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#### Abstract

The Turning Bands Method, introduced by G. Matherom, produces conditional simulations of a random function defined in $n$-space There are difliculties which make it less attractive for simulations in 2-space and for the the extension to the vector or co-regionalization case. The difficulties are both theoretical and computational. The decomposition of the covariance matrix method introduced more recently by M. Davis and F. Alabert is essentially independent of the dimension of the space and results in a straight forward extension to the vector case by using the general formulation of cokriging given by hlyers. As an alternative to the Cholesky decomposition, Davis proposed using a minimax polynomial approximation to the square root. The robustness of the simulation algorithm is examined with respect to the approximations for both the univariate and the vector form. Numerical results are given.


## 1. INTRODUCTION

Simulation is a tool that is widely used in many fields. When the experiment is replicable, sirnulation may be used as an alternative to complex analytical solutions. Albhough many applications in the earth sciences do not result in replicable data sets simulation is still useful because it provides a tool for quantifying the uncertainty that is obscured when estimation techniques are used. In mining. simulation has attracted interest as a tool for planning especially for scheduling the exploitation of mineral deposits, see for example Chiles (1984). The criteria imposed on the selection of waste disposal sites arc frequently given in terms of the probability of a lcakage; simulation of hydrological parameters allows a non-analytical estimation of such probabilities and takes into account the uricertainties associated with those parameters as illustrated in Silliman (1986). Although multivariate estimation, e.g., cokriging, has perhaps been of less interest than the univariate casc, even in mining applications multivariate simulations are of considcrablc importance as exemplified in Chiles (1984), Dowd (1984), Isaaks (1984) and Alabert (1987a). But interest in the problem pre-dates geostatistics as seen in Shinozuka (1971). In general the methods used arc not true multivariate simulations and do not condition the data by cokriging in a fashion fully analogous to the way kriging is used in the univariate case. The program given by Carr and Myers (1985) partly bridged this gap but it is a compromise since the intervariable dependence is ignored in the simulation stage. Many of the difficulties inlierent in the use of the Turning Bands method are avoided by the use of the covariance decomposition method developed by Davis $(1987 a, 198711)$ and Alabert (1987b). What remnincd then was to extend that method to the use of cokriging. One difficulty arises in thr multivariate case that does not occur in the univariate case, namely the undersampled problem, ie., not all variates are sanpled at all locations. It is seen that essentially the same algorithm given by Myers (1984), and then implemented in Carr, hlyers and Glass (1985), provides a resolution of the difliculties associated with multivariate simulation in the undersampled case.
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W. Armstrong (ed.j, Geostatistics, Vol. 1, 283-203
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### 1.1 The Turning Bands Method-Extensions

The fundamental characteristic of the Turning Bands method is that it produces a simulation of a random function defined in n-space as a linear combination of simulations of uncorrelated random functions defined in 1 -space such that the covariance function and first moment are preserved. Theoretically the linear combination is an integral with respect to a uniform probability measure on the unit $n$-sphere. In practice this integral is approximated by a finite linear combination of simulations corresponding to equally spaced directions and the simulations for the respective random functions defined in 1space may be obtained by one of several techniques although the Box-Jenkins Moving Average seems to be the one most commonly used. To preserve the covariance it is necessary to find a corresponding 1-dimensional covariance, i.e., one must solve an integral equation. It is easy to see that at least theoretically this formulation will extend easily to the vector case. Following the notation used in Myers (1982) let $\mathrm{Y}(\mathrm{t})=\left[Y_{1}(t), \ldots Y_{m}(t)\right]$ be a second order stationary vector random function defined in 1 space and $\mathrm{P}(\mathrm{s})$ a uniform probability measure on the unit $n$-sphere then

$$
\begin{equation*}
\stackrel{\rightharpoonup}{Z}(x)=\left[Z_{1}(x), \ldots, Z_{m}(x)\right]=\int \bar{Y}(\langle x, s\rangle) d P(s) \tag{1}
\end{equation*}
$$

is a second order stationary vector random function defined in $n$-space and the matrix covariance function for $\bar{Z}(x)$ is obtained from the integral (we assume without loss of generality that all components of $\bar{Z}(x)$ have zero means)

$$
\begin{align*}
& \bar{C}_{z}(h)=E\left\{Z(x+h)^{T} Z(x)\right\}=\int \bar{C}_{y, s}(h) d P(s)  \tag{2}\\
& \bar{C}_{y, s}(h)=E\left\{\bar{Y}(<x+h, s>)^{T} \bar{Y}(<x, s>)\right\} \tag{3}
\end{align*}
$$

and as in the univariate case we assume that any component of $\mathrm{Y}(<\mathrm{u}, s\rangle)$ and any component of $\mathrm{Y}(\langle v, \mathrm{r}\rangle)$ are uncorrelated for all $\mathrm{u}, v$ unless $\mathrm{r}=\mathrm{s}$. It is easy to see that exactly the same relationship is established between all the components of $\bar{C}_{Z}$ and $\bar{C}_{Y, s}$ as used in the univariate case. For the case of $n=3$ the 1 -dimensional covariances and cross-covariances are obtained easily from the corresponding 3-dimensional covariances and cross-covariances respectively. In the univariate case the practice is to represent, covariances as positive linear combinations of standard models and hence the problem of finding the 1 -dimensional covariance is reduced to finding the associated covariances for those standard models. However cross-covariances do not have to be positive linear combinations of covariances; the positive definiteness condition is more complicated as is shown in Myers (1984, 1987). In practice one models the cross-covariances by (general) linear combinations and the positive definiteness condition is satisfied by imposing sufficiency conditions on the coefficients. In this case although there are more relations, the problem of reducing the dimension on which the random vector is defined is solved in essentially the same way vector random function in 1-dimension still remains although even if this problem is solved the computational difficulty associated with producing simulations in 3-dimensions would have significantly escalated.

### 1.2 Linear Co-regionalizations

The use of a linear co-regionalization provides a solution to several problems arising out of the need to model cross- covariances (or cross-variograms) as well as the subsequent step of co-simulation of correlated random functions. More specifically let the rdndom vector $\bar{Z}(x)$ be represented in the form

$$
\begin{equation*}
\bar{Z}(x)=\bar{W}(x) B \tag{4}
\end{equation*}
$$

where $\bar{W}(x)$ is a random vector with p uncorrelated components and B is a $p \mathrm{x}$ m matrix, the covariance matrix function of $\bar{Z}(x)$ is given by

$$
\begin{equation*}
\bar{C}_{Z}(h)=B^{T} \bar{C}_{W}(h) B \tag{5}
\end{equation*}
$$

and $\bar{C}_{W}(h)$ is diagonal. The variogram matrix function has an analogous representation. Wackernagel (1988) has used a form of a principal components deromposition to obtain B. Given this representation it is then sufficient to simulate each component of $\bar{W}(x)$ independently and the (unconditional) simulation of $\bar{Z}(x)$ is obtained from (4). To condition $\bar{Z}(x)$ one might proceed in either of two ways, condition the components of $\bar{W}(x)$ which would require converting the data for $\bar{Z}(x)$ to data for $\bar{W}(x)$ or use cokriging to condition $\bar{Z}(x)$ directly in a manner analogous to the conditioning in the univariate case (this is the algorithm used in Carr and Myers, (1985)). In order to convert the data for $\bar{Z}(x)$ to data for $\bar{W}(x)$, B would have to be invertible and in particular it would have to be square. If $\bar{Z}(x)$, i.e., each component of $\bar{Z}(x)$, is defined in n - space then the components of $\bar{W}(x)$ are defined in $n$-space and hence it would still be necessary to use the Turning Bands Method or some other technique to produce the individual simulations. When $B$ is invertible the number of steps involved in the simulation process is directly proportional to the number of components in $\bar{Z}(x)$ (assuming that B and $\bar{C}_{W}(h)$ have already been determined).

### 1.3 Marginal Distributions

While it might seem plausible not to impose conditions on the univariate, i.e. marginal, frequency distribution, the alternative is to allow that distribution to be essentially indeterminate. All of the techniques currently in use for univariate simulation, as well as those proposed above and to follow, use finite linear combinations of uncorrelated random variables. It is then appropriate to require that the common distribution of these random variables be such that it is preserved under finite linear combinations. Although the normal is not the only distributional type with this property it is the one that is most frequently used. In turn this generally requires that a non-linear transformation first be applied to change the marginal to a standard normal then the inverse transformation is applied subsequently to the simulated values. In the univariate case the original margina distribution is preserved but the moments may not be, in general only the first two moments of the transformed data are preserved unless strong multivariate normality assumptions are invoked in order to be able to compute the bias adjustments. In the case of the simulation of a vector random function the concept of a marginal distribution is carried one step further, i.e. there is a marginal distribution for each component (not necessarily the same) and a joint distribution between components. Without multivariate distributional assumptions one can only transform the data for each component separately and hence preserve the separate marginal distributions. While it seems to be unavoidable, the construction of simulations by linear combinations of uncorrelated random variables places a severe limitation on the properties that can be preserved for the simulations.

## 2. THE COVARIANCE DECOMPOSITION

Using the formulation of cokriging given in Myers (1982) and the presentation of the simulation for the univariate case given in Davis (1987a, 1987b) the vector simulation using simple (co)kriging is easily obtained. We consider first the case where $\bar{C}_{Z}(h)$ is known, the function is full-sampled and simple cokriging is used. Subsequently ordinary cokriging with the undersampled form is considered and special results relating to the use of a regional co-regionalization are given.

### 2.1 Unconditional co-simulation

We begin by assuming that $\bar{Z}(x)$ is an m-component vector random function whose components are second order stationary and all with mean zero. The matrix covariance function is then iven by the middle term in (2) above. If $x_{1}, \ldots x_{n}$ are the locations where a simulate! value is required, form the matrix

$$
\begin{gather*}
\sum=\left[\begin{array}{cc}
\bar{C}\left(x_{1}-x_{1}\right) \ldots \ldots & \bar{C}\left(x_{1}-x_{n}\right) \\
\bar{C}\left(x_{n}-x_{1}\right) & \ldots \ldots \\
\bar{C}\left(x_{n}-x_{n}\right)
\end{array}\right] \\
=\left[\begin{array}{ccc}
\bar{C}_{11} \ldots \ldots . & \bar{C}_{1 n} \\
\vdots & \vdots \\
\bar{C}_{n 1} & \ldots \ldots & \bar{C}_{n n}
\end{array}\right] \tag{6}
\end{gather*}
$$

and let $\Sigma_{L}, \Sigma_{U}$ be a Cholesky decomposition of $\Sigma$. Then

$$
\begin{equation*}
\left\{\bar{Z}_{s}\left(x_{1}\right), \ldots . \bar{Z}_{s}\left(x_{n}\right)\right\}=\left\{\bar{V}_{1}, \ldots \bar{V}_{n}\right\} \Sigma_{U} \tag{7}
\end{equation*}
$$

is a vector of simulated values of the vector function $\bar{Z}(x)$ at the required locations whose covariance matrix is given by (6) when $\left\{\bar{V}_{1}, \ldots, \bar{V}_{n}\right\}$ is a nm-component vector of uncorrelated random variables. This of course is exactly the same as the result given in Davis (1987a) except that scalars are replaced in the appropriate places by vectors or matrices.

Likewise if A is a square root of $\Sigma$, then again the vector extension of Davis's construction is obtained. Moreover the Minimax polynomial construction for the square root of $\Sigma$ can still be used as in the scalar case.
2.1.1 Simulation Discrepancies-Approximation Errors. Although it is generally assurned or shown that a particular simulation algorithm has the minimal desired properties of reproducing the mean and covariance as well as the marginal distribution, little attention has been given to the question of whether simulations are equivalent in an appropriate sense. In the particular case of using a square root instead of the Cholesky decomposition, and moreover an approximation to the square root such as is given by the Minimax Polynomial, a more direct comparison is possible. We will state the results for the vector case but the scalar case is simply the case of $m=1$.

First suppose that the square root $A$, of $\Sigma$ is exact i.e., $A^{2}=\Sigma$. Consider then the difference of the vectors of simulated values; a strong form of equivalence would require that this difference be a zero vector for any choice of the vector of uncorrelated random variables $\left\{\bar{V}_{1}, \ldots, \bar{V}_{n}\right\}$.By equating the two, i.e., setting the difference equal to a zero vector, we see that this implies that $\mathrm{A}=\Sigma_{V}$ which is not possible. Consequently for a given simulated vector of uncorrelated random variables two different realizations are obtained. However it is possible for the two algorithms to be equivalent in another sense, for each vector might be another unique vector $\left\{\bar{V}_{1}^{\prime}, \ldots, \bar{V}_{n}^{\prime}\right\}$ such that

$$
\begin{equation*}
\left\{\bar{V}_{1}, \ldots \bar{V}_{n}\right\} \Sigma_{U}=\left\{\bar{V}_{1}^{\prime}, \ldots, \bar{V}_{n}^{\prime}\right\} A \tag{8}
\end{equation*}
$$

since A is invertible there is a unique solution. However unless the random variables are all uniformly distributed the probability of the one realization may not be the same as for the other and hence in terms of the (vector) random function the two methods are not equivalent even though the first and second order moments are preserved and the marginal distribution is also retained.

Now consider the possible discrepancies introduced by using an approximation to the square root. Let $f(t)=(t)^{1 / 2}$ and $g(t)$ be the approximating function, writing $\Sigma$ in diagonalized form

$$
\begin{equation*}
\Sigma=Q^{T} \operatorname{diag}\left\{\lambda_{1}, \ldots, \lambda_{n m}\right\} Q \tag{3}
\end{equation*}
$$

then we have

$$
\begin{equation*}
A=\mathrm{f}(\Sigma)=Q^{T} \operatorname{diag}\left\{f\left(\lambda_{1}\right), \ldots, f\left(\lambda_{n m}\right)\right\} Q \tag{10}
\end{equation*}
$$

and

$$
\begin{equation*}
g(\Sigma)=Q^{T} \operatorname{diag}\left\{g\left(\lambda_{1}\right), \ldots, g\left(\lambda_{n m}\right)\right\} Q \tag{11}
\end{equation*}
$$

Using $\boldsymbol{A}$ and $g(\Sigma)$ to construct simulations with the same vector of uncorrelated random variables we see that the covariance in the one case is $\Sigma$ and in the other it is

$$
\begin{equation*}
|g(\Sigma)|^{2}=Q^{T} \operatorname{diag}\left\{g^{2}\left(\lambda_{1}\right), \ldots, g^{2}\left(\lambda_{n m}\right)\right\} Q \tag{12}
\end{equation*}
$$

and the norm of the difference between (11) and (12) is given by

$$
\begin{array}{r}
\operatorname{tr}\left\{\Sigma-g^{2}(\Sigma)\right\}^{T}\left\{\Sigma-g^{2}(\Sigma)\right\} \\
=\sum_{j=1}^{n m}\left[\lambda_{j}-g^{2}\left(\lambda_{j}\right)\right]^{2} \leq(n m)\left\{\max \left\{\lambda^{j}-g^{2}\left(\lambda^{j},\right)\right\}^{2}\right. \tag{13}
\end{array}
$$

We may also consider how close the one realization is to the other when the same vector of uncorrelated random variables is used for both. While there are several different metrics that might be used the mean square distance would seem reasonable. Let $\left\{\bar{Z}_{s f}\left(x_{1}\right), \ldots, \bar{Z}_{s f}\left(x_{n}\right)\right\},\left\{\bar{Z}_{s g}\left(x_{1}\right), \ldots, \bar{Z}_{s g}\left(x_{n}\right)\right\}$ be the simulations obtained by using $f . g$ respectively. If we let $\bar{V}=\left\{\bar{V}_{1}, \ldots, \bar{V}_{n}\right\}$ then the distance between these two vectors is

$$
\begin{align*}
D= & \left\{\bar{Z}_{s_{f}}\left(x_{1}\right)-\bar{Z}_{s g}\left(x_{1}\right), \ldots, \bar{Z}_{s f}\left(x_{n}\right)-\bar{Z}_{\varepsilon g}\left(x_{n}\right)\right\} \\
& \left\{\bar{Z}_{s f}\left(x_{1}\right)-\bar{Z}_{s g}\left(x_{1}\right), \ldots, \bar{Z}_{s f}-\ddot{Z}_{s g}\left(x_{n}\right)\right\}^{T}  \tag{14}\\
= & \bar{V}\left\{\Sigma_{U}-g(\Sigma)\right\}\left\{\Sigma_{U}-g(\Sigma)\right\} \bar{V}^{T}  \tag{15}\\
= & \bar{V} K \bar{V}^{T}
\end{align*}
$$

This is a quadratic form and since $K$ is positive definite the largest cigenvalıe of $K$ can be used to obtain a bound on $D$ in terms of the values of $\bar{V}: \alpha_{1}, \ldots ., \alpha_{n m}$ more specifically we have

$$
\begin{equation*}
\mathrm{D} \leq \max \alpha_{j}\left\{\bar{V} \bar{V}^{T}\right\}^{1 / 2} \tag{16}
\end{equation*}
$$

but the eigenvalues of $K$ are of the form $\left[\mathrm{f}\left(\lambda_{i}\right)-g\left(\lambda_{i}\right)\right]^{2}$. If the components of $V$ arr uncorrelated standard normal random variables then the distribution of $\left\{\tilde{V}^{T} \bar{V}^{T}\right\}^{1 / 2}$ is that of the square root of a chi-square with $n m$ degrees of freedom. Alternatively we might consider the expected value of $D$ instead of just a bound. By re-writing $D$ in a more convenient form we have

$$
\begin{align*}
E(D) & =\operatorname{tr}\left\{g^{2}(\Sigma)-\Sigma\right\}^{T}\left\{g^{2}(\Sigma)-\Sigma\right\} \\
& =\sum_{i=1}^{n m}\left[\lambda_{i}-g^{2}\left(\lambda_{i}\right)\right\}^{2} \tag{17}
\end{align*}
$$

which is the same as the norrn of the differrnce between the covariance matrices.

Now consider the possible discrepancies introduced by using an approximation to the square root. Let $f(t)=(t)^{1 / 2}$ and $g(t)$ be the approximating function, writing $\Sigma$ in diagonalized form

$$
\begin{equation*}
\Sigma=Q^{T} \operatorname{diag}\left\{\lambda_{1}, \ldots, \lambda_{n m}\right\} Q \tag{9}
\end{equation*}
$$

then we have

$$
\begin{equation*}
A=f(\Sigma)=Q^{T} \operatorname{diag}\left\{f\left(\lambda_{1}\right), \ldots, f\left(\lambda_{n m}\right)\right\} Q \tag{10}
\end{equation*}
$$

and

$$
\begin{equation*}
g(\Sigma)=Q^{T} \operatorname{diag}\left\{g\left(\lambda_{1}\right), \ldots, g\left(\lambda_{n m}\right)\right\} Q \tag{11}
\end{equation*}
$$

Using $A$ and $g(\Sigma)$ to construct simulations with the same vector of uncorrclated random variables we see that the covariance in the one case is $\Sigma$ and in the other it is

$$
\begin{equation*}
[g(\Sigma)]^{2}=Q^{T} \operatorname{diag}\left\{g^{2}\left(\lambda_{1}\right), \ldots, g^{2}\left(\lambda_{n m}\right)\right\} Q \tag{12}
\end{equation*}
$$

and the norm of the difference between (11) and (12) is given by

$$
\begin{array}{r}
\operatorname{tr}\left\{\Sigma-g^{2}(\Sigma)\right\}^{T}\left\{\Sigma-g^{2}(\Sigma)\right\} \\
=\sum_{j=1}^{n m}\left[\lambda_{j}-g^{2}\left(\lambda_{j}\right)\right]^{2} \leq(n m)\left\{\max \left\{\lambda^{j}-g^{2}\left(\lambda^{j},\right)\right\}^{2}\right. \tag{13}
\end{array}
$$

We may also consider how close the one realization is to the other when the same vector of uncorrelated random variables is used for both. While there arc several different metrics that might be used the mean square distance would seem reasonable. Let $\left\{\bar{Z}_{s f}\left(x_{1}\right), \ldots, \bar{Z}_{s f}\left(x_{n}\right)\right\},\left\{\bar{Z}_{s g}\left(x_{1}\right), \ldots, \bar{Z}_{s g}\left(x_{n}\right)\right\}$ be the simulations obtained by using $f, g$ respectively. If we let $\bar{V}=\left\{\bar{V}_{1}, \ldots, \bar{V}_{n}\right\}$ then the distance between these two vectors is

$$
\begin{align*}
D= & \left\{\bar{Z}_{s_{f}}\left(x_{1}\right)-\bar{Z}_{s q}\left(x_{1}\right), \ldots, \bar{Z}_{s f}\left(x_{n}\right)-\bar{Z}_{s} g\left(x_{n}\right)\right\} \\
& \left\{\bar{Z}_{s f}\left(x_{1}\right)-\bar{Z}_{s q}\left(x_{1}\right), \ldots, \bar{Z}_{s f}-\bar{Z}_{s g}\left(x_{n}\right)\right\}^{T}  \tag{14}\\
= & \bar{V}\left\{\Sigma_{U}-g(\Sigma)\right\}\left\{\Sigma_{l V}-g(\Sigma)\right\} \bar{V}^{T}  \tag{15}\\
= & \bar{V} K \bar{V}^{T}
\end{align*}
$$

This is a quadratic form and since $K$ is positive definite the largest eigenvalue of $K$ can be used to obtain a bound on D in terms of the values of $\bar{V}: \alpha_{1}, \ldots \ldots \alpha_{n m}$ more specifically wc have

$$
\begin{equation*}
D \leq \max \alpha_{j}\left\{\bar{V} \bar{V}^{T}\right\}^{1 / 2} \tag{16}
\end{equation*}
$$

but the eigenvalues of $K$ are of the form $\left[f(A,)-g\left(\lambda_{2}\right)\right]^{2}$. If the components of V are uncorrclated standard normal random variables then the distribution of $\left\{\bar{V} \bar{V}^{T}\right\}^{1 / 2}$ is that of the square root of a chi-square with nm degrees of frccdorn. Alternatively we might consider the expected value of $D$ instead of just a bound. By re-writing $D$ in a more convenient form we have

$$
\begin{align*}
E(D) & =\operatorname{tr}\left\{g^{2}(\Sigma)-\Sigma\right\}^{T}\left\{g^{2}(\Sigma)-\Sigma\right\} \\
& =\sum_{i=1}^{n m}\left[\lambda_{i}-g^{2}\left(\lambda_{i}\right)\right]^{2} \tag{17}
\end{align*}
$$

which is the same as the norm of the difference between the covariance matrices.

Corresponding to the n data points $x_{1}, \ldots, x_{n}$ and thep unsampled points $x_{n+1}, \ldots, x_{n+p}$ partition the vector of values of $Z$ into $Z_{d}$ and $Z_{e}$, likewise partition the row vector $V$ of vectors of simulated uncorrelated random variables into $V_{d}$ and $V_{e}$. The covariance matrix for the full vector $Z$ and its Cholesky decomposition is given by

$$
\left[\begin{array}{cc}
\Sigma_{11} & \Sigma_{12}  \tag{23}\\
\Sigma_{21} & \Sigma_{22}
\end{array}\right]=\left[\begin{array}{cc}
L_{11} & 0 \\
L_{21} & L_{22}
\end{array}\right]\left[\begin{array}{cc}
U_{11} & U_{12} \\
0 & U_{22}
\end{array}\right]
$$

Using the simulation formulation given in (7) above we would have

$$
\begin{equation*}
\bar{Z}_{s d}=\bar{V}_{d} U_{11} \bar{Z}_{s e}=\bar{V}_{d} U_{12}+\bar{V}_{e} U_{22} \tag{24}
\end{equation*}
$$

and if we let $\bar{V}_{d}=\bar{Z}_{d} U_{11}^{-1}$ then $\bar{Z}_{s d}=\bar{Z}_{d}$ and the simulation is conditioned to the data. If the square root decomposition is used and the square root of the full covariance matrix is given in terms of a partitioning corresponding to the partitioning of the covariance matrix then we have

$$
\begin{equation*}
\bar{Z}_{s d}=\bar{V}_{d} A_{11}+\bar{V}_{e} A_{21}, \bar{Z}_{s e}=\bar{V}_{d} A_{12}+\bar{V}_{e} A_{22} \tag{25}
\end{equation*}
$$

and to condition the simulation we let $\bar{V}_{d}=\left\{\bar{Z}_{d}-\bar{V}_{e} A_{21}\right\} A_{11}^{-1}$
3.1.2. Ordinary Co-kriging. We might proceed in two ways to remove the assumption of zero means used above. One possibility is to assume that the means are known and modify the equations accordingly, thn second which is more realistic replaces simple kriging by ordinary kriging and we simply compute the adjustment necessary to make that change. To change from simple co-kriging to ordinary co-kriging we must add the difference between the ordinary co-kriged value and the simple co-kriged value. Writing as before $\bar{Z}_{d}$ as the row vector of data values of $Z$, let $\Gamma$ be the column of weight matrices in the simple co-kriging estimator and $\Gamma^{0}$ as the cnrresponding column of weight matrices in the ordinary co-kriging estimator. In addition let $\mathbf{M}=\left[M_{1}, \ldots, M_{m}\right]$ be the vector of means, $\bar{M} *$ be the estimated vector and E a column of identity matrices, then the true difference and its estimate are

$$
\begin{equation*}
\bar{Z}_{o k} *-\bar{Z}_{s k} *=\bar{M}\left\{I-E^{T} \Gamma\right\}=\bar{M} *\left\{I-E^{T} \Gamma\right\} \tag{26}
\end{equation*}
$$

It is then only necessary to add this term to $\bar{Z}_{s e}$ as given in (24) or (23) to compensate for the unknown non-zero means.

### 3.2 Under Sampled

When one component is not sampled at one location we must either shift a sub-column and a sub-row,i.e. a column of entries within a column of matrices and similarly for rows in corresponding to data to the part corresponding to locations to be estimated or alternatively we must further partition the covariance matrix to provide the separation. This problem only occurs in connection with conditioning. For simplicit we illustrate the algorithm for simple co-kriging with zero means and where there is on\& one component that is under sampled at only one location. We must partition $\Sigma_{11}$ into 3 sub-parts as follows

$$
\left[\begin{array}{ccc}
\Sigma_{11}^{11} & \Sigma_{11}^{12} & \Sigma_{11}^{13}  \tag{27}\\
\Sigma_{11}^{21} & \Sigma_{11}^{2} & \Sigma_{11}^{23} \\
\Sigma_{11}^{31} & \Sigma_{11}^{32} & \Sigma_{11}^{33}
\end{array}\right]
$$

and in turn we must partition $\Sigma_{12}$ and $\Sigma_{21}$ into three parts each corrcsponding to the partition in (27). These in turn induce partitions of the Cholesky decompositions of the
full covariance matrix. In turn we must partition $\bar{Z}_{d}$ into three parts $\bar{Z}_{d}^{1}, \bar{Z}_{d}^{2}, \bar{Z}_{d}^{3}$ and correspondingly partition $\bar{V}_{d}$ into three parts $\bar{V}_{d}^{1}, \bar{V}_{d}^{2}, \bar{V}_{d}^{3}$. Then we may write

$$
\begin{array}{r}
\bar{Z}_{s d}^{1}=\bar{V}_{d}^{1} U_{11}^{11}+\bar{V}_{d}^{2} U_{11}^{21}+\bar{V}_{d}^{3} U_{11}^{31} \\
\bar{Z}_{s d}^{2}=\bar{V}_{d}^{1} U_{11}^{12}+\bar{V}_{d}^{2} U_{11}^{22}+\bar{V}_{d}^{3} U_{11}^{32} \\
\bar{Z}_{s d}^{3}=\bar{V}_{d}^{1} U_{11}^{13}+\bar{V}_{d}^{2} U_{11}^{23}+\bar{V}_{d}^{3} U_{11}^{33} \\
\bar{Z}_{s e}=\bar{V}_{d}^{1} U_{12}^{11}+\bar{V}_{d}^{2} U_{12}^{21}+\bar{V}_{d}^{3} U_{12}^{31} \\
 \tag{31}\\
+\bar{V}_{e} U_{22}
\end{array}
$$

Since we want $\bar{Z}_{s d}^{1}=\bar{Z}_{d}^{1}$ and $\bar{Z}_{s d}^{3}=\bar{Z}_{d}^{3}$ we have for a given simulation of $\bar{V}_{d}^{2}$ two equations and two unknowns in the vectors $\bar{V}_{d}^{1}$ and $V_{d}^{3}$. Additional components being under sampled at the same or additional locations simply induces a more complex partitioning. In terms of a program these can be tracked by the use of counters.

## 4. SOME PRACTICAL ASPECTS

Any consideration of vector valued random functions must deal with the question of the modeling of cross-covariances. The most common practice either implicitly or explicitly uses a model of the form given by (5). In this case the actual functions used are all covariances (and in particular the positive definiteness condition is assured by imposing conditions on B). This is necessary because one can not impose sufficient conditions on a cross-covariance separately from the conditions imposed on the associated covariances and hence one can not easily identify standard cross-covariance models. Myers (1982, 1987) suggested an alternative method for more direct modeling of the cross-covariance< by considering the covariances of the sum and difference of the two components in question. Theoretically either of these is sufficient to construct the cross-covariance (in conjunction with the associated covariances) but since the modeling is not perfect both are necessary. This would appear to allow for more general models. Unfortunatcly if all covariances are modeled with finite linear combinations of standard models (no matter how large this set is) the requirement that the cross- covariance produced from the covariances of the sum and difference coincide reduces the technique to the use of a model like that given by ( 5 ). One has simply arrived at that point by a different process In turn this implies that in practice the distinction between "true" co-sirnulation and separate simulation of uncorrelated components used to re- construct the correlated components is more one of how the conditioning is done than how the simulation is done.

## 5 NUMERICAL RESULTS

As a test of the program, 20 runs were made of an unconditioned sirnulation for two variables. Likewise 20 runs were made conditioned on 100 points. In each case simulated values were roduced for a $10 \times 10$ grid. The variogram for each of the variables was spherical wit a sill of 1.0 and a range of 6.0 The cross-variogram was chosen so that the variogram of the difference of the two variables would also be spherical with the same parameters. The resulting sample variograms and variogram of the difference, plotted against the model, are shown in Figures 1,2. Computing time for 20 rins was less that 5 mirutes on a VAX 11/750.

## ACKNOWLEDGEMENTS

Portions of this paper were written while on sabbatical and visiting in the Departmentsof Statistics and Applied Earth Sciences, Stanford University. The program implementin?

VECTOR CONDITIONAL SIMULATION

the multivariate version of the matrix decomposition simulation algorithm was written by Jerry Jalkanen.

## NOTICE

Although the researcla described in this presentation has been supported by the United States Environmental Protection Agency through a Cooperative Research Agreement with the University of Arizona, it has not been subjected to Agency review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred.

## REFERENCES

Alabert, F., 1987a, 'Stochastic Imaging of Spatial Distributions using Hard and Soft Data', (unpublished), MS Thesis, Dept Applied Earth Sciences, Stanford University

Alabert, F., 1987, 'The Practice of Fast Conditional Simulations Through the LU Decomposition of the Covariance Matrix' Math. Geology 19 (5) 369-385

Borgman, L., Taheri, M. and Hagan, R., 1984, 'Three-Dimensional, Frequency-Domain Simulations of Geological Variables' in Geostatistics for Natural Resource Characterization, G. Verly et al (eds), D. Reidel Publishing Co., Dordrecht

Brooker, P., 1985, 'Two-dimensional Simulation by Turning Bands' Math. Geology 17 (1) 81-90

Carr, J. and Myers, D.E., 1985, 'COSIM:A FORTRAN IV Program for Co-conditional Simulation' Computers and Geosciences 11 (6) 675-705

Carr, J., Myers, D.E. and Glass, C., 1985, 'Co-kriging-A Computer Program' Computers and Geosczences 11 (2)

Chiles, J.P., 1984, 'Simulation of a Nickel Deposit: Problems Encountered and Practical Solutions' in Geostatistics for Natural Resource Characterization, G. Verly et a] (eds), D. Rcidel Publishing Co., Dordrccht 1015-1030

Christakos, G., 1987, 'Stochastic Simulation of Spatially Correlated Geo-processes' Math. Geology 19 (8) 807-831

Davis, M., 1987a, 'Production of Conditional Simulations via the LU Triangular Decomposition of the Covariance Matrix' Math. Geology 19 (2) 91-98

Davis, M., 1987b, 'Generating Large Stochastic Simulations - The Matrix Polynomial Approximation Method' Math. Geology 19 (2) 99-107

Dowd, P., 1984, 'Conditional Simulation of Interrelated Beds in an Oil Deposit' in Geostatistics for Natural Resource Characterization, G.Verly et al (eds), D. Reidel Publishing Co., Dordrecht 1031-1043

Isaaks, E.H., 1984, 'Indicator Simulation:Application to the Simulation of a High Grade Uranium Mineralization' in Geostatistics for Natural Resource Characterization. G.Verly et al (eds), D. Reidel Publishing Co., Dordrecht

Journel, A.G. and Huijbrechts, Ch., 1978, Mining Geostatistics Academic Press, London

Mantoglou, A. 1987, 'Digital Simulation of Multivariate 2 and 3 Dimensional Stochastic Processes with Spectral Turning Bands Method' Math. Geology 19 (2) 129-150
hlantoglou, A. and Wilson, J., 1982, 'The Turning Bands Method for Simulation of Random Fields using Line Generation by a spectral Method' Water Resources Research 18 (5) 1379-1394

Matheron, G., 1973, 'Intrinsic Random Functions and their Applications' Adv. Applied Probabzlzty 5 439-

Miller, S.M. and Borgman, L.E., 1985, 'Spectral-Type Simulation of Spatially Correlated Fracture Set Properties' Math. Geology 17 (1) 41-52

Myers, D.E., 1982, 'Matrix Formulation of Co-kriging' Math. Geology 14 (3) 249-257
Myers, D.E., 1984, 'Co-kriging-New Developments' in Geostatistics for Natural Resource Characterization, G.Verly et al (eds), D. Reidel Publishing Co., Dordrecht 295306
Myers, D.E., 1987, 'Multivariable Geostatistical Analysis for Environmental Monitoring' to appear in Sciences de la Terre
Shinozuka, M., 1971, 'Simulation of Multivariate and Multidimensional Random Processes' J. Acoustical Soc. Amer. 49 357-367

Silliman, S., 1986, 'Stochastic Analysis of High Permeability Paths in the Subsurface', (unpublished) Ph.D. Thesis, Department of Hydrology, University of Arizona

Wackernagel, H., 1988, 'Geostatistical Techniques for Interpreting Multivariate Spatial Information', in Quantitative Analysis of Mineral and Energy Resources, C.F. Chung et al (eds), D. Reidel Pub., Dordrecht 393-409

