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# Geostatistical Methods:

## Recent Developments and Applications in Surface and Subsurface Hydrology

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# SPATIAL-TEMPORAL GEOSTATISTICAL MODELING IN HYDROLOGY

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## ABSTRACT

Geostatistics has been utilized by a number of authors for the analysis of hydrological parameters such as permeability and hydraulic conductivity. The techniques are used in general to characterize the spatial variability for the variable of interest and to partially compensate for the late of state equations to model these parameters. These variables are considered to be temporally constant whereas other aquifer characteristics such as water table elevation are generally spatially and temporally dependent. If geostatistical methods are to be used to analyze these other characteristics then both spatial and temporally variablity must be incorporated. Although the presence of both types of dependence is not unique to hydrological problems, it also occurs in air pollution applications, there are very few examples of such analyses. In particular it is necessary to model variograms that incorporate both forms and the several of the published examples are now known to have theoretical defects (Myers and Journel, 1990, Rouhani and Myers, 1990). Since the variogram is the key component for the application of geostatistics, adequate modeling is essential. There are several possible approaches; incorporation of the temporal dependence only in the nonstationarity, incorporation of the spatial dependence only in the variogram parameters, separation of temporal and spatial dependence by treating different time points as separate variables whose interdependence and spatial dependence is characterized by variograms and cross-variograms, finally the model might be of the most general type wherein the value of the variogram is dependent on both the spatial and the temporal lags. Previous models have attempted to separate the dependence by modeling the variogram as a sum with spatial components and temporal components. It is the latter construction that is invalid. A review of all these constructions together with examples and applications is given.

## 1 INTRODUCTION

Unlike some areas of application for geostatistics such as ore reserve estimation, hydrology has a history of the use of both deterministic and probabilistic modeling. In particular state equations for fluid flow are wellknown and only require the separate determination of certain media parameters. These equations link in a natural way both spatial and temporal dependence. Geostatistics has been used most often either in applications where state equations are not known or where neither analytical nor numerical solutions of the state equations are easily obtained but where in some sense a sufficient amount of data is available. Some of the earliest applications of geostatistics were in hydrology, for example the monitoring of the aquifer underlying the lagoon at Venice. Most applications of geostatistics however have concentrated on spatial dependence and few have considered the link with temporal dependence. There are several possible reasons for this neglect; first of all temporal dependence has traditionally been modeled by time series with the associated emphasis on Fourier methods whereas Fourier techniques have had little impact on geostatistics, secondly variogram or covariance modeling is easiest in the isotropic case and geometric anisotropies can be easily modeled in terms of simple transformations on isotropic models. The extension of such methods to combined spatial-temporal dependence would require the use of a "natural" distance function in space-time. One possible approach is separate in some way the spatial dependence from the temporal dependence and model the two separately, for example to use the analogue of a zonal anisotropy, that is, the function of time and space is represented as a sum of two functions each depending on only one of the two. In subsequent sections various possible ways to model the combined dependence are examined together with the difficulties which occur, these are both theoretical and practical in that often it is a lack of the right kind of data that causes the problem.

## 2 THE GENERAL FORM

Particularly in the context of environmental problems where there may be many variables of interest, it is natural to consider $m$ functions $Z_1(x,t),\ldots,Z_m(x,t)$ where $x$ denotes a point in the appropriate dimensional space. For example these might represent different pollutant concentrations in an aquifer at location $x$ and time $t$. Although each has been written as though it depends on both time and space, one or more of these functions may be dependent on only one of the two. In the geostatistical context then the problem might be to estimate one or more of these functions at some point and time given spatial-temporal data. It may also be that we want to establish a causal relationship between some of these where the causality is expressed in statistical terms rather than deterministic. It may be that some or all of the data has non-point support in space or time or both, for example the data may represent pollutant concentrations at different locations but rather than being "instantaneous" levels they represent daily or weekly averages or perhaps maxima over the time upto $t$.

As shown in Rouhani and Myers (1990) each function $Z_j(x,t)$ separately could be considered as a random function with mean $M_j(x,t)$ and variogram $(h,s)$ or covariance $C(h,s)$, and if estimated separately the form of the kriging estimator(s) is unchanged by the incorporation of time. The kriging equations are likewise unchanged. Unfortunately there are both practical and theoretical problems associated with modeling such variograms and covariances.

Stein (1984) has considered a special case where the components are nearly uncorrelated and hence can nearly be separately estimated, that is $Z_i(x',t''), Z_j(x,t)$ are uncorrelated for all $x',t'',x,t$ except when $t''=t$ and $x'=x$. The cross-variograms have a very special form in that case.

The general form as presented above is in general so broad that it neither fits common applications nor lends itself to succinct analysis. It can perhaps be best described by examining various special cases.

1. Let $y(x,t)$ be a variable of interest defined in a region of space and also in a domain of time, for example y might be the infiltration rate at location $x$ and on day (or time) $t$. New variables can be defined in a number of ways, for example

$$z_1(x) = \int y(x,t)\,dt \text{ or } z_2(x) = (1/T)\int y(x,t)\,dt \tag{1}$$

Measuring time in days already suggests that the time dependence has been altered from instantaneous to the cumulative or average value for the day. This could be extended further to monthly or yearly averages, for sufficiently long periods the values might be treated as replications of the same variable in space. For a small number of intermediate length time periods the values might be treated as different variables.

2. Alternatively the spatial dependence might be removed by using areal averages usually leading to the use of time series methods.

$$w_1(t) = \int y(x,t)\, dx \tag{2}$$

$$w_2(t) = (1/A) \int y(x,t)\, dx \tag{2}$$

3. In some instances the dependence on space and time can be separated, for example the random function may be non-stationary but the random component depends only on location or time but not both as in the representations

$$Z_j(x,t) = M_j(x,t) + Y_j(x) \tag{3}$$

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While the variogram or covariance might be dependent on both $x, t$ it would differ from a variogram (or covariance) dependent only on one of the two by a deterministic function. Of course the random function might be non-stationary with respect to only one of $x, t$. The dependence on $x, t$ might be separated in other ways such as

$$Z_j(x,t) = Y_{j1}(x) Y_{j2}(t) \tag{4}$$

$$Z_j(x,t) = Y_{j1}(x) + Y_{j2}(t) \tag{4}$$

$$M_j(x,t) = m_{j1}(x) + m_{j2}(t) \tag{5}$$

$$M_j(x,t) = m_{j1}(x) m_{j2}(t) \tag{5}$$

As will be seen later, (4') seems very plausible but there are serious theoretical difficulties in modeling variograms for this decomposition.

In some instances one may only be interested in the functions at a finite number of time points (those represented in the data) in which case the temporal dependence can be suppressed as follows

$$W_{jk}(x) = Z_j(x, t_k);\ k = 1, \ldots, p \tag{6}$$

Sager (1977) has suggested other ways to remove or cope with the dependence on a spatial or temporal variable, for example

$$V_j(z) = \int_{t; U_j(t) < z} U_j(t) dt \tag{7}$$

$$D(t', t'') = \int [Z_j(x, t') - Z_j(x, t'')] dx \tag{8}$$

The difficulties incurred when both spatial and temporal dependence are incorporated are primarily those associated with modeling the variogram or covariance. While such modeling has not received a large amount of attention there are notable examples. Bilonick (1985,1987) used nested variograms to model and krige an atmospheric chemical deposition data set. Rouhani and Hall (1988) used intrinsic random functions for space-time kriging of piezometric data. Mizell (1980) used the state equation to derive a spatial-temporal covariance. As will be seen later some of these have a theoretical defect or weakness.

## 3 FUNDAMENTAL DIFFERENCES

As noted by Journel (1986), there are major differences between spatial and temporal phenomena. In the case of spatial phenomena the function or variable of interest is usually unique and the uncertainty or stochastic nature of the problem reflects a lack of knowledge about the values at unsampled locations or the functional form rather than a true randomness. While there may be some directional dependence, i.e., an anisotropy, there is in general no ordering whereas for temporal phenomena there is always the notion of past, present and future. Although in geostatistics spatial variables of interest are treated as realizations of a random function, that is,

$$z(x_i) = Z(x_i, \omega_j) \tag{9}$$

where $\omega_j$ is the element of the underlying probabilty space or index on the realizations, this stochastic dependence is usually suppressed. See for example DeMarsily and Ahmed (1987) with respect to the modeling of transmissitivity.

This practice or approach may not be fully satisfactory when time is treated as simply another dimension and when the variable of interest is considered as a unique realization of a random function defined in space and time. For example, piezometric head might represent a unique realization for the past and present but in the case of the future there is a truer stochastic dependence. For some variables this dilema can be resolved by taking advantage of a periodicity in time, when the variable is observed over multiple time periods these might be treated as multiple realizations. The difficulty lies in determining the temporal extent of each realization, in particular these may not be of constant length. Because the spatial extent of the region of interest is always taken to be finite and generally is considered fixed, periodicities in space are not often modeled. For example Journel and Froideveaux (1982) concluded in one instance that there was very little improvement in the estimator as the result of using a (spatial) hole-effect variogram. It seems less likely that this would be the case for temporal periodicities. A further complication may occur if the time domain is segmented to generate multiple realizations, these are often correlated and it becomes necessary consider the multiple "realizations" as single realizations of several correlated random functions. The analysis in this case requires the use of cross-variograms and co-kriging.

The most important difference is not so much that between spatial and temporal problems but rather that between spatio-temporal problems and either of the two simpler models. In either of these two simpler contexts the contruction of valid covariance or variogram models is fairly easy, i.e. through the use of nested models and in the case of covariances by products as well. There are as yet no known standard ways of constructing variograms or covariances in space-time, moreover some that are suggested by the representations (4), (4') lead to non-invertible kriging matrices.

## 4 DATA CHARACTERISTCS

One of the advantages usually cited for kriging is that it does not require data on a regular grid, in the spatial context this is very important because sampling is usually not on a regular grid and in fact it is not efficient either for variogram estimation or kriging. Relatively speaking the number of sample locations is usually small. In contrast temporal data is usually regularly spaced and the number of sampling points is large, Fourier or time series methods are strongly dependent on the regularity and the large sample size. Spatial-temporal data often exhibits both characteristics in that there will be a large number of observations in time at a small number of spatial locations. This leads to considerable difficulties in estimating and modeling variograms, Switzer (1989) has shown that the additional temporal data can be used to offset the lack of spatial data but in the process the spatial-temporal dependence is suppressed.

The well-known Borden data set illustrates a number of the problems associated with spatial-temporal dependent phenomena. While sampling tubes were installed at a large number of locations and data was collected daily for nearly two years, the movements of the pollutants was such that even modeling spatial variograms for fixed time points or temporal variograms at a few spatial locations was difficult because of sparcity of data as seen in Myers (1989), Myers et al (1990). Some of the difficulties may be seen in another way; if $(x, t)$ is considered a point in a higher dimensional space then the data may be concentrated in a very "thin" subspace. Estimation in this case is analogous to estimation in the plane when all the data is concentrated on a transect.

## 5 SPACE-TIME KRIGING

If time is simply considered as another dimension then there is no change in the form of the kriging estimator nor in the kriging equations, that is, if $(x_0, t_0)$ is an unsampled location-time and given data $Z(x_1, t_1), ..., Z(x_n, t_n)$ then $Z(x_0, t_0)$ could be estimated by

$$Z^*(x_0, t_0) = \sum \lambda_i Z(x_i, t_i) \tag{10}$$

where there are no assumptions about any interrelations between the space and the time coordinates of a point. That is, the estimator will interpolate in either space or time and will extrapolate in either space or time. The definition of the variogram or covariance for Y is completely analogous to the spatial case and (strict) conditional positive definiteness is sufficient for the kriging system to have a unique solution as shown in Myers (1988b).

$Z(x, t)$ is said to satisfy the Intrinsic Hypothesis (in time and space) if for any any increment $(h, k)$

$$\text{(i) } E[Y(x + h, t + k) - Y(x, t)] = 0$$

$$\text{(ii) } 0.5Var[Y(x + h, t + k) - Y(x, t)] = \gamma(h, k)$$

exists and does not depend on $h$ or $k$.

Note that it is not necessary to introduce a metric or distance in space-time, that is, to combine spatial and temporal distance in order to introduce variograms or for kriging although if it is desired to have some concept of isotropy then such a distance would be necessary. Such a form of isotropy seems unrealistic because of the intrinsic ordering for time and non-reversability. In the spatial context there is essentially no difference between interpolation and extrapolation, of course the kriging variances will be larger when extrapolating in either domain. In general in the spatial context one expects to find sample locations relatively uniformly spread around the location to be estimated (except on the border of a region) but in the temporal context the sample locations will always be on one side, the past, and hence the estimation is always a form of extrapolation. Again in the context of piezometric head data this results in serious problems, for example if the data is all taken during a wet season and the time to be estimated is in a subsequent dry season then the estimator can not adapt to the temporal transition without incorporating the temporal non-stationarity. This latter option will lead to all the indeterminancy problems known to be associated with the separate estimation of the drift (spatial or temporal) and the residuals as noted by Armstrong (1984). Where the estimator is written in the form of kriging or as a time series model some model assumptions must be incorporated when the objective is prediction into the future.

Computational problems may arise in a number of ways, in particular the coefficient matrix in the kriging system may be ill-conditioned for specific sample location patterns. The difficulty may be due to an insufficient number of sample locations compared to the order(s) of the drift(s) or because the locations are concentrated in a lower dimensional space, for example one will obtain poor estimates spatially if all the data is concentrated at one location but at different times. In other contexts this is referred to as the curse of higher dimensions and relatively speaking it is worse as the dimension increases, i.e., extending from 2-space spatially to space-time is worse than from 1-space spatially to space-time.

While the form of the Universal Kriging equations for space time kriging would be completely analogous to the spatial case, estimating and modelling the drift will likely cause much greater problems. If local neighborhoods are used for the estimation then low order non-stationarities can be ignored in the estimation process as suggested by Journel (1986). Seguret (1987) points out that if the drift is of low order, for example trigonometric, and the size of the kriging neighborhood is much smaller than the "period" of the drift function then the matrix will be ill-conditioned. Seguret suggests including additional sample locations corresponding to large time lags, these improve the efficacy of the inversion methods but have little impact on the estimated value. The most difficult problems occur however in the context of estimating and modeling variograms or covariances.

## 6 STRUCTURAL ANALYSIS

The simplest way to model a variogram in space-time is to separate the dependence on the two as suggested above in various forms. This runs counter to the practical techniques in common use for estimating and modeling variograms. For example the obvious analogue to the usual sample variogram would be as follows:

$$\gamma^*(h,k) = \frac{1}{2N(h,k)} \sum Z(x_i + h, t_i + k) - Z(x_i, t_i)^2 \tag{11}$$

While it is common practice in both 2, 3-dimensional space to consider sample variograms in various directions *including* those parallel to the coordinate axes one often finds that the number of pairs decreases to an extent that the directional variograms are not easy to model. Moreover the directional variograms are not really modeled separately but rather are only used to determine the angle of anisotropy and the ratio of the maximum to the minimum range. In the usual Euclidean space no one coordinate axis has any special character with respect to the others, this is of course not true in space-time. There are some examples in the literature wherein variograms have been modeled in space-time. These include the following:

$$C(h,t) = C_t(t)C_h(h) \text{ (Rodriquez-Iturbe and Mejia, 1974)}$$

$$\gamma(h,t) = \delta_0 + \gamma_t(t) + \gamma_h(h) + \gamma_{h,t}([gh^2 + t^2]) \text{ (Bilonick,1987)}$$

$$GC(h,t) = GC_t(t) + GC_h(h) \text{ (Rouhani and Hall,1988)}$$

where
$C$ = spatiotemporal covariance
$C_t$ =temporal covariance
$C_h$ = spatial covariance
$\gamma$ = spatiotemporal variogram

$\delta_0$ = pure nugget variogram
$\gamma_t$ = temporal variogram
$\gamma_h$ = spatial variogram
$\gamma_{h,t}$ = isotropic spatiotemporal variogram
$GC$ = spatiotemporal generalized (polynomial) covariance
$GC_t$ = temporal generalized covariance
$GC_h$ = spatial generalized covariance
$g$ = geometric coefficent of anisotropy between space and time
$t$ = time lag
$h$ = space lag
Each of these is obtained by assuming a decomposition as suggested in an earlier section. Unfortunately two of these are not completely valid as is shown by the following.

*An Example.* Several of the models listed above were constructed using the premise that a positive linear combination of valid models produces a valid model or in the case of covariances, the product of covariances is a covariance. Using an example due to Myers and Journel (1990) but transposed to the spatiotemporal domain it is seen that this is not quite correct when the models are dependent only on some of the coordinates.

Consider four points in $(x,t)$ space ($x$ in 1-dimensional space) with coordinates as follows; Point1:(0,0),Point2:(0,b), Point3:(a,0), Point4:(a,b) and a variogram model is constructed to represent a zonal anisotropy as follows

$$\gamma(h,t) = \gamma_1(h) + \gamma_2(t)$$

Suppose that $\gamma_1(0) = 0$, $\gamma_1(a) = u$, $\gamma_2(0) = 0$, $\gamma_2(b) = v$ and consider the coefficient matrix for ordinary kriging when using these four data locations

$$\begin{bmatrix} 0 & u & v & u+v & 1 \\ u & 0 & u+v & v & 1 \\ v & u+v & 0 & u & 1 \\ u+v & v & u & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

It is easily seen that this matrix is singular, the fallacy is that valid models which are made to depend on only some of the coordinates are not valid models in the higher dimensional space, that is, the transformation (x,t) to x (or to t) is not sufficiently well-behaved. This example shows that models such as those listed above may not be valid for particular data location patterns. Note that very little was assumed about the sub-models in the constructed model hence the counter-example is very general. If the variogram or covariance is continuous, for example it is given as linear combination of standard models but without a nugget term, then "near" sample location patterns will produce matrices that are ill-conditioned, hence even if the matrix is invertible there may be computational problems. This difficulty can arise even with a valid model, for example if the number of sample locations is small compared to the order of the drift or if the sample locations are concentrated in a lower dimensional space, e.g., all data collected at one location but at many different times. Unfortunately other simple methods for constructing zonal anisotropies are lacking and hence methods for modeling variograms in space-time are also lacking. One alternative of course is to simply use isotropic models and ignore any distinction between future, past times.

*A Special Case* Suppose that data is known only for a finite number of times $t_1, ..., t_m$ and the objective is only to estimate at an unsampled location for one or more of these times then one solution is to define m spatial variables $Z_1(x) = Z(x,t_1), \ldots, Z_m(x) = Z(x,t_m)$ and use co-kriging in either a full or undersampled form as described in Myers (1982,1984, 1988a). This will require the use of cross-variograms and modeling these produces a different set of problems.

## 7 CO-KRIGING

Recall that the co-kriging estimator can be written in the form

$$\overline{Z}^*(x_0) = \sum \overline{Z}(x_i)\Gamma_i \tag{12}$$

where $\overline{Z}(x) = [Z_1(x), ...., Z_m(x)]$ and the weight matrices, $\Gamma_i$, are obtained from a system of linear equations in which the coefficients are the values of the matrix valued variogram. That is, the entries in the matrix valued variogram are simply variograms on the diagonal and cross-variograms on the off-diagonal, covariances and cross-covariances can also be used. The problem of modeling the variogram in space-time is replaced by one of estimating and modeling cross-variograms. Two problems occur; first there is the question of valid models for cross-variograms and secondly a sufficient number of spatial locations for which data is collected at all the times. The first problem can be addressed by the use of "sums" and "differences" as described in Myers (1984, 1988a). The second problem can be addressed by the use of pseudo-cross variograms which were first introduced by Clark et al (1989). Clark et al did not resolve a number of questions concerning valid models but these are covered in Myers (1990). As defined by Clark et al, the pseudo-cross variogram is given by

$$\hat{g}_{jk}(h) = 0.5E[Z_j(x) - Z_k(x+h)]^2 \tag{13}$$

and generalized by Myers (1990) as

$$g_{jk}(h) = g_{kj}(-h) = 0.5\mathrm{Var}[Z_j(x) - Z_k(x+h)] \tag{14}$$

If $Z_j(x), Z_k(x)$ are second order stationary with covariances $C_{jj}(h), C_{kk}(h)$ and cross-covariance $C_{jk}(h)$ then (14) can be re-written in the form

$$g_{jk}(h) = 0.5[C_{jj}(0) - 2C_{jk}(0) + C_{kk}(0)] + \gamma_{jk}(h) \tag{15}$$

where $\gamma_{jk}(h)$ is the usual cross-variogram. If further $m_j, m_k$ are the means then

$$\hat{g}_{jk}(h) = g_{jk}(h) + 0.5[m_j^2 - 2m_j m_k + m_k^2] \tag{16}$$

If moreover $m_j = m_k$ then (13) and (14) coincide. Although neither (13) nor (14) is a variogram or a covariance they are "close" to being cross-variograms except that both are non-negative valued and need not be zero when $h = 0$ as is necessary for a variogram. It is necessary to examine for symmetry otherwise the model for negative lags may be different for positive lags. Clark et al obtained the co-kriging estimator for one variable using data on all variables although they did not give sufficient conditions to ensure the existence of a solution to the co-kriging equations. In Myers (1990) it is shown that the general co-kriging estimator is the same as given in (12) and the cokriging equations are the same as when cross-variograms are used except that the off-diagonal entries in the matrix variogram are the pseudo-cross variograms. By their definitions either (13) or (14) may be estimated by sample analogues but it is not necessary that data be available for both variables at any common points. This is easily implemented in standard variogram software. The pseudo-cross variogram can be modeled as a cross-variogram plus a positive constant, namely the value at $h = 0$.

## 8 SUMMARY

There is increasing interest in applying geostatistics to problems where there is both spatial and temporal dependence, perhaps intervariable dependence well. The underlying assumptions of stationarity, the form of the kriging estimator and the kriging equations do not change but there are practical and theoretical difficulties associated with the modeling of variograms. When treated as simply another dimension certain important aspects of the temporal dependence are lost. Various alternatives and partial solutions have been presented.

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