (NRC) Waste Management Program and partially by the Lawrence Livermore National Laboratory (LLNL) Containment Test Program. The program is primarily concerned with investigating the geologic properties of potential underground repositories which can be used to store nuclear waste material. The first problem to be solved is that of site characterization, i.e., the determination of various parameters like transmissivity, porosity and subsurface structures necessary to evaluate the integrity of the particular site. Initially exploratory boreholes are drilled at a potential site and this data is evaluated to determine the critical parameters. Usually contour maps of groundwater flows and other parameters are developed and site characteristics can be derived from this information. Thus, it is necessary for the NRC to evaluate various techniques which can be used to produce reliable contour maps in order to characterize a site.

Spatial estimation is a technique to estimate points or volumes on a grid when the data is spatially correlated. Once the grid is generated, contouring follows directly using simple interpolation techniques. It is the purpose of this study to investigate the applicability of a specific spatial estimator developed in the mining industry to groundwater and geological data. The investigation consists of applying the estimator to simple groundwater

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structures and evaluating the results. In one case a model developed by a hydrologist for a particular aquifer was used to generate a grid which was used as "truth" and the performance of the estimator given a sparse number of measurements was evaluated. It was shown that the estimator could reliably reproduce the grid for this simple aquifer. The estimator was then applied to more complex geological formations and found to produce reasonable results in this case as well. In summary, we feel that the spatial estimator can be used with confidence to produce reliable contours if the investigator carefully identifies the proper statistical model from the data set.

ABSTRACT

In this report we consider the application of spatial estimation techniques or kriging to groundwater aquifers and geological borehole data. We investigate the adequacy of these techniques to reliably develop contour maps from various data sets.

The estimator is developed theoretically in a simplified fashion using vector-matrix calculus. The practice of spatial estimation is discussed and the estimator is then applied to two groundwater aquifer systems and used also to investigate geological formations from borehole data. It is shown that the estimator can provide reasonable results when designed properly.

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I. INTRODUCTION

The need for alternate energy sources has propelled the use of nuclear energy as a feasible means for generating power. Nuclear technology has been utilized in many military and non-military applications such as fuel fabrication, medicine, weapons, etc. One perplexing problem has evolved - the disposal of radioactive waste products. It is the responsibility of the Nuclear Regulatory Commission (NRC) to assure that wastes be disposed in a manner non-detrimental to public health and welfare.

One proposed solution to the disposal problem is to isolate the waste in deep geological repositories. The waste is to be contained until they are no longer radiotoxic. Some elements will take a long time to decay - up to a few million years. For these slowly decaying elements the primary containment vessel will have deteriorated and therefore the geological structure of a repository will serve as the ultimate containment vessel. The question of contamination of the water supply becomes of prime concern. The magnitude of the disposal problem can be realized from the fact that only a single curie of ^{90}Sr , a common fission by-product, if dissolved in water could render 10^{11} liters unacceptable as drinking water according to the U.S. Public Health Service Standards [1]. Disposal practices depend on the radioactivity of the waste, the general chemical character of the waste, and the

physical environment in the area of disposal. All plans for terrestrial storage have stressed the need for careful hydrogeologic studies to insure that the wastes will not contaminate existing or future water supplies. Thus, prior to construction and regulation of a repository, a site must be selected, characterized, and evaluated.

The repository site evaluation process consists of two stages: elimination of sites prior to performance evaluation and the selection of sites by comparison of predicted performance. Once the number of candidate sites are screened, the most promising systems must be evaluated by developing a performance model, which ultimately yields as output the radioactive flux dosage to the average man compared to existing radiation standards [2].

Since the most likely release of radionuclides in the long term will be via the groundwater system, it is obvious that hydrogeology will form a major component of any performance evaluation model. The geological framework, the output of the repository excavation performance model, and the hydrogeologic parameters will form the input to the hydrogeological model. During different stages of the process, two types of parameters will be required: general site characterization parameters during preliminary evaluation and model input parameters for performance evaluation. Thus prior to site selection, much information about the geological and hydrogeological structures of the site must be obtained. For example, size, shape,

faults, groundwater properties, and chemical composition - this process is called site characterization. This report addresses itself to the site characterization problem, i.e., the problem of determining various geological and hydrogeological parameters necessary to characterize a potential repository.

Unfortunately, the evaluation of repository performance involves considerable uncertainties. These uncertainties arise from several sources: (i) measurement uncertainty in specifying geological parameters; (ii) spatial variability of the subsurface environment, and, (iii) uncertainty in analytic performance models. Any treatment of repository regulations must account for these uncertainties and therefore, any techniques used to characterize a potential site must also give some measure of the potential uncertainties in parameters generated.

The determination of hydrogeological parameters requires an understanding of the piezometric surface of a potential site, i.e., the water levels. Water levels measured in wells are conveniently studied by means of maps and graphs. Most frequently used are water-level contour maps. The elevation to which water rises in wells defines the piezometric surface. The surface may be either above or below the water table. The piezometric surface is determined by both water pressure and elevation of the aquifer. Where water levels in wells reliably reflect the water table, contour maps of the water

table can be drawn. The force potential causing groundwater flow is directly proportional to the elevation of water levels in wells drilled in aquifers. The general direction of groundwater flow can be shown on water table maps. This map indicates the elevation of the water table by means of contours. Various hydrogeological parameters can be obtained directly from the contours. Thus, one of the important tasks in groundwater study is to produce reliable contour maps of the water table.

Information about hydrogeological parameters can be obtained by borehole sampling. Too many boreholes at a site are not only expensive but they can tend to deteriorate the integrity of the site as a possible repository. Two approaches are possible: first, the use of nonintrusive measurements (e.g., seismic) or second, make statistical inferences on the suitability based on few data points. In this report we evaluate a technique which can be used to solve the site characterization problem. The fundamental problem is to generate a grid of control points from a set of sparse, irregular, uncertain, but spatially-correlated, measurements - this is called the fundamental spatial estimation problem. Spatial estimation techniques can be useful as a statistical interpolation/extrapolation method to derive more information from sparse data sets and they can also be used to combine different types of data (seismic, depth, gravity, etc.) to give a more complete characterization of geological and hydrogeological parameters.

Spatial estimation is rooted on ore estimation problems. In the early 1950's a South African mining engineer, D. G. Krige applied moving-average techniques to the problem of ore estimation [3,4]. Later a French engineer, G. Matheron formalized the approach in the early 1960's [5]. Matheron introduced the concept of "regionalized variables" to represent functions whose known values do not follow any simple deterministic function over a wide range. He expanded Krige's empirical observations into a theory of the behavior of these spatially distributed variables which was applicable to any phenomenon satisfying certain basic assumptions. Currently, this theory has been used in mining, meteorology, forestry, mapping of groundwater potentials, air pollution concentrations, geologic surfaces and oil field delineations [6-12]. To honor Krige for his pioneering work, Matheron referred to the spatial estimation techniques as "kriging" and later as universal kriging when used to estimate a variable with a trend in the data. In this report, we refer to the estimator as the spatial or kriging estimator, interchangeably.

Kriging is a particular statistical spatial estimation technique similar in principle to the Box-Jenkins approach of time series analysis [13]. It makes no attempt to describe the physical mechanism of the underlying phenomenon in contrast to the Kalman filter approach [14]; instead it models, using statistical principles, the structure of the available spatially-distributed data to estimate contours of geologic phenomenon. Kriging is essentially a stochastic technique of

interpolating sparse data assumed to be spatially correlated. It consists of two parts: estimation of a variogram, which describes the degree of correlation between two observations as a function of the distance between them, and calculation of the kriging weights, which indicate the relative influence of each of the data observations on the interpolations.

A potential geological repository must be evaluated from very sparse data. The relevant questions are: What is the minimum measurement density requirement? What is the uncertainty associated with the estimate? How is the selection of additional sampling locations optimized? Kriging is a spatial estimation technique which can produce answers to these questions. First, kriging can be used to produce a contour map of the geological formation (or any other spatially-distributed phenomena) of a potential site with an associated measure of uncertainty (kriging error). For a given variogram, by maneuvering the data set, kriging will provide insights into the effect of data density on the associated uncertainty of the contour map as well as a rationale for selection of additional sample-locations. Secondly, kriging can be used to combine different types of data from a suite of geological and geophysical measurements to produce a more complete characterization of the geological parameters than provided by conventional methods.

The objective of the report is to evaluate the effectiveness of kriging as a potential tool for site characterization of deep geological repositories. The basic criterion for evaluation is how realistically the estimator predicts the geological phenomenon. This can be judged in two ways: by comparing the estimated value with the measured value for the point which is removed from the data set, or by comparing the estimated map with the "real" contour map based on other information in addition to the estimated data set. By using representative data sets, the uncertainty in the estimation of the variogram can be assessed. Furthermore the effect of faults on estimation can also be investigated.

We evaluate kriging by experimenting on representative data sets. We selected three particular data sets to study: (i) Toppenish Creek Basin, (ii) Todd Lake, and (iii) Nevada Test Site. The first two cases are simple groundwater aquifers and the final set is a complex geological formation.

The Toppenish Creek Basin, Washington is a simple aquifer system. The data set consists of 76 water level measurements at various wells in the region during September 1971. The data was obtained from J. A. Skrivan of the USGS, Tacoma, Washington. The main purpose of this study is to evaluate how realistically the spatial estimator could produce contours of a well-known aquifer system.

The Todd Lake, Pennsylvania data set represents a region well known to a LLNL hydrologist, W. A. Murray. From a set of ten actual well-measurements and 18 known water levels (pond, lake, etc.) he was able to develop a groundwater model (partial differential equations) and generate a regular grid of data points for contouring purposes. In this case study we assume the grid generated by his model is the true representation of levels in the region, hereafter called "truth" grid. Here we would like to determine how well the spatial estimator can reproduce the "truth" grid using the same sparse data set of 28 points.

Finally, we studied the depth to the top of the paleozoic rocks from 93 borehole data from the Nevada Test Site (NTS). The Geologic Data Base from the Nevada Test Site maintained by LLNL [7] contains parameters describing the location coordinates, the lithologic contacts (alluvium, volcanic tuffs, and paleozoic rocks), the distance to known and inferred faults, the depth to the water table, etc., from over 1000 drill holes. In addition, there is a data base of 9000 files of processed geophysical data versus depth from logs and samples. Other geophysical data such as seismic reflections and gravity are also available for the area. We also investigated the effect of faults on the estimated depth.

In this report, we develop spatial estimators to solve the site characterization problem. The estimators are developed simply from

well-known regionalized variable theory [5] using vector-matrix calculus techniques in Section II. The practice of spatial estimation is discussed in Section III primarily to answer the question of "how". It is shown in this section that the most crucial area of spatial estimation is the development of the statistical structural model - the variogram and drift. Techniques to estimate and identify the underlying variogram and drift from raw measurement data are discussed along with techniques to validate the model. The spatial estimators are developed for the three representative data sets in Section IV. It will be shown that the estimator performs well on the groundwater aquifers, i.e., reasonable contours were produced. In the case of the sparse Todd Lake data, the estimator reproduces the "truth" grid with a maximum relative error of approximately one percent. Applying the estimator to the complex geological data from the Nevada Test Site produces reasonable maps for subsurface paleozoic rock depth in the region. Results of the estimator are compared with that obtained from gravity measurements. It will also be shown that image display techniques can be used to interactively investigate properties of regional maps.

We show that spatial estimation techniques can be used effectively to characterize proposed repository sites from limited data provided that care is taken when identifying the statistical structural model from raw data. Using a statistical model the estimator provides reasonable estimates and predicts associated uncertainties from irregularly

distributed data with measurement errors and underlying trends. The spatial estimator gives an optimum (minimum error variance) estimate and can be used to provide information on the design of optimum sampling networks.

II. THEORETICAL BACKGROUND

In this section we briefly develop the fundamental theory of spatial estimation. Mathematical details will be kept to a minimum and deferred to Appendix A. Only the fundamental relations will be presented. Our ultimate goal is to use the spatial estimator to produce a reasonable contour map with some measure of confidence. For the water level data, once the map is produced other hydrogeological parameters can be derived.

Construction of contour maps of areally distributed data presents problems because the data are often irregularly located in a region. The first step in contouring is usually to produce a regular mesh or grid of control points through interpolation. The grid may be produced in a variety of ways, ranging from estimates at grid points based on the nearest observation, to estimates derived from trend surfaces of all observations. Once the grid is generated contours or isopleths (i.e., lines connecting points of equal value) are produced by simple interpolation between grid points. Finally, the contours are drawn by a plotter to yield the desired results.

In this section we discuss the development of an "optimal" estimator which can be used to estimate control points on a grid for eventual contouring. In section 1, we define the spatial estimation problem. An estimator to solve this problem is discussed in section 2. The problem of drift estimation is discussed and solved in sections 3 and 4.

II-1. Spatial Estimation Problem

In this section we define the spatial estimation problem and assumptions necessary to obtain a reasonable solution. Recall the most critical part of contour map generation lies in the generation of the grid of control points - this is the fundamental spatial estimation problem, simply stated (see Figure 1)

GIVEN a set of irregularly located measurement points in a well-defined region, FIND the "best" (minimum error variance) linear estimates of control points at desired locations within the region.

Actually spatial estimation can be thought of as "stochastic interpolation", since a minimum variance estimator is designed to provide point estimates between and around existing measurements.

Figure 1. Spatial Estimation Problem for Grid Generation

A natural phenomena can be characterized by the distribution in space of one or more variables, e.g. the distribution of altitude in a horizontal space characterizes a topological surface. Let $z(\underline{x}_i)$ be the value of the variable z at point $\underline{x}_i$ in space (1, 2, or 3 dimensional). In the estimation approach, $z(\underline{x}_i)$ is interpreted as a particular realization of a random function $Z(\underline{x})$. More formally, $z(\underline{x}_i)$ is defined as a regionalized variable, i.e., a function with spatial distribution which varies randomly from one location to another. Spatial estimation theory is based on the observation that the variabilities of all regionalized variables have a particular structure, i.e., they are similar and the measure of similarity can be expressed in some way. For example, if we make three measurements of water potential, two that are in close proximity to one another and one not as close, we may find that the close measurements agree and even the third measurement is also related to the other two measurements, to some extent. The statistical measure of similarity or correlation and continuity between measurements as a function of distance between them is called the variogram and it forms the basic "model" which must be determined before estimation can commence. Before we get into the practical aspects of spatial estimation, let us develop the theoretical basis of the techniques.

In most cases of spatial estimation, the number of measurements or data points are sparse for a given region, e.g. borehole data in an exploratory ore deposit. Thus, in order to make the technique

mathematically reasonable we impose the following constraints on the function called the intrinsic hypothesis. The regionalized variable satisfies the intrinsic hypothesis if for all h (a spatial distance increment) the first and second moments of the difference $Z(\underline{x+h}) - Z(\underline{x})$ depend only on the distance between the two points $\underline{x+h}$ and $\underline{x}$ and not on their individual locations, i.e. [3,4]

$$E\{Z(\underline{x+h}) - Z(\underline{x})\} = m(h)^{\dagger} \quad (2.1)$$

$$\text{Var}\{Z(\underline{x+h}) - Z(\underline{x})\} = E\{(Z(\underline{x+h}) - Z(\underline{x})) - m(h)\}^2 = 2\gamma(h) \quad (2.2)$$

where $\gamma(h)$ is the variogram of the difference. This hypothesis means that the expected value of Z is a constant and that two different locations separated by the same distance h have the same probability distribution. The intrinsic hypothesis need only hold over the distance used to make an estimate, not throughout the entire field of interest. This property is called local stationarity.

We define the following general measurement model for the data as

$$Z(\underline{x}) = r(\underline{x}) + m(\underline{x}) + e(\underline{x}) \quad (2.3)$$

[†] E is the standard expected value operation.

where

- $r(\underline{x})$ is the residual value at location $\underline{x}$;
- $m(\underline{x})$ is the systematic error or drift at $\underline{x}$; and
- $\epsilon(\underline{x})$ is the random measurement error at $\underline{x}$.

In this model we relax the assumption of constant mean (equation (2.1)) and assume that the drift is a slowly varying function which can be approximated by a polynomial, i.e.,

$$m(\underline{x}) = \sum_{j=0}^M a_j f^j(\underline{x}) \quad (2.4)$$

where

- a_j are unknown coefficients; and
- f^j are monomials in the space under consideration.

The residual is defined to be zero mean with stationary increments as in (2.2). The random measurement errors are assumed to be zero mean, uncorrelated with $z(\underline{x})$, and itself, i.e.,

$$\begin{aligned} E\{\epsilon(\underline{x}_i)\} &= 0 \quad \forall i, \\ \text{Cov}\{\epsilon(\underline{x}_i), \epsilon(\underline{x}_j)\} &= \sum_{(N \times N)} = \text{diag} [\sigma_\epsilon^2(1) \dots \sigma_\epsilon^2(N)] \\ \text{Cov}\{\epsilon(\underline{x}_i), z(\underline{x})\} &= 0 \quad \forall i, \underline{x}. \end{aligned} \quad (2.5)$$

Using the measurement model of (2.3) we can now precisely define the spatial estimation problem as

GIVEN a set of measurement data $\{z(\underline{x}_i)\}$, $i = 1, \dots, N$ and the measurement model of equations (2.3 - 2.5)

$$z(\underline{x}_k) = r(\underline{x}_k) + m(\underline{x}_k) + \epsilon(\underline{x}_k), \quad (2.6)$$

FIND the "best" linear, unbiased, minimum error variance estimate $\hat{z}(\underline{x}_k)$ of z at point $\underline{x}_k$.

This completes the definition of the spatial estimation problem in the next section, we discuss a solution to this problem.

II-2. Spatial Estimation Theory

The spatial estimation problem can be solved using optimization theory results by formulating the problem properly. Here we show how to solve the problem using Lagrange multiplier techniques. To be more precise, we would like to find the linear estimator

$$\hat{z}(\underline{x}_k) = \sum_{i=1}^N \lambda_i z(\underline{x}_i) = \underline{\lambda}^T \underline{z} \quad (2.7)$$

where $\underline{\lambda}^T := [\lambda_1 \dots \lambda_N]$ and $\underline{z}^T := [z(\underline{x}_1) \dots z(\underline{x}_N)]$

such that

$$E\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} = 0 \quad (\text{unbiased}) \quad (2.8)$$

and

$$\sigma_k^2 = \text{Var}\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} \text{ is minimum (minimum variance).} \quad (2.9)$$

The solution to the spatial estimation problem is found by minimizing the error variance of (2.9) subject to the constraint of (2.8). The optimum linear estimator of (2.7) is found using Lagrange multiplier techniques. It is shown in Appendix A that the estimation problem can be reduced to solving the linear equations

$$A\theta = \underline{D}_k \quad (2.10)$$

where A is an $(N+M+1) \times (N+M+1)$ matrix with entries specified by the variogram and drift models;

θ is an $(N+M+1)$ vector of unknown weights and multiplier coefficients, i.e.,

$$\theta^T := [\underline{\lambda} \mid \underline{\mu}]^T; \text{ and}$$

$\underline{d}_k$ is an $(N+M+1)$ vector reflecting distances between control data at position $\underline{x}_k$.

It is also shown that the associated error variance can be estimated from the weights as

$$\sigma_k^2 = \underline{w}^T \underline{d}_k \quad (2.11)$$

This error variance is a theoretical model and it can be interpreted as a prediction of how much different realizations of the surface can vary with the same underlying variogram and drift.

Thus, the technique generates point estimates $\hat{z}(\underline{x}_k)$ and a measure of the precision σ_k^2 . Note that if the error is assumed Gaussian, i.e., $(z - \hat{z}) \sim N(0, \sigma_k^2)$, then we can construct a 95% confidence interval $(\hat{z}(\underline{x}_k) - 2\sigma_k, \hat{z}(\underline{x}_k) + 2\sigma_k)$ to evaluate the estimator quality.

We will examine the practical aspects of spatial estimation in another section, here we would like to investigate some properties and extensions of the technique.

Property 1: The linear point and variance estimator $(\hat{z}, \sigma)$ take into account four essential and intuitive facts.

- (i) Geometry (location) of the sample configuration in A ;
- (ii) A structural (statistical) model of the phenomenon variability characterized by the variogram model, γ ;
- (iii) Geometry of the domain to be estimated, $\text{Var}(z-\hat{z})$ expressed in σ_k^2 ; and
- (iv) Distances between control points to be estimated and samples in $\underline{u}_k$.

Property 2: Assume no measurement error ϵ_i ; then $\hat{z}$ is an exact interpolator, i.e., $\hat{z}_k = z_k$ and $\sigma_k^2 = 0$. Thus, the spatial estimates pass directly through the measurement points.

Property 3: The error variance estimate σ_k^2 does not depend on the particular values of the data $\{z(\underline{x}_k)\}$ but only the locations $\{\underline{x}_k\}$.

Property 4: The matrix A depends only on the locations of the samples, i.e., $\{\underline{x}_i\}$, $i = 1, \dots, N$.

This property indicates that two identical sample configurations produce the same matrix A . This property is important if we use the same data set to estimate points on a grid because we need only invert

At once, since for $\hat{z}(\underline{x}_p)$ and $\hat{z}(\underline{x}_q)$ we solve

$$\underline{\theta}_p = A^{-1} \underline{b}_p \text{ and } \underline{\theta}_q = A^{-1} \underline{b}_q .$$

It can be shown that the solution $\underline{\theta}$ is invariant under a change of coordinates, i.e., the same weights $(\{\lambda_i\}, \{\mu_i\})$ result if all sampled points $\{z(\underline{x}_i) - z(\underline{x}_j)\}$ are translated the same amount $\underline{h}$. Thus, if data are collected on a regular pattern, it is not necessary to solve the equations repeatedly as before. This procedure is usually true when N is small; however, for large N a "neighborhooding" technique is applied and A changes for each estimate.

Before we digress from this discussion, it should be noted that we have been concerned primarily with "punctual" spatial estimation, i.e., minimum variance estimation of a "point" in space. The general theory [5] has been developed for the estimation of $z(\underline{x}_k)$ at location $\underline{x}_k$ from samples $\{z(\underline{x}_j)\}$, $j = 1, \dots, N$ when

- (i) z_k is a point value taken by z at $\underline{x} = \underline{x}_k$; or
- (ii) $z_k = \frac{1}{v} \int_{v_0} z(\underline{x}) d\underline{x}$ is the average of $z(\underline{x})$ over the block v_0 of volume v and centered at $\underline{x} = \underline{x}_k$; or
- (iii) $z_k = \frac{1}{V} \int_V z(\underline{x}) d\underline{x}$ is the average value of $z(\underline{x})$ over the whole field V ; or

(iv) $z_k = \int z(x_1 + \alpha) \rho(\alpha) d\alpha$ is a weighted moving average of $z(\underline{x})$; or

(v) $z_k = \text{grad } z(\underline{x})$ is components of the gradient at $\underline{x} = \underline{x}_k$
 $\underline{x} = \underline{x}_k$ (i.e., dip and strike of a geological layer).

Thus, spatial estimation techniques are not only limited to punctual estimation. In the next section we discuss the problem of drift estimation and show how it can also be used alternately to solve the spatial estimation problem.

11-3. Drift Estimation Problem

In cases where the variable to be measured shows a systematic fluctuation along certain directions we say there is drift present. For example, in hydrology, estimation of water potential in a sloping (linear) plane requires one to account for the large regional systematic trend. Drifting can occur in two different manners

- (1) regional or slow varying systematic behavior over a given region or large neighborhood; or
- (2) punctual or local fluctuations which vary from neighborhood to neighborhood.

Previously we found it necessary in our measurement model of (2.6) to account for the drift when deriving the spatial estimator. The spatial estimator did not produce estimates of the drift coefficients $\{a_i\}$ of (2.4); however, in some situations it is necessary to estimate the precise drift model and identify these coefficients. The estimation of drift is used to provide residuals for variogram analysis. In this instance we must obtain an analytical expression for drift which is valid over the region under investigation. Drift can also be used for map analysis; i.e., examination of smooth changes or general tendencies of the variable of interest. Punctual estimates are required to contour the drift for this type analysis.

The "regional" and "punctual" drift estimation problem is

GIVEN a set of measurement data $\{z(\underline{x}_i)\}$, $i = 1, \dots, N$ the measurement model of (2.3) - (2.5), and corresponding assumptions, i.e.,

$$Z(\underline{x}) = r(\underline{x}) + m(\underline{x}) + e(\underline{x}).$$

FIND the "best" linear, unbiased, minimum error variance estimate $\hat{m}(\underline{x}_k)$ of $m(\underline{x})$ at a point $\underline{x}_k$ or over the entire data region defined by $\{z(\underline{x}_i)\}$.

In the next section, we show how to solve this problem using the same approach as the spatial estimator. In fact, we show that after estimating the drift the spatial estimation problem can be solved with a simplified set of linear equations which yield results identical to those derived previously. Therefore, drift estimation leads to an alternate approach for solving the spatial estimation problem as well.

II-4. Drift Estimation Theory

In this section, we solve the drift estimation problem - first, for punctual drift estimates and second for regional drifts. We follow the technique of Lagrange multipliers used in Appendix A.

II-4.1 Punctual Drift Estimation

As before this problem can be formulated as finding the linear, minimum variance, unbiased estimate

$$\hat{m}(\underline{x}) = \sum_{i=1}^N \lambda_i z(x_i) = \underline{\lambda}^T \underline{Z}^{\dagger} \quad (2.12)$$

such that

[†]Here we use the same notation as before to only show the mathematical similarity of the problems.

$$E\{m(\underline{x}) - \hat{m}(\underline{x})\} = 0 \quad (\text{unbiased})$$

and

$$\sigma_M^2 = \text{Var}\{m(\underline{x}) - \hat{m}(\underline{x})\} \text{ is minimum} \quad (\text{minimum variance}) \quad (2.13)$$

It is easy to show that the optimal drift estimator can be found by minimizing the error variance subject to the unbiasedness constraint. Again using Lagrange multipliers the drift estimation problem reduces to solving the set of linear equations (see Appendix A for details).

$$D\underline{\eta} = \underline{\beta}_k \quad (2.14)$$

where D is an $(N+M+1) \times (N+M+1)$ matrix with entries specified by the variogram and drift models;

$\underline{\eta}$ is an $(N+M+1)$ parameter vector given by

$$\underline{\eta}^T := [\underline{\lambda}^T \mid \underline{\mu}^T]; \text{ and}$$

$\underline{\beta}_k$ is an $(N+M+1)$ vector at position $\underline{x}_k$.

The associated error variance equivalent to (2.11) is given by

$$\sigma_M^2 = \underline{\eta}^T \underline{\beta}_k \quad (2.15)$$

It then follows from (2.14) that the desired estimates of the $\{a_i\}$ of (2.4) can be found as (see Appendix A for details)

$$\underline{\hat{a}} = W\underline{z} \quad (2.16)$$

where W is an $(M+1) \times N$ matrix of weights, and the associated error variance can also be estimated as well.

Thus, with the optimal drift coefficients estimated, the residuals can then be calculated at each data point since

$$\hat{r}(\underline{x}) = z(\underline{x}) - \hat{m}(\underline{x})$$

For point estimates, not at data points, the residuals must be estimated from a simple set of linear equations. The optimal spatial estimate is given by

$$\hat{z}(\underline{x}_k) = \hat{r}(\underline{x}_k) + \hat{m}(\underline{x}_k) \quad (2.17)$$

It has been shown by Matheron, that spatial estimates obtained in this fashion produce identical results to those of Section II-2. This equation is the result of the so-called additivity theorem [5] which shows that

$$\hat{z}(\underline{x}_k) = \hat{m}(\underline{x}_k) + \underline{\lambda}^T (\underline{z} - \hat{m})$$

II-4.2 Regional Drift Estimation

Following the same strategy for "regional" drift, i.e., one drift function to model the trend of the entire region, it is possible to derive similar equations to (2.14). Thus, to estimate drift over a region we must construct

$$\hat{m}(\underline{x}) = \sum_{i=0}^M \hat{\alpha}_i f^i(\underline{x}) = \underline{\hat{\alpha}}^T \underline{f} \quad (2.18)$$

The relation implies that we must calculate the $\{\alpha_s\}$, $s = 0, \dots, M$ and $m(\underline{x})$ is the drift of $z(\underline{x})$ for any $\underline{x}_i$ such that $|\underline{x} - \underline{x}_i| \leq \rho$ where ρ defines the regional neighborhood. We assume that N punctual samples of $Z(\underline{x})$ at $\underline{x}_j$, $j = 1, \dots, N$ are drawn. We define M estimates $\hat{\alpha}_s$ for each α_s which are a linear combination of the N samples inside the neighborhood of radius r around some $\underline{x}_k$, i.e.,

$$\hat{\alpha}_s = \sum_{i=1}^N \lambda_i^s z(\underline{x}_i) = \underline{\lambda}_s^T \underline{z} \quad s = 0, \dots, M \quad (2.19)$$

subject to the usual unbiased, minimum variance constraints.

After minimizing as in Appendix A, we obtain the linear equations

$$D\phi_s = \underline{\xi}_s, \quad s = 0, \dots, M \quad (2.20)$$

where D is given in (2.14) and

$$\begin{aligned} \phi_s^T &= (\lambda_s^T : \mu_s^T), \quad s = 0, \dots, M \\ \xi_s^T &= (\underline{u}_s^T : \underline{e}_s^T), \quad \underline{e}_s^T \text{ a unit row vector} \end{aligned}$$

Thus solving (2.20), $M+1$ times we obtain estimates for $\{\alpha_s\}$ and the corresponding error variance is given by

$$\sigma_{\alpha_s}^2 = \underline{\phi}_s^T \underline{\xi}_s = \mu_s^s$$

Once the $\{\alpha_s\}$ are estimated the drift can be removed from samples and the residuals can be estimated using simple spatial estimation techniques as before. This completes the theoretical discussion on spatial estimation theory, we summarize the results in Table I. In the next chapter we discuss the practical issues involved in spatial estimation.

III. PRACTICE OF SPATIAL ESTIMATION

In this section we discuss some of the more practical issues involved in spatial estimation. Theoretically, once the variogram and drift

TABLE 1. SPATIAL AND DRIFT ESTIMATOR SUMMARY

TYPE	ESTIMATOR	λ -SOLUTION	ERROR VARIANCE	EQUATIONS
SPATIAL	$\hat{z}(\underline{x}_k) = \underline{\lambda}^T \underline{z}$	$A\underline{\theta} = \underline{D}_k$	$\sigma_k^2 = \underline{\theta}^T \underline{D}_k$	(2.10, 2.11)
PUNCTUAL DRIFT	$\hat{m}(\underline{x}_k) = \underline{\lambda}^T \underline{z}$ $\hat{\underline{a}} = \underline{W} \underline{z}$	$D\underline{\eta} = \underline{D}_k$ ---	$\sigma_M^2 = \underline{\mu}^T \underline{r}_k$ $\sigma_a^2 = \text{Cov}(\underline{a} - \hat{\underline{a}})$	(2.14, 2.15) (2.16)
REGIONAL DRIFT	$\hat{m}(\underline{x}) = \underline{\hat{a}}^T \underline{r}$ $\hat{\underline{a}} = \underline{\lambda}_S^T \underline{z}$	--- $D\underline{\phi}_S = \underline{\epsilon}_S$	--- $\sigma_{\alpha_S}^2 = \underline{\mu}_S^S$	(2.18, 2.19, 2.20)

are determined, one need only solve a set of linear equations.

Besides the numerical difficulties of matrix inversion etc., the major problem in spatial estimation is "identifying" the spatial model - variogram and drift. In fact, it is necessary to know the drift in order to calculate the variogram. Typically, this impasse is resolved by iteration until satisfactory results are achieved.

We will discuss the problem of "fitting" a spatial model to samples in this section. First, we describe properties and procedures to estimate the variogram and drift from samples in sections 1 and 2. Then we discuss some of the practical aspects of spatial estimation which can be used. Finally we discuss some graphical techniques to display the spatial results.

III-1. Variogram

In this section we discuss the properties of the variogram - the fundamental spatial model relating (statistically) the similarity of samples. Recall that the variogram is defined as the variance in the increment of regionalized variables, i.e.,

$$\gamma(\underline{n}) := 1/2 \text{ Var}\{z(\underline{x}+\underline{n}) - z(\underline{x})\} \quad (3.1)$$

where the increments satisfy the stationarity requirements of the intrinsic hypothesis of (2.2). Note that in dealing with the

increments rather than the spatial variables themselves, the variogram is more general than the usual covariance because in cases that the covariance does not exist the variogram does (e.g. Wiener process). The variogram is related to the covariance by (see Figure 2).

$$\gamma(\underline{n}) = C(0) - C(\underline{n}) \quad (3.2)$$

where $C(h) := \text{Cov}(z(\underline{x}+h), z(\underline{x}))$.

Let us examine some of the fundamental properties of the variogram

Property 1: The variogram starts at 0, i.e., $\gamma(\underline{n}) = 0^+$

Property 2: The variogram is a positive definite, even function, i.e.,

$$\gamma(\underline{n}) = \gamma(-\underline{n}) \geq 0 \quad \forall \underline{n}$$

Property 3: When the variance exists, the variogram has a limit or sill, i.e.,

$$\lim_{\underline{n} \rightarrow \infty} \gamma(\underline{n}) = \text{Var}\{z(\underline{x})\} = C(0)$$

⁺ In some cases, the variogram may not start at zero, but some other positive value then it is said to be discontinuous and exhibit the "nugget effect" (see [4] for details), i.e., $\gamma(\underline{n}) = C_0$ for $\underline{n} > \underline{\epsilon}$ and $\underline{\epsilon}$ small.

$$\gamma(h) = C(0) - C(h)$$

Figure 2. Covariance and Variogram

Property 4: The variogram possesses a range - the point "a" on the variogram (Figure 2) beyond which the samples are no longer related or correlated, i.e., there exist an a such that for $|n| \geq a$, $\text{Cov}(z(\underline{x}), z(\underline{x}+n)) = 0$.

Property 5: The variogram grows more slowly than a parabola, i.e.,

$$\lim_{|n| \rightarrow \infty} \frac{\gamma(n)}{|n|^2} = 0 \quad \text{when } |n| \rightarrow \infty$$

The first four properties of the variogram are depicted in Figure 2 along with the corresponding covariance function. Note that for values of z with $|n| \geq a$ the samples are uncorrelated. Property 5 can be used to detect the presence of "drift", if not satisfied.

Table II depicts some of the common variograms which satisfy the properties discussed. Note that some variograms do not possess all of these properties (e.g. a linear variogram does not possess a sill).

Finally we note that if the regionalized variables do not exhibit the same behavior in every direction (isotropy) they are called anisotropic, i.e., the variograms calculated in different directions of space differ. When they are identical, the variogram is termed isotropic. Departure from isotropy can be classified as geometric and zonal - both can be corrected. These classifications evolved from the manner in which the variograms can be reduced to isotropic

TABLE 11. VARIOGRAM MODELS

TYPE	FORMULA	SLOPE AT THE ORIGIN	RANGE	SILL
Nugget effect	$\gamma(h) = C(1-\delta)$	∞	0	C
Power	$\gamma(h) = \omega h ^\lambda$	$\begin{cases} 0 < \lambda < 1 & \infty \\ \lambda = 1 & \omega \\ 1 < \lambda < 2 & 0 \end{cases}$	∞	∞
Spherical	$\gamma(h) = \begin{cases} \omega \left[\frac{3}{2} \frac{h}{a} - \frac{1}{2} \left(\frac{h}{a} \right)^3 \right] & h \leq a \\ \omega & h > a \end{cases}$	$3\omega/2a$	a	ω
Gaussian	$\gamma(h) = \delta [1 - \exp(- h ^2/a^2)]$	0	$\sqrt{3}a$	ω
Exponential	$\gamma(h) = \delta [1 - \exp(- h /a)]$	ω/a	$3a$	ω
Logarithmic or de Wijsian	$\gamma(h) = 3a \ln(h/a)$	$3a$	∞	∞

Geometric anisotropy - is the case where anisotropy can be corrected by a linear transformation of coordinates (see [4]); and

Zonal anisotropy - the variogram is a nested structure in which each component has a variogram of its own structure.

This completes the discussion of variogram properties. In the next section we discuss the problem of estimating or identifying the variogram from raw sample data.

III-2. Variogram Estimation/Identification

Variogram identification from raw data is the most crucial part of the spatial estimation process and probably the least understood. Prior to the actual estimation, it is necessary to fit an experimental variogram to a theoretical model which will ensure mathematical consistency of the calculations. Thus, the practice of variogram identification is concerned with:

- (i) estimating the "raw" or experimental variogram and drift from sample data;
- (ii) fitting a theoretical variogram and drift to the experimental; and
- (iii) checking the validity of the fit.

An unbiased estimator for the variogram is [9]

$$\hat{\gamma}^*(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (z(\underline{x}_i+h) - z(\underline{x}_i))^2 \quad (3.3)$$

where $N(h)$ is the number of pairs of points separated by distance h .

If drift is present, then it can be shown that (3.3) is a biased[†] estimator for the variogram. The drift can also be estimated using the experimental drift estimator on the sample data, i.e.,

$$\hat{m}^*(h) = \frac{1}{N(h)} \sum_{i=1}^{N(h)} (z(\underline{x}_i+h) - z(\underline{x}_i)) \quad (3.4)$$

The experimental variogram can then be drift-corrected and fit. The drift corrected variogram is given by

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z(\underline{x}_i+h) - z(\underline{x}_i) - \hat{m}^*(h)]^2$$

An interactive computer algorithm called VARIFIT was developed based on the K603 Kriging algorithm developed at USGS, Tacoma [15].[†] VARIFIT enables the user to:

[†] If the drift is constant, then it is unbiased.

- (1) Calculate the estimated variogram, drift, and corrected-variogram; and
- (2) Interactively fit a theoretical variogram (Table II) to the estimated data; and
- (3) Check the validity of the fit.

A typical VARIFIT output is shown in Figures 3, 4, 5. In Figures 3 and 4, we see the estimated variograms and drift calculated from the sample data. In Figure 5, we see the result of a theoretical (interactive) fit of a spherical variogram to the experimental variogram of Figure 3. It should be noted that anisotropic variograms in four directions can also be identified using this algorithm.[†]

Another approach to the drift and structure identification problem is to make use of an algebraic property that higher order differencing of variables filters out polynomials in the expectation. The original random function $Z(x)$ is called an intrinsic random function of order k (abbreviated k -IRF) where k is the highest degree polynomial filtered. The purpose of taking increments is to produce a stationary regionalized variable from one with a drift. This is the n -dimensional analog of the Box-Jenkins approach to time series

[†] The algorithm is on the CDC 7600 and can be obtained by typing
.292100:SPACEST[VARIFIT].

Figure 3. Experimental Variogram Estimates

Figure 4. Experimental Drift Estimate

Figure 5. Theoretical Variogram Fit of Estimated Variogram

analysis [13]. The advantage is that the covariance structure of the spatial variable can be estimated without the effects of the drift. This is done by developing the generalized covariance of the k-IRF which differs from the variogram, which is only legitimate for the 0-IRF case.

There are various classes of functions that satisfy the conditions of a generalized covariance, but one class with nice properties for identification purposes (that is, linear in the coefficients) is the class of polynomial generalized covariances. The form of these generalized covariances, which depends on the order of the increment, is listed in Table III.

Note that for $k = 0$, the only covariance function is a linear one which is much more restrictive than the variograms given in Table II. How does the generalized covariance compare to the variogram in the 0-IRF case? Let $Z(\lambda) = Z(\underline{x}_i) - Z(\underline{x}_j)$; then it can be shown that

$$K(\underline{x}_i - \underline{x}_j) = -\gamma(\underline{x}_i - \underline{x}_j)$$

Thus, for a non-stationary process, we can produce a stationary one by forming the k^{th} order increments. We can then estimate, from the generalized covariance, the covariance structure of the stationary process. It can be shown that the estimators designed previously are still valid (i.e., same structure equation) with the generalized

TABLE III. GENERALIZED COVARIANCE MODELS

DRIFT	k	POLYNOMIAL GENERALIZED COVARIANCE MODEL*
Constant	0	$K(\underline{h}) = C\delta - b_0 \underline{h} $
Linear	1	$K(\underline{h}) = C\delta - b_0 \underline{h} + b_1 \underline{h} ^3$
Quadratic	2	$K(\underline{h}) = C\delta - b_0 \underline{h} + b_1 \underline{h} ^3 - b_2 \underline{h} ^5$

*With coefficient constraints:

(Two-dimensional space):

$$C \geq 0, b_0 \geq 0, b_2 \geq 0, b_1 \geq -(10/3) \sqrt{b_0 b_2};$$

(Three-dimensional space):

$$C \geq 0, b_0 \geq 0, b_2 \geq 0, b_1 \geq -10 \sqrt{b_0 b_2}.$$

covariance replacing the variogram and only a simple system (no drift equations need be solved (see [8] for details).

Once we have decided on the type of a theoretical variogram or generalized covariance, we must make sure that the fit is reasonable. Tests must be performed to insure the validity of the variogram and drift models [11]. The technique employed is the successive estimation of all of the data points, ignoring each of them in turn, one by one. We then verify that there is no systematic error and compare the calculated errors (difference between the estimated and real values) with the theoretically predicted standard deviations (σ_k) to assure consistency. A statistical analysis is carried out on the standard errors, checking that they are zero mean and unit variance. This technique can be utilized for comparing several models and determining the best fit. The first selection criterion is minimum mean squared error and secondly the standard error is close to unity. The successive estimation technique is depicted in Figure 6. Here we see that data point 1 has been eliminated from the data set and estimated based only on the remaining data values. The deviation from the actual values, i.e., $\Delta z_i = z_i - \hat{z}_i$ are calculated for the entire data set and then the sample error statistics are estimated. The sample statistics are:

Figure 6. Successive Estimation Technique

- (i) Systematic Error is zero. ($E(\Delta z_i) = 0$);
- (ii) Standard Error is unit variance. ($\Delta z_i \sim N(0,1)$);
- (iii) RMS Error is minimum ($\min \sqrt{\Delta z_i^2}$)

The validity test results are summarized in Table IV where the practical estimators used to validate the models are shown. This completes the discussion of variogram estimation. In the next section we discuss the more pressing problem - that of estimating the variograms when a drift is present.

III-3. Variogram Estimation In The Presence Of Drift

In this section we briefly discuss the problem of identifying the variogram from samples when drift is present. Let us assume that there exists a drift and we ignore it, then the variogram estimate of (3.3) is biased due to the neglected drift, i.e.

$$\hat{\gamma}(h) = \gamma_{KDE}(h) + E\{[\mu(x+h) - \mu(x)]^2} \quad (3.4)$$

when there exists a simple regional drift, we can subtract $\mu(x)$ from $Z(x)$ to obtain the residuals and identify the residual variogram. It is known that identifying the variogram of the residuals gives a biased estimate of the true variogram; however, this bias can be neglected for small distances. The closeness of the residual

TABLE IV. SUCCESSIVE ESTIMATION VALIDITY TEST

TEST	THEORY	PRACTICE
SYSTEMATIC ERROR	$E(\Delta z_i) = 0$	$\frac{1}{N} \sum_{i=1}^N \Delta z_i \approx 0$
STANDARD ERROR	$\frac{\Delta z_i}{\sigma_i} \sim N(0,1)$	$\frac{1}{N} \sum_{i=1}^N \left(\frac{\Delta z_i}{\sigma_i} \right)^2 \approx 1$
MINIMUM ROOT MEAN SQUARED ERROR	$\min \sqrt{\Delta z_i^2}$	$\left[\frac{1}{N} \sum_{i=1}^N \Delta z_i^2 \right]^{1/2}$ is minimum

where $\Delta z_i := z(\underline{x}_i) - \hat{z}(\underline{x}_i)$

variogram to the true variogram depends on the appropriateness of the functions selected to represent the drift and variogram as well as the size of the chosen neighborhood.

A method to estimate the drift and variogram can be summarized [9] as:

- (i) Assume a theoretical variogram and drift function;
- (ii) Estimate the coefficients of the drift polynomial $\{a_i\}$ (2.19);
- (iii) Using this drift calculate the residuals of (2.3);
- (iv) Estimate the variogram of the residuals using (3.3);
- (v) Validate the results using Table IV; and
- (vi) If acceptable, stop. If not go to (i).

Local or punctual drift estimation can be performed using the standard spatial estimator setup of section II and then estimating the corresponding drift coefficients. In the next section, we discuss various techniques to display the data.

III-4. Data Display Techniques

Two-dimensional spatial data has traditionally been displayed in contour maps, which was the basic idea in introducing the spatial estimation. Skipping ahead, a typical contour map for a particular groundwater aquifer is shown in Figure 12. For simple structures like

these aquifers the contours provide an effective means of displaying the data. Also, contours are a convenient way of displaying the one-sigma error maps (see Figure 13) since the investigator can overlay both maps (estimated and one sigma) to decide on the regions of highest confidence.

Unfortunately, for more complex structures it is sometimes difficult to identify the value represented by a contour (see Figure 32). An alternative to contours are gray or pseudo color images. The Signal and Image Processing Research Group (SIPRG) at LLNL has the capability to generate displays of two dimensional data either in gray or color. Representative color images of the simple aquifer and corresponding one-sigma error map is shown in Figures 15 and 16. The advantage of color is that various colors can be assigned to various values of Z displayed (see the spectrum shown on the image) which are easy to interpret. In fact regions of minimum error can easily be located by the black assignments in Figure 16. The SIPRG also has an "interactive" capability which enables the user to dynamically select various color assignments and rotate them through the image. In the near future, capability will be developed to generate color images of the data and overlay the one-sigma error contours (in white) so that the investigator can easily analyze the data. This completes the discussion of display techniques. In the next section we discuss the application of these techniques to representative data sets.

IV. APPLICATION OF SPATIAL ESTIMATORS

In this section we discuss the application of the spatial estimation techniques to real data sets. We apply the "practice" of spatial estimation to representative measurements of water and geological formation depth data in order to evaluate the performance of the estimator and produce contour maps for comparative purposes. First, we evaluate the estimator performance on two groundwater aquifer systems and then investigate the subsurface structure of a geological formation from borehole data. The aquifer system structures are simple, while the rock depth information is much more complex. The first aquifer we investigate is located in Toppenish Creek, Washington.

IV-1 CASE STUDY: Toppenish Creek Basin, Washington

The purpose of this study is to investigate the performance of spatial estimation techniques on a simple groundwater aquifer system. The data was obtained from J. Skrivan, USGS, Tacoma, Washington. The data set is a measure of the September 1971 water levels at Toppenish Creek Basin, Washington.

The Toppenish Creek data is shown in Figure 7. We see that the 76 measurements are distributed irregularly in the region and contours of the raw data shows that the major hydraulic gradient is from the SE to NW direction.

FEET

Figure 7. Toppenish Creek Basin Raw Data (In Feet).

The spatial estimator will be applied to generate a grid of (22 x 22) uniformly spaced sample estimates and then contoured. Note that the estimator will be used to "interpolate" between measurement points and "extrapolate" in regions without data.

First, we must identify a structural model (variogram and drift) from the data. Following the procedure outlined in section III-2, the estimated variograms $\hat{\gamma}^*$, $\hat{\gamma}$ and drift $\hat{m}^*$ are calculated. A set of sample anisotropic/isotropic variograms are estimated and as expected the NW/SE variogram (direction of the hydraulic gradient) increased at a rate faster than h^2 (Property 5 of III-2) indicating the presence of a drift (see Figure 8). Note that the average variogram is dominated by the NW/SE and N/S variogram. An examination of the estimated drift-corrected variograms (Figure 9) still indicate a biased estimate (all drift not removed); therefore we decided to visually fit (using VARLFIT) the NE/SW variogram, since it should be essentially drift free (appears perpendicular to the major hydraulic gradient).

The estimated NE/SW variogram is shown in Figure 10. We note that a large number of pairs (~ 120) are at distances between 0 and 2 feet, which indicates that a careful fit of the initial points should be made, since the estimator will weight these closest points most heavily. The drift appears linear; however, it could be modeled either as linear or a constant since it is not very severe. We used

Figure 8. Anisotropic/Isotropic Estimated Variograms for Toppenish Creek Data

Figure 9. Drift-Corrected Anisotropic/Isotropic Estimated Variogram for Toppenish Creek Data

Figure 10. Estimated NE/SW Variogram for Toppenish Creek Basin, Washington

the automatic (generalized covariance) fit feature of the estimation algorithm[†] and also selected power function, linear, and spherical variograms with constant and linear drifts. After fitting these structures visually we applied the successive estimation method for validation. Each model was fit visually to the estimated NE/SW variogram and then the parameters of each particular structural model were adjusted until the standard error was approximately unity. Those with the smallest root mean-squared error (RMSE) were retained. These results are summarized in Tables V and VI. We found that the successive estimation technique appears to fit the closest points with most pairs. This is apparent when we examine Figure 11 which shows the "best" fits from Tables V and VI: generalized covariance, spherical, and linear variograms with constant drift. Note that in this figure we plot the "fits" to the NE/SW variogram since it is approximately drift-free. Note also that the initial slopes of the linear and spherical are practically identical, thus they yield similar validations. We also found that most pairs (range, sill) with initial slope 25 yielded identical statistics again confirming the heavy dependence on closely spaced pairs.

After the structural identification was completed, the spatial estimator was run over the data set. We chose the linear variogram

[†] We used the algorithm BLUEPACK [16] for our case studies and VARFIT for this variogram identification.

TABLE V. TOPPENISH CREEK STRUCTURAL MODEL SUMMARY

TYPE	MODEL	DRIFT
GENERALIZED COVARIANCE (AUTO)	$K(h) = 20.56 - 1.76 h $	Linear
VARIOGRAM 1	$\gamma(h) = 95 h ^{1.7}$	Constant
2	Same	Linear
VARIOGRAM 3	$\gamma(h) = 600L^{3/2} \frac{ h }{35} - 1/2 \left(\frac{ h }{35} \right)^3$	Constant
4	Same	Linear
VARIOGRAM 5	$\gamma(h) = 25 h $	Constant

TABLE VI. TOPPENISH CREEK STRUCTURE IDENTIFICATION/VALIDATION

TYPE	STANDARD ERROR	ROOT MEAN-SQUARED ERROR (ft)	MEAN ERROR (ft)
GENERALIZED COVARIANCE (AUTO)	0.84	4.77	0.03
VARIOGRAM 1	0.96	5.16	0.15
2	0.96	5.39	0.16
VARIOGRAM 3	0.99	4.67	0.05
4	0.98	4.97	0.09
VARIOGRAM 5	1.02	4.66	0.06

Figure 11. Identified Variograms (Near Origin) Against NE/SW Experimental Variograms for Toppenish Creek Basin, Washington

with a constant drift since it had the minimum RMS error and generated the contours shown in Figures 12 and 13. We could have selected the generalized covariance, or spherical model as well since the validation statistics were very close. In fact maps generated from these models were almost identical.

An examination of the resulting contour map of the Toppenish Creek Basin, indicates that most of the major features have been maintained. Note that the normalized map coordinates must be converted back to problem coordinates and the conversion factors are shown as (Δx , Δy) on Figures 12 and 13.

An examination of the standard errors indicates that the sample distribution appears symmetric; thus, a Gaussian approximation is reasonable, so the one-sigma values can be used to construct confidence intervals in various regions of the area. A close examination of the one-sigma error map in Figure 13 indicates that the upper NE corner and lower SW corners are the most uncertain areas. This is expected since no measurements are available in those regions.

A contour was also constructed for fitting a linear drift to the data. The results of this run using the linear variogram are shown in Figure 14. The contour represents a simplified fit to the raw data and it is close to the estimated contour of Figure 12 again indicating

Figure 12. Contour of Groundwater Levels (in Feet) at Toppenish Creek Basin, Washington, Using Spatial Estimation Techniques (Linear Variogram)

Figure 13. One Sigma Estimation Error Contours (in Feet) of Toppenish Creek Basin, Washington, Using Linear Variogram

Figure 14. Drift (Trend) Contours (In Feet) of
Toppenish Creek Basin, Washington Using
Linear Drift and Spatial Estimation Techniques

the simplicity of the structure. Pseudo-color image displays of the estimated region and corresponding one sigma error values were generated using SIPRG facility. These images are shown in Figures 15 and 16.

Summarizing the results of this case study, it appears that the spatial estimator can be used with confidence to reconstruct a regional contour map of a simple groundwater aquifer system. In the next section we consider another simple aquifer; however, this time with a limited number of data points.

IV-2. CASE STUDY: Todd Lake, Pennsylvania Natural Flow Conditions

The purpose of this case study is to investigate the performance of spatial estimation techniques on a simple groundwater aquifer system when the data are sparse. Todd Lake data was obtained from W. Murray, a hydrologist at LLNL, who worked on the aquifer. He developed a two-dimensional (partial differential equation) groundwater model of the Todd Lake region which we used as "truth" data to evaluate the performance of the spatial estimator over a limited data set. We used a set of 28 measurements (ten well measurements and 18 other inferred from the map) corresponding to the data derived by the hydrologist from measurements and a-priori knowledge of the region. A general layout of the Todd Lake region is shown in Figure 17. The major landmarks are shown, i.e., the lake, pond, and quarry. We decided to

Figure 15. Pseudo-color image of spatially estimated Toppenish Creek Basin, Washington using linear variogram.

Figure 16. Pseudo color image of one sigma errors for spatially estimated Toppenish Creek data using linear variogram

eliminate the quarry, since this data would create unnecessary problems for the estimator. It would require more data to resolve and not really provide anymore useful information for this analysis. The "truth" contour of the Todd Lake region is shown in Figure 18. The major hydraulic gradient appears to be from the SW to the NE. Contours from the measurement set are shown in Figure 19 for comparative purposes. Again note that the major features are preserved because of the particular measurement locations selected.

As before, we use the 28 data points and identify a structural model from the data. Anisotropic/isotropic variograms were estimated first indicating a drift in the NE/SW direction (hydraulic gradient) as shown in Figure 20. Again, the estimated drift-corrected variograms (Figure 21) appear biased due to inadequate drift estimation. We chose to use the NW/SE variogram to fit because it appears perpendicular to the major hydraulic gradient and essentially drift-free. The estimated variogram is shown in Figure 22. Note that the apparent drift-correction is small (difference between $\hat{\gamma}^*$ and $\hat{\gamma}$ curves) indicating the drift-free variogram structure.

The variogram and drift identification were again performed and the resulting variograms are given in Tables VII and VIII. After adjusting the model parameters to yield a standard error of unity, the "best" fit is a power variogram with a linear drift (variogram 2 in Table VIII), since it yields the minimum RMS error. The fit of this

Figure 18. Todd Lake "Truth" Groundwater Level Contour (In Feet)

Figure 19. Todd Lake Groundwater Level Contour Based on 28 Measurements (In Feet)

Figure 20. Anisotropic/Isotropic Estimated Variograms for Todd Lake Data

Figure 21. Drift-Corrected Anisotropic/Isotropic Variograms for Todd Lake Data

Figure 22. Estimated NW/SE Variogram for Todd Lake Data Using 28 Measurements

TABLE VII. TODD LAKE STRUCTURAL MODEL SUMMARY

TYPE	MODEL	DRIFT
GENERALIZED COVARIANCE (AUTO)	$K(h) = 2.17 - 0.04 \ln h + 6.07 \times 10^{-9} \ln h^3$	Linear
VARIOGRAM 1	$\gamma(h) = 3.0 \times 10^{-3} \ln h^{1.45}$	Constant
2	$\gamma(h) = 2.3 \times 10^{-3} \ln h^{1.45}$	Linear
VARIOGRAM 3	$\gamma(h) = 1.4 \times 10^{-2} \ln h^{1.2}$	Constant
4	$\gamma(h) = 8.0 \times 10^{-3} \ln h^{1.2}$	Linear
VARIOGRAM 5	$\gamma(\ln h) = 5.0 \times 10^{-2} \ln h$	Constant
6	$\gamma(\ln h) = 2.7 \times 10^{-2} \ln h$	Linear

TABLE VIII. TODD LAKE STRUCTURE IDENTIFICATION/VALIDATION

TYPE	STANDARD ERROR	RMS ERROR (ft)	MEAN ERROR (ft)
GENERALIZED COVARIANCE (AUTO)	0.51	4.12	0.76
VARIOGRAM 1	1	5.0	0.42
2	0.94	3.94	0.62
VARIOGRAM 3	0.94	5.6	0.48
4	1.04	4.04	0.73
VARIOGRAM 5	0.97	6.08	0.5
6	0.98	4.16	0.85

variogram to the NW/SE variogram data is shown in Figure 23 and it appears quite reasonable.

Contours of the Todd Lake region were produced using the model identified from the 28 data points. The map as well as the one-sigma errors are shown in Figures 24 and 25. Again the main features are preserved and the map looks reasonable (visually) when comparing it to the "truth" map of Figure 18. The error map indicates the regions of highest confidence (again closest to data points) and least confidence (edges).

The performance of the "sparse" structural model derived from the 28 data points was evaluated on the set of truth data and the results are shown in Table IX. The RMS and mean error are quite small as compared to the original statistics (in parenthesis) based only on 28 points; however, the standard error is no longer close to unity. This result is expected since that structural model was "identified" from the sparse 28 point data set. A "truth" variogram was fit to the truth data for comparative purposes and the validation results are also shown in Table IX. Note that the error statistics are invariant but the standard error is now unity. The invariance of the error statistics implies that both models are functions of the exponent (1.45 fixed) only. The truth variogram more closely fits the initial points. This result is confirmed in Figure 26. The identified "truth" variogram was run over the 28 point data and the estimated

Figure 23. Estimated NW/SE Variogram for Todd Lake
Using 28 Measurements

Figure 24. Contour of Groundwater Levels (In Feet) at Todd Lake Using Spatial Estimation Techniques (Power Variogram)

Figure 25. One-Sigma Estimation Error Contours (In Feet) of Todd Lake (Power Variogram)

Figure 26. Identified Truth and Sparse for the NW/SE Todd Lake Truth Data

TABLE IX. TODD LAKE STRUCTURAL ANALYSIS USING TRUTH DATA

MODEL	TYPE*	STANDARD ERROR	RMS ERROR (ft)	MEAN ERROR (ft)
SPARSE	$\gamma(n) = 2.3 \times 10^{-3} n^{1.45}$	0.16 (0.98)	0.63 (3.94)	0.015 (0.6)**
TRUTH	$\gamma(n) = 3.8 \times 10^{-4} n^{1.45}$	0.98	0.63	0.015

* Both with linear drift.

** Numbers in parenthesis based only on sparse data (28 points)

values were identical to those obtained from the sparse model. These results confirm again that the initial fit of close data points dominate the performance of the estimator.

The final analysis of estimator performance is shown in Figure 27 where relative error[†] contours are displayed. Here we see that the largest relative error is only about one percent which is quite good. In fact, the RMS error was only about 4.4 ft. with mean error of -1.9 ft. which is good for this data set. The largest regions of uncertainty appear where the estimator must extrapolate and there is no measurement data. The estimated values appear to give good estimates for the true values. Psuedo-color images of Todd Lake are shown in Figures 28 and 29 for comparative purposes.

Summarizing, it appears that for simple groundwater aquifers that reasonable contours can be obtained even with sparse data. In the next section we investigate a more complex structure - the paleozoic rock depths at the Nevada Test Site.

$$^{\dagger} \epsilon_{REL} = \frac{Z_{TRUE} - \hat{Z}}{Z_{TRUE}} .$$

Figure 27. Relative Error Contours for
Todd Lake Spatial Estimation

Figure 28. Pseudo-color images of spatially estimated Todd Lake.

Figure 29. Pseudo color image of one-sigma errors for spatially estimated Todd Lake data.

IV-3 CASE STUDY: Nevada Test Site, Paleozoic Rock Formations

The purpose of this study is to evaluate the performance of the spatial estimator on data from a complex but well known geological formation - the paleozoic rock at the Nevada Test Site (NTS).

The 1350 square mile NTS is one of the most exhaustively studied areas in existence. The NTS Geologic Data Base maintained by LLNL contains parameters describing the location coordinates, the lithologic contacts (alluvium, volcanic tuffs, and Paleozoic rocks), the distance to known and inferred faults, the depth to the water table, representative values for physiochemical properties of the rocks, etc. from over 1000 drill holes [17]. In addition, there is a data base of 4000 files of processed geophysical data vs. depth from logs and samples. Other geophysical data such as seismic reflections and gravity are also available for the area. These data are ideal for experimenting with spatial estimation techniques because of the following reasons:

1. Being computerized, they are readily available and easily accessible.
2. There is a very large quantity of data.
3. There is quite a variety of types of data.
4. General geology of the area is well understood.

5. Data are for properties similar to those relevant for the evaluation of a waste repository site, i.e., fault locations, density, lithologic units, basement depth, and water table location.

We studied the depth to the top of the Paleozoic rocks from 93 borehole data. The principal rock types and the studied area at NTS are shown in Figure 30. The Yucca Fault running roughly N-S divides the area into two parts. We studied the effect of fault on the estimated depth by considering no fault in the area for one case and with fault for another case.

First, we calculated the estimated variogram from the data following the procedure outlined in section III-2. A set of sample anisotropic variograms are shown in Figure 31. These variograms are biased because of the presence of drift in all directions.

Various tested structural models are summarized in Table X and the identification and validation results are summarized in Table XI. The RMS errors for those models without fault are slightly smaller than those for the equivalent models with fault. There are probably two reasons behind this observation. First, the vertical throw due to fault is relatively small as compared with the error. Second, there are fewer data points to estimate with when a fault is present because the fault effectively divides the data into two sets and no

Figure 30. Map shows principal rock types and studied area at NTS.

(From Ramspott and Howard:[18])

Figure 31. Anisotropic Variograms for Paleozoic Rock Depth at NTS

TABLE X. NTS PALEOZOIC ROCK DEPTH STRUCTURAL MODEL SUMMARY

TYPE	MODEL	DRIFT
WITH FAULT		
Generalized Covariance (Auto)	$k(h) = -4.4115 h + 2.1088 \times 10^{-6} h ^3$	Linear
Linear 1	$\gamma(h) = 9.15 h $	Constant
Linear 2	$\gamma(h) = 9.15 h $	Linear
Spherical A1	$\gamma(h) = 11700 \left[\frac{3}{2} \frac{ h }{2000} - \frac{1}{2} \left(\frac{ h }{2000} \right)^3 \right]$	Constant
Spherical A2	$\gamma(h) = 11900 \left[\frac{3}{2} \frac{ h }{2000} - \frac{1}{2} \left(\frac{ h }{2000} \right)^3 \right]$	Linear
WITHOUT FAULT		
Generalized Covariance (Auto)	$k(h) = -5.0885 h + 2.7081 \times 10^{-6} h ^3$	Linear
Linear 1	$\gamma(h) = 8.70 h $	Constant
Linear 2	$\gamma(h) = 8.70 h $	Linear
Linear 3	$\gamma(h) = 9.15 h $	Quadratic
Spherical A1	$\gamma(h) = 11100 \left[\frac{3}{2} \frac{ h }{2000} - \frac{1}{2} \left(\frac{ h }{2000} \right)^3 \right]$	Constant
Spherical A2	$\gamma(h) = 10800 \left[\frac{3}{2} \frac{ h }{2000} - \frac{1}{2} \left(\frac{ h }{2000} \right)^3 \right]$	Linear
Spherical A3	$\gamma(h) = 11250 \left[\frac{3}{2} \frac{ h }{2000} - \frac{1}{2} \left(\frac{ h }{2000} \right)^3 \right]$	Quadratic
Spherical B3	$\gamma(h) = 16800 \left[\frac{3}{2} \frac{ h }{3000} - \frac{1}{2} \left(\frac{ h }{3000} \right)^3 \right]$	Quadratic
Spherical C1*	$\gamma(h) = 16800 \left[\frac{3}{2} \frac{ h }{3000} - \frac{1}{2} \left(\frac{ h }{3000} \right)^3 \right]$	Constant

*Drift Removed Residuals

TABLE XI. NTS PALEOZOIC ROCK STRUCTURE IDENTIFICATION/VALIDATION

TYPE	STANDARDIZED ERROR	RMS ERROR (m)	MEAN ERROR (m)
WITH FAULT			
Generalized Covariance (Auto)	1.756	84	1.115
Linear 1	0.999	76	1.398
Linear 2	1.023	79	1.733
Spherical A1	1.009	76	0.388
Spherical A2	1.009	80	-0.374
WITHOUT FAULT			
Generalized Covariance (Auto)	0.991	83	-5.234
Linear 1	1.003	73	-2.089
Linear 2	1.012	74	-5.404
Linear 3	1.010	77	0.508
Spherical A1	1.004	75	0.819
Spherical A2	1.003	73	-6.711
Spherical A3	1.005	78	-0.373
Spherical B3	1.075	79	0.332
Spherical C1*	0.941	69	-0.403

* Drift Removed Residuals

correlation is assumed between them. Nevertheless, the RMS error from all models are not too different from the RMS error of 77.8 m estimated from gravity data based on 20 measurements of depth between 500 and 1000 m.

The contour maps based on the estimated depth for both cases of with and without fault together with their uncertainty maps are shown in Figures 32 to 35. Two cross-sections running E-W demonstrate the effect of fault on the estimated depth (Figures 36 and 37). Although the estimated depths show discontinuity near the fault, the contour routine smooths out these differences. The contour map has the gross features of a map based on gravity data, surface geology data as well as the borehole data. The color images of the depths are shown in Figures 38 and 39. These figures dramatically indicate the presence of the fault in the data.

The contour maps indicate a quadratic drift. We calculated this drift with a spherical variogram of range 3,000 m and sill 16,800 m. The variograms of the drift removed residuals are shown in Figure 40. It is evident that the anisotropy has been greatly reduced. The standard error for the drift removed residues (see Table XI) using the same initial variogram but constant drift is quite good (0.941) indicating that the estimated drift is correct.

Figure 32. Paleozoic Rock Depth at NTS From
Model Linear 1 with Fault

Figure 33. One-Sigma Error for Paleozoic Rock Depth at NTS From Model Linear 1 with Fault

Figure 34. Paleozoic Rock Depth at NTS from
Model Linear 1 without Fault

Figure 35. One-Sigma Error for Paleozoic Rock Depth at
NTS from Model Linear 1 without fault

Figure 36. Cross-Section of AA' in Figure 32

FROM THE 'A' SERIES THE CURVE AND THE 'B' SHOWS THE CONVENTIONAL CONSIDERED INTERVALS 2' TO 10'

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CHARACTERISTICS OF 106.414'S CONSIDERING				
SECT	NO.	COORDINATES OF ORIG.	NO.	POINT SPACING
1	1	2.012424E+00	2.012424E+00	2.012424E+00
2	2	2.012424E+00	2.012424E+00	2.012424E+00

Figure 37. Cross-Section of BB' in Figure 35

Figure 38. Pseudo-color image of paleozoic rock depth at the Nevada test site.

Figure 39. Pseudo-color image of one-sigma estimation errors of paleozoic rock depths at the Nevada test site.

Figure 40. Anisotropic Variograms for Residuals of Drift-Corrected Paleozoic Rock Depth at NTS

These calculations are preliminary. They are presented here to demonstrate the procedures and the potential of the technique. The structure for the rock depth is much more complicated than those from the two water level cases studied before. However, with simple linear variogram and constant drift, the Paleozoic rock depth can be reasonably reproduced.

There are many other parameters in the NTS data bank. Further research of these parameters using the spatial estimation approach is needed. This concludes the application of spatial estimation techniques to simple groundwater aquifer system and complex geological formations. In the next section we propose future research and application of this approach.

V. SUMMARY AND FUTURE WORK

In this report we developed spatial estimators for correlated data irregularly distributed in a region. Using the well known regionalized variable theory we were able to (simply) develop the estimator using vector-matrix calculus techniques. Once the theory was developed, the practice of spatial estimation was then discussed and it was shown that the most crucial area of spatial estimation is the identification of the statistical structural model - the variogram and drift. Techniques to estimate and identify the underlying variogram and drift from raw data were discussed and a validation

technique discussed. The code VARIFIT available at LLNL was used for this identification.

The spatial estimators were applied to three case studies: (i) Toppenish Creek Basin, (ii) Todd Lake, and (iii) Nevada Test Site. The first two cases were simple groundwater aquifers and the final case was a complex geological formation. The spatial estimator yielded reasonable contour maps of the regions under investigation. In the case of Todd Lake sparse data was taken from a known "truth" grid. The estimated grid reconstructed from the sparse data set yields a maximum relative error of approximately one percent. The complex NTS paleozoic rock depth maps were generated with and without faults for comparative purposes. It was shown that the estimator performed equally well. Results of the estimator were confirmed by using additional information (gravity measurements). It was also shown that image display techniques can be used to effectively investigate properties of regional maps. Spatial estimation techniques can be an effective tool to characterize proposed repository sites from limited data; however, much care must be taken when identifying the structural model from the raw data.

There is still more work which must be completed to evaluate the potential of applying this particular spatial estimation technique. The subsequent list shows areas which must be investigated or developed further:

1. Structural model identification;
2. Spatial estimation combining various types of data;
3. Extension of punctual parameter estimates to volumetric estimates;
4. Design of optimal measurement networks;
5. Grid simulations from a given data set with known statistical properties;
6. Development of interactive data display techniques; and
7. Development of hydrogeological parameters used model-based estimation techniques.

The identification of a structural model from various data sets is the most crucial aspect of the spatial estimation technique due to the need to first identify the drift and then characterize the variogram. The technique using generalized covariances is a compromise in that models are fit to "drift-free" data after successive differencing. Although this technique appears to give reasonable results most intuition is lost in the process. The identification problem formulated from the parametric optimization viewpoint (applying various theoretical models) may prove to yield more satisfying results.

The combination of more measurement information in the spatial estimation problem will yield more reliable results. For example, combining various measurements like borehole data along with seismic measurements in the site characterization problem should produce

better results. Similar problems have been approached in different areas and should be investigated further [8].

The extension of punctual parametric estimates to volumetric estimates has been investigated thoroughly and applied to grade estimation in the mining industry [4]. These techniques appear quite reasonable in the site characterization problem. For example, the extension of porosity estimated measured in a core can be extended to a block using the existing theory. We feel that this technique should be investigated on a given data set.

The optimization of a measurement network based on the error variances predicted by the spatial estimator should be investigated. In this case the variance of the estimator can be used as an index to determine the optimal location of a possible additional measurement point [10]. Model-based estimation techniques can also be used in this application and should also be investigated.

The ability to simulate a given region with the same structural variability passing through the measurement points can provide valuable information about areas where little information is present [10]. The various simulations depict possible variations of the true area. Generation of many simulations can serve to produce an average of the results and generate more confidence.

The development of effective interactive display techniques provide a valuable tool to the NRC site analyst by providing a geologic structure. These techniques can be improved further to simultaneous display estimate grid values and uncertainty maps. This technique would prove very useful when used in conjunction with an optimal measurement design.

Finally, the feasibility of using model-based estimators to directly estimate the model parameters from noisy measurements has been demonstrated for temporally correlated data [14]. These techniques are quite powerful and replace the structural model with a physical phenomenological model (e.g., groundwater flows). We feel that these techniques should be compared for a generated data set.

In summary, we feel that the application of modern spatial estimation techniques to spatially correlated measurement data can provide a useful tool in the NRC site characterization and evaluation process. The spatial estimator applied in this report yields reasonable results for the data sets investigated. More work must be performed (listed above) before the final analysis can be completed.

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APPENDICES

APPENDIX A

SPATIAL AND DRIFT ESTIMATION THEORY

In this Appendix we derive the necessary equations for spatial and drift estimation reported in Section II. Here we use the vector-matrix calculus techniques of Appendix B and C to derive the estimators. First we derive the basic spatial (kriging) estimator in Section A-1 and then the drift estimators in A-2 and A-3.

A-1. Spatial Estimation Theory

The spatial estimation problem can be solved using optimization theory results by formulating the problem properly. Here we show how to solve the problem using Lagrange multiplier techniques. To be more precise, we would like to find the linear estimator

$$\hat{z}(\underline{x}_k) = \sum_{i=1}^N \lambda_i z(\underline{x}_i) = \underline{\lambda}^T \underline{Z} \quad (A-1)$$

where $\underline{\lambda}^T := [\lambda_1 \dots \lambda_N]$ and $\underline{Z}^T := [z(\underline{x}_1) \dots z(\underline{x}_N)]$

such that

$$E\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} = 0 \quad (\text{unbiased}) \quad (A-2)$$

and

$$\sigma_k^2 = \text{Var}\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} \text{ is minimum (minimum variance).} \quad (\text{A-3})$$

The unbiased constraint, sometimes called the universality condition (unconditionally unbiasedness) leads to the following non-bias constraint

$$\sum_{i=1}^N \lambda_i f^j(\underline{x}_i) - f^j(\underline{x}_k) = 0^\dagger \quad j = 0, \dots, M \quad (\text{A-4})$$

which is obtained by solving (A-2) with (2.6) and (2.7) and

$$E\{z(\underline{x})\} := m(\underline{x})$$

To minimize the variance of (A-3) subject to the constraint of (A-4), we use the Lagrange multiplier technique. First, we define the function J in terms of the Lagrange multipliers $\{\mu_j\}$, $j = 0, \dots, M$

[†] It is important to note that this constraint is independent of the $\{a_j\}$, $j = 0, \dots, M$ of (2.4) and therefore, the actual drift coefficients need not be estimated!

$$J(\lambda, \mu) = \text{Var}\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} \\ - 2 \sum_{j=0}^M \mu_j \sum_{i=1}^N \lambda_i f^j(\underline{x}_i) - f^j(\underline{x}_k) = 0 \quad (\text{A-5})$$

but

$$\text{Var}\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} = 2 \sum_{i=1}^N \lambda_i \gamma_{ik} - \sum_{i=1}^N \sum_{\ell=1}^N \lambda_i \lambda_\ell (\gamma_{i\ell} - \sigma_\epsilon^2(i)) \quad (\text{A-6})$$

where $\gamma_{i\ell} := \gamma(\underline{x}_i - \underline{x}_\ell) := \text{Var}\{z(\underline{x}_i) - z(\underline{x}_\ell)\} = \text{variogram at } (i, \ell)$

and recall $\sigma_\epsilon^2(i) = \text{Var}\{\epsilon(\underline{x}_i)\}$

or

$$\sigma_k^2 = \text{Var}\{z(\underline{x}_k) - \hat{z}(\underline{x}_k)\} = 2\lambda^\top \gamma_k - \lambda^\top (\Gamma - \Sigma) \lambda \quad (\text{A-7})$$

where

$$\lambda^\top := [\lambda_1, \dots, \lambda_N]; \gamma_k^\top := [\gamma_{1k} \dots \gamma_{Nk}]; \text{ and } \Sigma = \text{diag} [\sigma_\epsilon^2(1) \dots \sigma_\epsilon^2(N)]$$

$$\Gamma := \begin{bmatrix} \gamma_{11} & \dots & \gamma_{1N} \\ \vdots & & \vdots \\ \gamma_{NN} \end{bmatrix} ; \text{ symmetric}$$

(NxN)

We can also write the constraint (A-4) in vector-matrix form as

$$F^T \underline{\lambda} - \underline{f}_k = \underline{0} \quad (A-8)$$

where

$$F := \begin{bmatrix} f^0(\underline{x}_1) & \dots & f^M(\underline{x}_1) \\ \vdots & & \vdots \\ f^0(\underline{x}_N) & \dots & f^M(\underline{x}_N) \end{bmatrix} ; \underline{f}_k := [f^0(\underline{x}_k) \dots f^M(\underline{x}_k)]$$

(Nx(M+1))

Using (A-7) and (A-8), we can rewrite (A-5) in vector-matrix notation, i.e.,

$$J(\underline{\lambda}, \underline{\mu}) = 2\underline{\lambda}^T \underline{\gamma}_k - \underline{\lambda}^T (\Gamma - \Sigma) \underline{\lambda} - \underline{\mu}^T (F^T \underline{\lambda} - \underline{f}_k) \quad (A-9)$$

$$\text{and } \underline{\mu}^T := [\mu_0 \dots \mu_M]$$

The function J is minimized by differentiating (see Appendix B) with respect to the λ 's and μ 's, setting the results to zero and solving, i.e.,

$$\frac{\partial J}{\partial \underline{\lambda}} = 2\underline{y}_k - 2(\Gamma - \Sigma) \underline{\lambda} - 2F\underline{\mu} = 0$$

$$\frac{\partial J}{\partial \underline{\mu}} = -2(F^T \underline{\lambda} - \underline{f}_k) = 0 \quad ,$$

a set of $(N+M+1)$ linear equations for $\underline{\lambda}$ and $\underline{\mu}$. Thus, we have to solve for

$$A\underline{\theta} = \underline{b}_k \quad (A-10)$$

$$A \in \mathbb{R}^{(N+M+1) \times (N+M+1)}; \quad \underline{\theta}, \underline{b}_k \in \mathbb{R}^{N+M+1}$$

or

$$\left[\begin{array}{c|c} \Gamma - \Sigma & F \\ \hline F^T & 0_{M+1} \end{array} \right] \begin{bmatrix} \underline{\lambda} \\ \underline{\mu} \end{bmatrix} = \begin{bmatrix} \underline{y}_k \\ \underline{f}_k \end{bmatrix} \quad (A-11)$$

Solving the linear equation of (A-11) gives the "optimal" weights $(\{\lambda_i\}, \{\mu_j\})$ of the spatial estimator. Using this relation we can rewrite (A-7) in terms of the optimal solution. Premultiplying the first equation of (A-11) by $\underline{\lambda}^T$ we can replace the second term of (A-7) after substituting the second equation of (A-11) to obtain

$$\sigma_k^2 = \underline{\theta}^T \underline{b}_k \quad (A-12)$$

Thus, a solution to the spatial estimation problem is given by the linear, unbiased, minimum variance estimator[†]

$$\hat{z}(\underline{x}_k) = \sum_{i=1}^N \lambda_i z(\underline{x}_i) = \underline{\lambda}^T \underline{z} \quad (A-13)$$

where the λ_i 's are the solution of (A-11) given by

$$\underline{\lambda} = (\Gamma - \Sigma)^{-1} [(I + F \Delta F^T (\Gamma - \Sigma)^{-1}) \underline{y}_k - F \Delta \underline{f}_k]$$

and

$$\Delta = -(F^T (\Gamma - \Sigma)^{-1} F)^{-1} \quad \dagger\dagger$$

The associated error variance is given by (A-12). Thus, the technique generates point estimates $\hat{z}(\underline{x}_k)$ and a measure of the precision σ_k .

[†] Historically this is called the "kriging estimator" in honor of D. G. Krige, a mining engineer who applied statistics to ore estimation. The technique without measurement errors is called "universal kriging," since it removes the trend as well (see [3,4] for details).

^{††} See Appendix C for details.

In the next section we discuss the problem of drift estimation and show now it can also be used alternately to solve the spatial estimation problem.

A-II. Drift Estimation Theory

In this section, we solve the drift estimation problem - first, for punctual drift estimates and second for regional drifts. We follow the technique of Lagrange multipliers used in Section A-I.

A-II-1 Punctual Drift Estimation

As before this problem can be formulated as finding the linear, minimum variance, unbiased estimate

$$\hat{m}(\underline{x}) = \sum_{i=1}^N \lambda_i z(x_i)^T \quad (A-14)$$

such that

^THere we use the same notation as before to only show the mathematical similarity of the problems.

$$E\{m(\underline{x}) - \hat{m}(\underline{x})\} = 0 \quad (\text{unbiased})$$

and

$$\sigma_M^2 = \text{Var}\{m(\underline{x}) - \hat{m}(\underline{x})\} \text{ is minimum} \quad (\text{minimum variance}) \quad (\text{A-15})$$

The unbiased condition leads to the constraint of (A-4) which can be expressed in vector-matrix notation as before

$$F^T \underline{\lambda} - \underline{f}_k = \underline{0} \quad (\text{A-16})$$

Similarly, the variance can be expressed as

$$\sigma_M^2 = \underline{\lambda}^T (\Gamma - \Sigma) \underline{\lambda} \quad (\text{A-17})$$

We define the function to be minimized as a function of the variance and unbiased constraint of (A-16), (A-17)

$$L(\underline{\lambda}, \underline{\mu}) = \underline{\lambda}^T (\Gamma - \Sigma) \underline{\lambda} - 2 \underline{\mu}^T (F^T \underline{\lambda} - \underline{f}_k)$$

Performing the required minimization $(\frac{\partial L}{\partial \underline{\lambda}}, \frac{\partial L}{\partial \underline{\mu}})$ as in Appendix B we obtain the set of linear equations similar to (A-11)

$$U\bar{u} = \bar{u}_k \quad (A-18)$$

where

$$U := \begin{bmatrix} \Gamma - \Sigma & 1 & F \\ & 1 & \\ F^T & & 0_{M+1} \end{bmatrix} ;$$

$$\bar{u}^T = [\bar{\lambda}^T : \bar{\mu}^T] ; \quad \bar{u}_k^T = [u_k^T : f_k]$$

Solving this set of linear equations yield the optimal point drift estimate

$$\hat{m}(x_k) = \sum_{i=1}^N \lambda_i z(x_i) = \bar{\lambda}^T \bar{z}$$

where

$$\bar{\lambda} = -(\Gamma - \Sigma)^{-1} F (F^T (\Gamma - \Sigma)^{-1} F)^{-1} f_k^{\dagger}$$

with error variance as before

$$\sigma_M^2 = \bar{u}^T \bar{u}_k = \bar{\mu}^T f_k \quad (A-19)$$

[†] See Appendix C for details.

Estimates of $\{a_i\}$ can easily be found from

$$\hat{m}(\underline{x}_k) \approx \underline{f}_k^T \hat{\underline{a}}$$

or letting $k = 1, \dots, N$

$$\hat{\underline{m}} = \underline{F} \hat{\underline{a}} \quad (\text{A-20})$$

Solving (A-18) for $\underline{\lambda}$ it is easy to show that

$$\hat{\underline{m}} = \underline{\lambda}^T \underline{Z} = (\underline{f}_k^T \underline{W}) \underline{Z} \quad (\text{A-21})$$

where

$$\underline{W} \text{ is } (M+1) \times N \text{ and } \underline{W} = (\underline{F}^T (\underline{I} - \underline{\Sigma})^{-1} \underline{F})^{-1} \underline{F}^T (\underline{I} - \underline{\Sigma})^{-1}$$

From (A-20) and (A-21) the drift coefficients can be obtained as

$$\hat{\underline{a}} = \underline{W} \underline{Z} \quad (\text{A-22})$$

with

$$\text{Cov}(\underline{a} - \hat{\underline{a}}) = (F^T(\Gamma - \Sigma)^{-1}F)^{-1}$$

This completes the results for punctual drift estimation, in the next section we consider the regional case.

A-II.2 Regional Drift Estimation

Following the same strategy for "regional" drift, i.e., one drift function to model the trend of the entire region, it is possible to derive similar equations to (A-18). Thus, to estimate drift over a region we must construct

$$\hat{m}(\underline{x}) = \sum_{i=0}^M \hat{\alpha}_i f^i(\underline{x}) = \hat{\underline{\alpha}}^T \underline{f} \quad (\text{A-23})$$

The relation implies that we must calculate the $\{\alpha_s\}$ $s = 0, \dots, M$ and $m(\underline{x})$ is the drift of $Z(\underline{x})$ for any $\underline{x}_i$ such that $|\underline{x} - \underline{x}_i| \leq \rho$ where ρ defines the regional neighborhood. We assume that N punctual samples of $Z(\underline{x})$ at $\underline{x}_j$, $j = 1, \dots, N$ are drawn. We define M estimates $\hat{\alpha}_s$ for each α_s which are a linear combination of the N samples inside the neighborhood of radius r around some $\underline{x}_k$, i.e.,

$$\hat{\alpha}_s = \sum_{i=1}^N \lambda_i^s Z(\underline{x}_i) = \underline{\lambda}_s^T \underline{Z} \quad s = 0, \dots, M \quad (\text{A-24})$$

subject to the usual unbiased, minimum variance constraints. The unbiasedness condition leads to

$$F^T \underline{\lambda}_s - \underline{e}_s = 0 \quad \text{for each } \alpha_s, s = 0, \dots, M \quad (A-25)$$

and $\underline{e}_s$ a unit column vector.

The cost function becomes for each s

$$R_s(\underline{\lambda}_s, \underline{\mu}_s) = \underline{\lambda}_s^T (I - Z) \underline{\lambda}_s - 2 \underline{\mu}_s^T (F^T \underline{\lambda}_s - \underline{e}_s) \quad , \quad s = 0, \dots, M \quad (A-26)$$

After minimizing (A-26) as in Appendix C, we obtain

$$D \underline{\phi}_s = \underline{\xi}_s \quad , \quad s = 0, \dots, M \quad (A-27)$$

where D is given in (A-18) and

$$\underline{\phi}_s^T = [\underline{\lambda}_s^T : \underline{\mu}_s^T] \quad , \quad s = 0, \dots, M$$

$$\underline{\xi}_s^T = [\underline{0}_N^T : \underline{e}_s^T]$$

The optimal weight vector of (A-24) is given by

$$\underline{\lambda}_S = -(\Gamma - \Sigma)^{-1} F (F^T (\Gamma - \Sigma)^{-1} F)^{-1} \underline{e}_S^{\dagger}$$

Thus solving (A-27), $M+1$ times we obtain estimates for $\{\alpha_S\}$ and the corresponding error variance is given by

$$\sigma_{\alpha_S}^2 = \underline{\psi}_S^T \underline{e}_S = \mu_S^S$$

Once the $\{\alpha_S\}$ are estimated the drift can be removed from samples and the residuals can be estimated using simple spatial estimation techniques as before. This completes the theoretical discussion on spatial estimation theory, we summarize the results in Table I.

[†] See Appendix C for details

APPENDIX B
MATRIX CALCULUS RULES

In this Appendix we define the basic rules of matrix calculus which are required in this work. These results are taken from Deutsch [9]. First we define the gradient vector operator

$$\frac{\partial}{\partial \underline{\theta}}^T := [\frac{\partial}{\partial \theta_1} \dots \frac{\partial}{\partial \theta_N}] \text{ for } \frac{\partial}{\partial \underline{\theta}} \in \mathbb{R}^N \quad (B-1)$$

and $\underline{a}, \underline{b} \in \mathbb{R}^N, C \in \mathbb{R}^{N \times M}$.

The gradient operation on a vector $\theta \in \mathbb{R}^N$ and matrix C is

$$\frac{\partial}{\partial \underline{\theta}} (\underline{\theta}^T C) = C \quad \text{for } C \text{ not a function of } \underline{\theta} \quad (B-2)$$

and for a vector $\underline{b}$

$$\frac{\partial}{\partial \underline{\theta}} (\underline{b}^T \underline{\theta}) = \underline{b} \quad \text{for } \underline{b} \text{ not a function of } \underline{\theta} \quad (B-3)$$

and finally the "chain rule"

$$\frac{\partial}{\partial \underline{\theta}} (\underline{a}^T \underline{b}) = (\frac{\partial}{\partial \underline{\theta}} \underline{a})^T \underline{b} + (\frac{\partial}{\partial \underline{\theta}} \underline{b})^T \underline{a} \quad (B-4)$$

for $\underline{a}, \underline{b}$, functions of $\underline{\theta}$.

APPENDIX C

DERIVATION OF SPATIAL ESTIMATOR WEIGHTS

In this Appendix we use a theorem from linear algebra to explicitly calculate the weights λ for the spatial estimators. The following theorem (Noble and Daniel [20]) shows how to calculate the inverse of a partitioned matrix.

Theorem C-1 Let A be a partitioned matrix such that

$$A = \left[\begin{array}{c|c|c} P & I & Q \\ \hline R & I & S \end{array} \right]$$

where $P \in \mathbb{R}^{N \times N}$, $S \in \mathbb{R}^{M \times M}$ and A and P are nonsingular, then

$$A^{-1} = \left[\begin{array}{c|c|c} X & I & -P^{-1}QW \\ \hline -WRP^{-1} & I & W \end{array} \right] \quad (C-1)$$

for $W = (S - RP^{-1}Q)^{-1}$, $X = P^{-1} + P^{-1}QWRP^{-1}$.

Proof: This theorem is easily proved using the block Gaussian elimination technique. Elementary row transformations are performed on A until the identity matrix is obtained, i.e., $TA = I$; thus T is the inverse of A given by (C-1).

If we apply this theorem to the general form of our linear equations for spatial estimation, we obtain the following corollary

Corollary C-1 Let

$$A = \begin{bmatrix} K & | & L \\ \hline L^T & | & 0_M \end{bmatrix}$$

where $K \in \mathbb{R}^{N \times N}$, $L \in \mathbb{R}^{N \times M}$, 0 is $M \times M$ null matrix and A , K are nonsingular, then

$$A^{-1} = \begin{bmatrix} Y & | & -K^{-1}L\Delta \\ \hline -\Delta L^T K^{-1} & | & \Delta \end{bmatrix} \quad (C-2)$$

for $Y = K^{-1} + K^{-1}L\Delta L^T K^{-1}$ and $\Delta = -(L^T K^{-1}L)^{-1}$.

Proof: Using Theorem C-1 with $K = P$, $L = Q = R$, $S = 0$, we obtain $Y = X$ and $\Delta = W$.

Now if we apply this corollary to our three cases: (i) spatial estimation; (ii) punctual drift estimation; and (iii) regional drift estimation, we obtain the desired results for the optimal weights, $\underline{\lambda}$, i.e., from (A-10) we have

$$\underline{\theta} = A^{-1} \underline{b}_k \quad (C-3)$$

Thus, substituting (C-2) into (C-3), we obtain

$$\begin{bmatrix} \underline{\lambda} \\ \underline{\mu} \end{bmatrix} = \begin{bmatrix} Y & -K^{-1}L\Delta \\ -\Delta L^T K^{-1} & \Delta \end{bmatrix} \begin{bmatrix} \underline{y}_k \\ \underline{f}_k \end{bmatrix} \quad (C-4)$$

or

$$\underline{\lambda} = Y \underline{y}_k - K^{-1} L \Delta \underline{f}_k = K^{-1} [(I + L \Delta L^T K^{-1}) \underline{y}_k - L \Delta \underline{f}_k] \quad (C-5)$$

$$\underline{\mu} = -\Delta L^T K^{-1} \underline{y}_k + \Delta \underline{f}_k. \quad (C-6)$$

We can now solve our specific cases:

Case (i) Spatial Estimator

Using matrix A of (A-11), we see that with

$$K = I - \Sigma \text{ and } L = F$$

so substituting into (C-5) we have

$$\underline{\lambda} = (I - \Sigma)^{-1} [(I + F \Delta F^T (I - \Sigma)^{-1}) \underline{y}_k - F \Delta \underline{f}_k] \quad (C-7)$$

and

$$\Delta = -(F^T(\Gamma - \Sigma)^{-1}F)^{-1}.$$

Case (ii) Punctual Drift Estimator

Using matrix D of (A-18), we see that

$$K = \Gamma - \Sigma, L = F, \underline{y}_k = \underline{0}$$

so

$$\underline{\lambda} = -(\Gamma - \Sigma)^{-1}F(F^T(\Gamma - \Sigma)^{-1}F)^{-1}\underline{f}_k \quad (C-8)$$

Case (iii). Regional Drift Estimator

Using D of (A-27), we see that

$$K = \Gamma - \Sigma, L = F, \underline{y}_k = \underline{0} \text{ and } \underline{f}_k = \underline{e}_s$$

so

$$\underline{\lambda}_s = -(\Gamma - \Sigma)^{-1}F(F^T(\Gamma - \Sigma)^{-1}F)^{-1}\underline{e}_s \quad (C-9)$$

This completes the derivation of explicit expressions for the optimal weight vector, $\underline{\lambda}$.