A Numerical Spectral Approach for the Derivation of Piezometric Head Covariance Functions

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Relating the variability of permeability to the variability of head is a central part of linear estimation techniques such as cokriging. Only a few analytic relationships between log permeability covariances and head covariances presently exist. This paper describes a general numerical procedure which computes head covariances (ordinary or generalized) and cross covariances for any proper log permeability covariance. The numerical spectral method, a discrete analog of Fourier-Stieltjes analysis, employs the pertinent linearized (small-perturbation approximation) equations describing the physics of flow. The domain is taken as finite, with boundary effects considered negligible. The numerical spectral method can reproduce all pertinent analytic results with excellent agreement. Furthermore, we demonstrate the method's generality by finding the covariance relations for a case where no analytical results presently exist.

1. INTRODUCTION

Groundwater mechanics has traditionally dealt with "deterministic" or fully specified problems: fully specified geometry, parameters, boundary conditions, and initial conditions. Given this information, application of the principles of fluid mechanics, such as continuity and Darcy's law, produces a unique solution. However, in geohydrologic applications, one is seldom able to specify precisely all inputs to the problem. For example, one may only have measurements of the piezometric head and transmissivity at a few locations, some geologic logs, and less frequently, results of some tracer tests. With this information the geohydrologist is faced with the task of predicting the movement of a contaminant plume and of recommending a cost-effective remediation scheme.

The available information is incomplete, that is, insufficient for a precise deterministic prediction. However, by combining available measurements, applying fluid mechanics principles or models, and analyzing the spatial variability of geologic formations, one can achieve the next best thing: quantifying the likelihood of possible events. These predictions can be used, for example, to design the most economical remediation scheme for a prescribed reliability level. Rigorous probabilistic analysis using groundwater models and measurements can be extremely complicated. A practical approach, which is adequate for many applications, is to use linear estimation methods [see Kitanidis and Vomvoris, 1983; Hoeksema and Kitanidis, 1984; Dagan, 1985a; Rubin and Dagan, 1987a, b]. This family of methods, also known as kriging, cokriging, Gaussian conditional mean, etc., only require specification of mean values, variances, and correlation coefficients of the hydrogeologic properties, such as the piezometric head or the logarithm of the hydraulic conductivity (log permeability). This estimation procedure is usually implemented as follows:

1. The correlation structure of the log permeability is specified on the basis of data and other information. For example, the log permeability may be represented through a stationary process with an exponential covariance function.

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2. The flow equation is used to relate the head to the log permeability. The correlation structure of the head and the cross correlation between head and log permeability are derived.

3. The parameters of the spatial variability model are estimated, and the consistency of the overall model with the data is tested.

4. The best estimates of the head or log permeability at any point and the variance of the estimation error can then be calculated with a best (minimum variance) linear unbiased estimator, such as cokriging.

This work focuses on the second step, i.e., the derivation of the covariance function of the head and the cross-covariance function of the head and log permeability, which are needed for the third and fourth steps.

The physical relationship between head and log permeability can be described by a stochastic partial differential equation; that is to say a partial differential equation with statistically specified coefficients. Because this mathematical relation cannot be expressed in a closed form, many approximate methods have been proposed. Freeze [1975] used a Monte Carlo technique to relate the log permeability and head covariances, as did others [Smith and Freeze, 1979a, b; Schwartz, 1977; Smith and Schwartz, 1980, 1981a, b]. Monte Carlo methods appear very general, but their usefulness is somewhat limited because of their computational costs. Dagan [1979, 1981] developed the self-consistent embedding matrix approximation, and Chirlin and Dagan [1980] applied the method to a two-dimensional field to find the head variograms.

When approximate methods are used to solve the stochastic equation describing groundwater flow, the computational cost can be significantly reduced if the variance of log permeability is small. In this case, the so-called "small perturbation" assumption allows us to avoid the cost of repeated simulations. Numerical methods for approximately solving the stochastic equation for groundwater flow have been developed. Sagar [1978] proposed a Galerkin finite element method to find the head variance from permeability information, while Hoeksema and Kitanidis [1984] used a finite difference scheme. Dikow [1988] used spectral methods to compute fluxes at outflow boundaries. Under certain
conditions, analytical solutions relating head and log permeability covariances can be developed. One of the most important analytical techniques are spectral methods, which make use of an integral transform to produce closed-form solutions. Among the assumptions made in this approach is that the domain is infinite [Baker et al., 1978; Gutjahr and Gelhar, 1981; Mizell et al., 1982] or semi-infinite [Naff and Vecchia, 1986]. Dagan [1982a, b, 1985a] has developed other analytical methods, also assuming unbounded domains. Developing analytical solutions is far from a trivial matter and closed-form solutions are not yet available for most log permeability covariances.

In these analytical solutions the rationale for using an unbounded domain is that (1) boundary conditions are often not well defined, and (2) the effect of head boundary conditions is limited to within a few correlation lengths from the boundary so they can be neglected if the boundary is located far enough from the area of interest. Although the assumption of an infinite domain makes analytical solutions easier to develop, the unbounded domain assumption seems to have a limitation: the need to place restrictions on the permissible log permeability functions so that for one- and two-dimensional flow, head variances remain finite [Baker et al., 1978; Gutjahr and Gelhar, 1981; Mizell et al., 1982]. However, an infinite head variance simply means that the expected value of the squared difference between the head fluctuations at two different points increases without bound as the distance between these two points increases. Since all cases of practical interest involve finite distances, this is not a serious limitation. The approach followed by Dagan [1985a] and Rubin and Dagan [1988] is to use the head semivariogram. This is adequate for purposes of carrying out minimum variance unbiased linear estimation.

Analytical solutions are possible only in special cases: where covariance functions are convenient analytical expressions. This paper presents an efficient computer-based numerical approach which can compute results for any valid log permeability covariance function and for any dimension. In fact, the covariance function does not have to be an ordinary one; it can also be a generalized function or a variogram. Furthermore, it can be given in analytical form or through any other means. For example, the experimental variogram, usually computed as a piecewise linear function, would be an acceptable way to specify log permeability covariances. Derivation of analytical solutions for all these cases would be a major undertaking; the method discussed here can handle them easily.

2. BACKGROUND ON SPECTRAL METHODS

"Spectral" or integral transform methods for solving differential equations are well known; Fourier and Laplace transforms are common spectral methods. The integral transform converts a problem from the "functional" domain to a "spectral" domain. Spectral methods are useful for solving differential equations because the transforms are designed so that differential equations in the functional domain become algebraic equations in the spectral domain. For many problems, the expressions in the spectral domain are easily solved and back-transformed to yield a solution in the functional domain. This section reviews elements from spectral theory needed in the development of our method.

Begin by defining a domain. For the numerical spectral method this domain is finite. We have found that the notation is simpler when the domain is taken as a unit "volume," i.e., the maximum distance in any principal direction is 1. For example, when the number of dimensions is 3, the domain would be the unit cube. The origin of the Cartesian coordinate system is placed at the center of the unit cube, thus giving $-\frac{1}{2} \leq x \leq \frac{1}{2}$ in every dimension $i$. The actual dimensions of the section of the aquifer under study can be scaled to conform to the unit cube convention.

Within this domain, let $g(x)$ be a random function or process, defined in one, two, or three dimensions ($n = 1, 2, 3$). Let $g(x)$ have zero mean

$$E[g(x)] = 0$$

where $E[ ]$ stands for "expected value of" or "mean value of." The function $g(x)$ is called stationary (or wide-sense stationary) if

$$E[g(x + \xi)g(x)] = R_{gg}(\xi)$$

where $\xi$ is the vector of the separation vector and $R$ is the covariance function. That is, a zero-mean random function is stationary if its covariance depends only on the separation vector and not the actual spatial location.

Using this finite domain, the following Fourier transform can be defined:

$$S(k) = \int_{-1/2}^{1/2} R(\xi)e^{-2\pi i \cdot \xi \cdot k} d\xi$$

where $S(k)$ is called the "spectrum," $i$ is $\sqrt{-1}$, and $k$ is an $n$-dimensional vector of integers known as the wave number. For example, if the analysis is for three-dimensional flow ($n = 3$), then $k$ can be $[0, 0, 0], [-1, 0, 0], [0, 1, 0]$. The integration is over a "volume" defined $-\frac{1}{2} \leq \xi_1 \leq \frac{1}{2}, -\frac{1}{2} \leq \xi_2 \leq \frac{1}{2}, -\frac{1}{2} \leq \xi_3 \leq \frac{1}{2}$. Note that in (3) a single integral appears as shorthand notation of a double integral (if $n = 2$) or a triple integral ($n = 3$). The term $\xi \cdot k$ is the inner or dot product of $\xi$ and $k$. In an inverse fashion we can obtain $R(\xi)$ from $S(k)$ through

$$R(\xi) = \sum_{k} S(k)e^{2\pi i \cdot \xi \cdot k} - \frac{1}{2} \leq \xi \leq \frac{1}{2}$$

In classical Fourier analysis the inverse transform (4) would be termed a Fourier series, with $S(k)$ being the Fourier coefficients. Thus our analysis makes use of classical calculus familiar to many engineers.

Since $R(\xi)$ is a covariance function, the Fourier transform (3) can be expressed in a form not involving complex exponentials. Because $R(\xi)$ is evenly symmetric about the origin, $R(\xi) = R(-\xi)$, and because for any real $\theta$, $e^{i\theta} = \cos \theta + i \sin \theta$, we may write in the three-dimensional case

$$S(k) = 2 \int_{0}^{1/2} d\xi_1 \int_{-1/2}^{1/2} d\xi_2 \int_{-1/2}^{1/2} d\xi_3 R(\xi) \cos (2\pi \xi \cdot k)$$

Similarly, for formulations in one and two dimensions, integrations are over half the unit volume ($0 \leq \xi \leq \frac{1}{2}$). Equation (5), referred to as a Fourier cosine transform, is of practical use when finding spectra.

Now consider a set of random complex variables $G(k)$
(that is, complex variables whose real and imaginary parts are random variables) with the following properties:

$$E[G(k)] = 0$$

$$E[G^*(k)G(k')] = S(k) \quad k = k'$$

$$E[G^*(k)G(k')] = 0 \quad \text{otherwise}$$

where the asterisk denotes complex conjugation. Consider the process defined in the bounded domain as follows:

$$g(x) = \sum_{k} G(k)e^{i2\pi x \cdot k}$$

Since $G(k)$ are random, $g(x)$ is a complex-valued random process. The mean of the process is exactly zero:

$$E[g(x)] = \sum_{k} E[G(k)]e^{i2\pi x \cdot k} = 0$$

and the covariance function of this function is

$$E[g(x)g(x + \xi)] = \sum_{k} \sum_{k'} E[G^*(k)G(k')] e^{-i2\pi x \cdot k} e^{i2\pi (x + \xi) \cdot k'} = \sum_{k} S(k)e^{i2\pi \xi \cdot k} = R(\xi)$$

Consequently, $g(x)$ is a stationary process with covariance $R$. The practical consequence of this analysis is that if we limit our attention to a finite domain (the unit cube in this case), the appropriate Fourier transform pair is (3) and (4). This transform preserves the covariance function $R$ for all distances of interest, which is, for $-\frac{1}{2} \leq \xi_i \leq \frac{1}{2}, i = 1, 2, 3$.

A similar procedure can be used to analyze the behavior of the cross-covariance function, which for two zero-mean stationary functions $g_1(x)$ and $g_2(x)$ is

$$R_{g_1, g_2}(\xi) = E[g_1(x)g_2(x + \xi)]$$

with a transform pair given by

$$R_{g_1, g_2}(\xi) = \sum_{k} S_{g_1, g_2}(k)e^{i2\pi \xi \cdot k} = \frac{1}{2} \leq \xi_i \leq \frac{1}{2}$$

$$S_{g_1, g_2}(k) = \int_{-\frac{1}{2}}^{\frac{1}{2}} R_{g_1, g_2}(\xi)e^{-i2\pi \xi \cdot k} d\xi$$

Let us describe the processes in functional forms similar to (8),

$$g_1(x) = \sum_{k} G_1(k)e^{i2\pi x \cdot k}$$

$$g_2(x) = \sum_{k} G_2(k)e^{i2\pi x \cdot k}$$

where $G_1(k)$ and $G_2(k)$ are random variables with these properties:

$$E[G_1(k)] = E[G_2(k)] = 0$$

$$E[G_1^*(k)G_1(k')] = S_{g_1, g_1}(k) \quad k = k'$$

$$E[G_1^*(k)G_1(k')] = 0 \quad \text{otherwise}$$

Multiplying equations in (14) and taking expected values gives

$$E[g_1(x)g_2(x + \xi)] = \sum_{k} E[G_1^*(k)G_2(k')] e^{-i2\pi x \cdot k} e^{i2\pi (x + \xi) \cdot k'}$$

$$E[g_1(x)g_2(x + \xi)] = \sum_{k} S_{g_1, g_2}(k)e^{i2\pi \xi \cdot k} = R_{g_1, g_2}(\xi)$$

Note that this analysis is free of the conventional Fourier-Stieltjes notation commonly found in infinite domain derivations. In infinite domains, Fourier-Stieltjes notation is required to describe the transform of a random process, since the transform is everywhere continuous but nowhere differentiable [Priestley, 1981]. In the finite domain case, however, the transform $G(k)$ of a random process $g(x)$ is a set of random variables, with the first two moments as already described.

3. THE FLOW MODEL

In order to obtain a relationship between head and log permeability fluctuation covariances based upon the physics of flow, we must predicate the analysis upon the pertinent groundwater flow equation. Consider a locally isotropic, spatially heterogeneous aquifer, assuming (as in other works), no sources or sinks. We will focus on this case, although the method we present is more general. The governing equation is

$$\sum_{j=1}^{n} \frac{\partial}{\partial x_j} \left( K \frac{\partial \phi}{\partial x_j} \right) = 0$$

where $n$ is the dimension of the flow domain ($n = 1, 2, 3$), and where $K$, the hydraulic conductivity, and $\phi$, the head, are both functions of the spatial location, $x$. In this paper we will use Einstein’s notation, which means that the summation sign is not shown:

$$\frac{\partial}{\partial x_j} \left( K \frac{\partial \phi}{\partial x_j} \right) = 0$$

In modeling the aquifer, it is not practical to model every detail of the spatial variables $K$ and $\phi$. Rather, we limit ourselves to describing the first two statistical moments of these functions. The head and the permeability can both be expressed as a mean function plus a random perturbation about the mean:

$$\phi(x) = \bar{\phi}(x) + h(x) \quad E[h(x)] = 0$$

$$\ln K = \bar{K} + f(x) \quad E[f(x)] = 0$$

The $\ln K$ is referred to as the “log permeability.” We shall take the log permeability and head perturbations to be stationary, with the covariance functions defined as
\begin{align}
R_{ff}(\xi) &= E[f(x)f(x+\xi)] \\
R_{hh}(\xi) &= E[h(x)h(x+\xi)]
\end{align}

These covariance functions depend only on \( \xi \), the separation vector. The cross covariance between the log permeability and head fluctuations is defined as

\[ R_{fh}(\xi) = E[f(x)h(x+\xi)] \]

and is assumed to depend only on \( \xi \).

We adopt the assumption of Bakr et al. [1978] and Mizell et al. [1982], who take the mean log permeability \( \Psi \) in (22b) as constant and the flow field as macroscopically uniform,

\[ J_j = \frac{\partial \Phi}{\partial x_j} = \text{const} \]

Neglecting products of perturbations and discarding all terms of higher than first order, (21), (22), and (25) can be combined to give

\[ \frac{\partial^2 h}{\partial x_i \partial x_j} = J_j \frac{\partial f}{\partial x_j} \]

This result was obtained by Bakr et al. [1978] and more formally by Gelhar [1986]. The small-perturbation approximation implicit in (26) is recognized as a limitation to the applicability of spectral methods to date. Dagan [1985b] showed that the small-perturbation approximation was valid for log permeability variances up to about unity, assuming an exponential log permeability covariance. Recently, Ababou et al. [1988] used numerical experiments to support their contention that small-perturbation spectral methods are valid to log permeability variances of at least 2. In this paper we will not address the validity of the small-perturbation approximation for log permeability variances greater than unity.

We turn now to the domain description. In groundwater modeling an infinite domain assumption is made for the sake of convenience, usually to free the analysis from boundary effects. The assumption is that the formation is much larger than some area of interest and therefore infinite for all practical purposes. For a bounded domain the same effect can be accomplished by specifying the size of the domain as large as needed.

Consider, for example, the case of two-dimensional flow. Assume that the “area of interest” is the shaded portion of Figure 1. This area contains all the locations where measurements are available or where predictions are to be made. One may select this area so that it contains the whole formation. It is convenient to select the orientation of the Cartesian system of coordinates and the unit lengths so that the area of interest is \(-\frac{1}{4} \leq x_1 \leq \frac{1}{4}, -\frac{1}{4} \leq x_2 \leq \frac{1}{4}\). Now consider the unit square area \(-\frac{1}{2} \leq x_1 \leq \frac{1}{2}, -\frac{1}{2} \leq x_2 \leq \frac{1}{2}\). This is the area which will be used for the numerical derivation of the head covariance function.

Restricting the domain of interest to between \(-\frac{1}{4} \leq x_i \leq \frac{1}{4}\) is not crucial to the analysis; it was done primarily to ease notational complexity. Recall that we wanted our covariances in terms of separation distances, with \(-\frac{1}{4} \leq \xi \leq \frac{1}{4}\). Since the covariances are in terms of separation distances, and not the domain coordinates themselves, we must make sure that the domain coordinates have a maximum separation distance of \(\frac{1}{2}\). This is most easily accomplished by specifying that the area enclosed by \(-\frac{1}{4} \leq x_i \leq \frac{1}{4}\) be the area of interest.

We specify that the boundary conditions of the bounded domain, \(-\frac{1}{4} \leq x_i \leq \frac{1}{4}\), be periodic, that is,

\[ f(x + n) = f(x) \]
\[ h(x + n) = h(x) \]

where \(n = \{n_1, n_2, n_3\}\) and \(n_i = 0, \pm 1, \pm 2, \ldots\). The period is of unit length in all principal directions and is twice the size of the domain of interest. In this analysis the assumption of periodicity is not limiting because we have made no assumptions about the boundary conditions on the area of interest, \(-\frac{1}{2} \leq x_i \leq \frac{1}{2}\), other than the flow field is macroscopically uniform. Furthermore, our choice of periodic boundary conditions allows direct comparison to previous work which used Fourier spectral methods, since no other boundary condition parameters cloud the analysis. Readers familiar with Fourier analysis will recognize the periodicity assumption as fundamental to the development of a Fourier transform. The continuous Fourier transform is defined in the limit as the period goes to infinity.

Assume that \(f(x)\) and \(h(x)\) are stationary random fields with covariance functions \(R_{ff}(x)\) and \(R_{hh}(x)\), respectively. (We shall later see how we can relax the stationarity assumption.) Then, as in section 2, we may write expressions for the head and log permeability fields within the unit cube

\[ f(x) = \sum_{k} F(k)e^{i2\pi x \cdot k} \]
\[ h(x) = \sum_{k} H(k)e^{i2\pi x \cdot k} \]

where \(F(k)\) is a complex random variable with

\[ E[F(k)] = 0 \]
4. The Generalized Covariance Function

Expressions (34) and (35) can be used to calculate $S_{hh}(k)$ and $S_{ff}(k)$. Then the inverse Fourier transform (4) could be used to find $R_{hh}(\xi)$ and $R_{ff}(\xi)$. However, for $k = 0$ these expressions result in indeterminate forms 0/0. (Incidentally, a similar problem arises in flow in one- and two-dimensional unbounded domains [e.g., Mizell et al., 1982] where it has motivated the use of a particular class of covariance function $R_{ff}$ which results in a finite variance for $h(x)$, the head fluctuation.) However, we will see that as in the case of unbounded domains this is not an important limitation. By using appropriately defined increments of head, a practice common in geostatistics, the head covariance function is needed only to within a constant.

Let us see the meaning of determining $R_{hh}(\xi)$ to within a constant. Because of (22) and (25), the head, $\phi(x)$, must take the form

$$
\phi(x) = m + J_j x_j + h(x)
$$

The slope coefficients $J_j$ are assumed known. For $m$ to be perfectly known, the head at a given location would have to be given. Because it is not, $m$ is not known. Consequently, we will focus on linear combinations of head values which do not depend on $m$, such as $\phi(x_i) - \phi(x_j)$. More generally, define an authorized increment as any linear combination of $\phi(x)$ values at $p$ locations,

$$
y = \sum_{i=1}^{p} \mu_i \phi(x_i)
$$

which does not depend on $m$. A necessary and sufficient condition for such an authorized increment is that $\sum_{i=1}^{p} \mu_i = 0$. The variance of the authorized increments is

$$
\text{Var}[y] = \sum_{i=1}^{p} \sum_{j=1}^{p} \mu_i \mu_j R_{hh}(x_i, x_j)
$$

Using (4), the head covariance, $R_{hh}(\xi)$, can be written as

$$
R_{hh}(\xi) = C + K_{hh}(\xi)
$$

where

$$
C = S_{hh}(0)
$$

and where

$$
K_{hh}(\xi) = \sum_{k \neq 0} S_{hh}(k)e^{i2\pi\xi\cdot k}
$$

The function $K_{hh}(\xi)$ is called the generalized covariance function and differs from the ordinary covariance function by an arbitrary constant. From (40) the value of this constant is the value of the spectrum at $k = 0$. The variance of $y$ is expressed in terms of the generalized covariance as

$$
\text{Var}[y] = \left( \sum_{i=1}^{n} \mu_i \right) \left( \sum_{i=1}^{n} \mu_i \right) C + \sum_{i=1}^{n} \sum_{j=1}^{n} \mu_i \mu_j K_{hh}(x_i - x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} \mu_i \mu_j K_{hh}(x_i - x_j)
$$
Thus the variance of the authorized increment \( y \) depends only on the generalized covariance, \( K_{hh}(\xi) \).

In linear estimation we only have to deal with authorized increments of head. This is achieved by imposing the unbiasedness constraint: the expected value of the estimation error vanishes, no matter what the value of \( m \). In this case \( K_{hh}(\xi) \) suffices for the calculation of all desired second moments of \( h(x) \). Thus for purposes of linear estimation the value of the spectrum at \( k = 0 \) can be an arbitrary constant, and the resulting generalized covariance is adequate for finding all second moments of interest.

In geostatistics the variogram is a common way of expressing the second moment of variability. For stationary increments the relation between the head semivariogram and the head generalized covariance can be simply expressed as

\[
\gamma_{hh}(\xi) = \frac{1}{2} E[(h(x + \xi) - h(x))^2] = K_{hh}(0) - K_{hh}(\xi) \tag{43}
\]

When two or more authorized increments are used for linear estimation, such as in cokriging, then a cross covariance between the two increments is needed. Similar to (39), we begin by noting that the cross covariance of log permeability and head can be written using (19) as

\[
R_{\phi h}(\xi) = C' + K_{\phi h}(\xi) \tag{44}
\]

where \( C' \) is some arbitrary constant

\[
C' = S_{\phi h}(0) \tag{45}
\]

and where \( K_{\phi h}(\xi) \) is the generalized cross covariance,

\[
K_{\phi h}(\xi) = \sum_{k \neq 0} S_{\phi h}(k) e^{i2\pi \xi \cdot k} \tag{46}
\]

We can build authorized increments of \( Y \), the log permeability, and of \( \phi \), the head, by

\[
y_1 = \sum_{i=1}^{p} \eta_i Y(x_i) \tag{47}
\]

\[
y_2 = \sum_{i=1}^{q} \mu_i \phi(x_i)
\]

If \( \sum_{i=1}^{p} \eta_i = 0 \) or \( \sum_{i=1}^{q} \mu_i = 0 \), then the covariance of increments \( y_1 \) and \( y_2 \) becomes

\[
\text{Cov} [y_1, y_2] = \sum_{i=1}^{p} \sum_{j=1}^{q} \eta_i \mu_j K_{\phi h}(x_j - x_i) \tag{48}
\]

Thus the generalized cross covariance suffices when the cross covariance of two authorized increments is needed.

While the generalized covariance of the head and a semivariogram had the simple relation expressed in (43), no such simple relation exists between the generalized cross covariance and the cross semivariogram. In cokriging, the cross variogram is defined [Journel and Huijbregts, 1978] as

\[
2\gamma_{\phi h}(\xi) = E[(f(x) - f(x + \xi))(h(x) - h(x + \xi))] \tag{49}
\]

Expressions (44) and (49) can be combined to give a relation between the cross variogram and the generalized cross covariance of log permeability and head fluctuations

\[
2\gamma_{\phi h}(\xi) = 2 K_{\phi h}(0) - K_{\phi h}(\xi) - K_{\phi h}(-\xi) \tag{50}
\]

Since the cross spectrum \( S_{\phi h}(k) \) is imaginary and odd, the generalized cross covariance must also be odd, that is, \( K_{\phi h}(\xi) = -K_{\phi h}(-\xi) \), and \( K_{\phi h}(0) \) must be exactly zero. Substitution into (50) of this symmetry gives simply \( \gamma_{\phi h}(\xi) = 0 \). Thus when using log permeability and head fluctuations and when boundary conditions are specified as in section 3, the cross semivariogram as defined in (49) is not useful. The generalized cross covariance is the proper formulation for use in cokriging.

5. NUMERICAL APPROXIMATION

Equations (34) and (35) of section 3 gave us closed-form relations between the head and log permeability fluctuation spectra. The relations were valid for finite domains with periodic boundary conditions. However, in order to find the covariance function of the head, the value of the head spectrum must be known at an infinity of wave numbers before the inverse transform can be applied. This, of course, is not possible with digital computers. In this section we present a method for approximately solving the spectral relationships obtained in (34) and (35) that is amenable for use on a digital computer. The method is computationally inexpensive and places no restrictions upon the nature of the log permeability covariance functions, save those which arise from the physics of flow.

As stated earlier, the inverse transform needed to convert (34) and (35) into covariance and cross-covariance functions is equivalent to an infinite Fourier series. However, applied mathematicians and engineers have found that functions can be approximately represented by a finite number of terms in the expansion. This leads directly to an approximation for the inverse transform defined in (4),

\[
R(\xi) = \sum_{|k| \leq K_c} S(k) e^{i2\pi \xi \cdot k} \tag{51}
\]

where \( K_c \) is some finite cutoff wave number. This allows us to find the head spectrum at a finite number of points using (34),

\[
S_{hh}(k) = \frac{(|J_k|)^2}{4\pi^2 k^2} S_{\phi}(k) \quad |k| \leq K_c \tag{52}
\]

and for the cross spectrum (35),

\[
S_{\phi h}(k) = \frac{-i|J_k|}{2\pi k^2} S_{\phi}(k) \quad |k| \leq K_c \tag{53}
\]

The error introduced by the use of (51) depends upon the value of the cutoff wave number. In (52) we can see that the error decays with the squared modulus of the wave number, indicating an \( O(k^2) \) convergence for large wave numbers. Therefore the head spectrum will quickly decay with wave number, indicating that the number of terms required will be reasonable for computation even on a microcomputer.

The steps needed to find the head variogram can be summarized as follows:

1. Scale the area containing log permeability data points into the cube \(-\frac{1}{2} \leq x_i \leq \frac{1}{2}\) for every dimension \( i \). The log permeability covariance is then estimated, either as a covariance function, or a variogram.

2. A value of the cutoff, \( K_c \), is chosen. For each wave
number $|k| \leq K_c$, (30) is used to compute the value of the log
permeability spectrum. The value at $k = 0$ need not be
computed.

3. Equations (52) and (53) are used to compute the value
of the head spectrum and cross spectrum for every $|k| \leq K_c$.
Advantage is made where possible of symmetries in the
spectral domain, especially the relation $S(k) = S^*(-k)$; this
will reduce the number of computations by approximately
half. For cross spectra the relation $S(k) = -S^*(-k)$ is used to
reduce the number of computations.

4. The inverse transforms are made using (51), thus
giving an approximation for the head covariance (to within a
constant) and the cross covariance (also to within a constant).

When the log permeability spectrum cannot be directly
determined, there is an alternative procedure to steps 2 and
4 which can dramatically reduce the computational expense
associated with the numerical spectral method, especially
for problems in two and three dimensions. Instead of numerically
or analytically evaluating the integral required in the
Fourier transform (3) or the inverse transform approximation
(52), discrete Fourier transforms are used. The discrete
Fourier transform pairs compatible with the transforms (3)
and (4) are

In one dimension

$$S(k) = \frac{1}{N_1} \sum_{n=0}^{N_1-1} R \left( \frac{n}{N_1} \right) \exp \left( -i2\pi \frac{n}{N_1} k \right) \quad (54)$$

$$R \left( \frac{n}{N_1} \right) = \sum_{k=0}^{N_1-1} S(k) \exp \left( i2\pi \frac{n}{N_1} k \right) \quad (55)$$

In two dimensions

$$S(k_1, k_2) = \frac{1}{N_1N_2} \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} R \left( \frac{n_1}{N_1}, \frac{n_2}{N_2} \right) \exp \left( -i2\pi \left( \frac{n_1}{N_1} k_1 + \frac{n_2}{N_2} k_2 \right) \right) \quad (56)$$

$$R \left( \frac{n_1}{N_1}, \frac{n_2}{N_2} \right) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} S(k_1, k_2) \exp \left( i2\pi \left( \frac{n_1}{N_1} k_1 + \frac{n_2}{N_2} k_2 \right) \right) \quad (57)$$

In three dimensions

$$S(k_1, k_2, k_3) = \frac{1}{N_1N_2N_3} \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \sum_{n_3=0}^{N_3-1} R \left( \frac{n_1}{N_1}, \frac{n_2}{N_2}, \frac{n_3}{N_3} \right) \exp \left( -i2\pi \left( \frac{n_1}{N_1} k_1 + \frac{n_2}{N_2} k_2 + \frac{n_3}{N_3} k_3 \right) \right) \quad (58)$$

$$R \left( \frac{n_1}{N_1}, \frac{n_2}{N_2}, \frac{n_3}{N_3} \right) = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} S(k_1, k_2, k_3) \exp \left( i2\pi \left( \frac{n_1}{N_1} k_1 + \frac{n_2}{N_2} k_2 + \frac{n_3}{N_3} k_3 \right) \right) \quad (59)$$

Note that the covariance function $R$ has a period of unity,
while the spectrum $S$ has period of $N_1$ in each principal
direction. The values of $N_1$, $N_2$, and $N_3$ are very much
related to the cutoff wave number $K_c$ used in the approxi-
mation (51). $N_1$ represents the number of wave numbers in
each of the principal directions, equal to $2K_c + 1$. Also, the
truncated spectral domain using the discrete Fourier trans-
form is "rectangular" defined by the set of the $N_i$, while (52)
takes a "circular" domain, defined with the radius $K_c$.
The choice of $N_i$ is not arbitrary. A general rule is that the
smaller the value of the integral scale with respect to the area
of interest, the larger $N_i$.

As a result of an inverse discrete Fourier transform, the
covariance is known only at sampled values. However, if $K_c$
is large, the covariance function will be sampled at a density
that should closely approximate the true covariance. Use of the
discrete transform does not affect the behavior of the
numerical approximations when $K_c$ is large. Furthermore,
the discrete Fourier transforms are more amenable to com-
puter implementation. The discrete Fourier transform pairs
(54)–(59) will approach the exact pair defined in (3) and (4)
when $N_i \to \infty$ for all $i$. The forward transforms (54), (56),
and (58) represent discrete approximations to the integral in (3),
while the inverse transforms (55), (57), and (59) are trunca-
tions of the infinite series (4).

The major advantage of a discrete transform is that fast,
efficient algorithms known as fast Fourier transforms (FFTs)
exist to drastically decrease the effort required to convert
between spectra and covariances. Many types of FFT algo-
rithms exist, and codes are widely available [e.g., Press et al.,
1986]. If the discrete Fourier transform is used to
approximate (3), the computation would require $O(N^2)$ com-
plex multiplications and additions. FFT algorithms require
only $O(N \log N)$ such operations. As an example of the savings
this yields, consider the three-dimensional problem
where 32 wave numbers are required in each of the principal
directions. On a typical microcomputer the discrete Fourier
transform approximation to (3) would require 2.1 central
processor days. The FFT implementation would require
87 CP seconds. This 2000-fold reduction in effort makes FFT
versions of the numerical spectral method feasible on micro-
computers.

6. Applications

In this section we examine the behavior of the numerical
spectral method when applied to problems of interest. For
purposes of verification of the numerical spectral method,
we first compare it to analytical solutions which have been
previously developed. The starting point for analytical in-
vestigations has usually been the one-dimensional problem.
This case is useful for demonstration because it can be used to
test methods and to illustrate the most important charac-
teristics of a problem-solving methodology. Thus we begin
the investigation of the applications with a one-dimensional
case.

Bakr et al. [1978] used the following function to describe
the log permeability fluctuation covariance

$$R_{\xi}(\xi) = \sigma_{\xi}^2 \left( 1 - \frac{|\xi|}{l} \right) e^{-|\xi|l} \quad (60)$$

where $\sigma_{\xi}^2$ is the log permeability variance, $\xi$ is the separation
distance, and $l$ is a length parameter. The spectrum associ-
Fig. 2. Comparison of log permeability fluctuation spectra for an unbounded domain and bounded domains.

Fig. 3. Head fluctuation variograms in a one-dimensional domain. Log permeability fluctuations covariance given by (60).

with (60) can be found by application of a Fourier transform. In an infinite domain the spectrum is given by

\[ S_f(k) = 4 \sigma_f^2 \frac{(2\pi k)^2}{1 + (2\pi k)^2} \]

(61)

where \( k \) is the wave number. For a finite domain the spectrum can be found using the cosine transform defined in (6). The result of the transform of (60), defined only at integer values of the wave number, is

\[ S_f(k) = 4 \sigma_f^2 \frac{(2\pi k)^2}{1 + (2\pi k)^2} \cdot \left\{ 1 + (-1)^k e^{-\frac{1}{4}(2\pi k)^2} \right\} \]

(62)

Application of (34) would lead directly to a head spectrum; finding the head covariance function is problematic. The inverse Fourier transform is (4), an infinite series representation; solving this series in closed form is difficult.

Figure 2 compares the spectra obtained from the finite domain and the infinite domain. One aspect arising from the finite domain requirement is that the value of the log permeability spectrum at \( k = 0 \) is no longer identically zero. The integral scale in our finite domain is related to \( S(0) \) by

\[ \lambda = \int_0^{\lambda/2} R(\xi) \frac{S_f(0)}{2\sigma_f^2} d\xi = e^{-\frac{1}{4}(2\pi k)^2} \]

(63)

Gutjahr and Gelhar [1981] demonstrated that for an unbounded domain in one dimension the log permeability integral scale must be identically zero, in addition to other restrictions. Since the value of the head and log permeability spectra at \( k = 0 \) does not affect the variogram, a nonzero integral scale does not impede finding the generalized covariances.

The numerical spectral method can be used to find the variogram of the head fluctuations, given (60) as the log permeability covariance. The results are seen in Figure 3. At small separation distances, the infinite and finite domain solutions are nearly identical, especially for small values of \( l \). As \( l \) increases, the range of agreement between the solutions decreases. One characteristic of the finite domain solutions is that the computed head variogram approaches a constant sill, i.e., the slope of the variogram is zero at \( \xi = \pm \frac{\lambda}{2} \). In the finite domain the stationary log permeability fluctuations resulted in stationary head fluctuations.

In addition to computing the head variogram one can also compute the generalized cross covariance of head and log permeability fluctuations. The unbounded-domain solution for the cross covariance corresponding to log permeability covariance (60) is

\[ R_{fh}(\xi) = \kappa_f^2 J_\xi e^{-\frac{1}{4}(2\pi k)^2} \]

(64)

Figure 4 compares the infinite domain solution to that predicted from the numerical spectral method. To date, only Dagan [1985a, b] and Rubin and Dagan [1988] have developed analytical methods for determining the cross covariances needed in cokriging. The numerical spectral method provides a computational scheme which can find the cross covariance for any case of interest.

Figure 4 also provides insight into the behavior of the cross-covariance functions at separation distance of 0 and \( \pm \frac{\lambda}{2} \). When these separation distances are substituted into (46), the expressions for cross covariance in terms of its cross spectrum become

\[ K_{fh}(0) = \sum_{k \neq 0} S_{fh}(k) \]

(65)

\[ K_{fh}(\pm \frac{\lambda}{2}) = \sum_{k \neq 0} S_{fh}(k)(-1)^k \]

(66)
The flow equation implies that $S_{Rh}(k)$ is an odd function, that is, $S_{Rh}(k) = S_{Rh}(-k)$; this can be seen in (35). Since the cross spectrum $S_{Rh}(k)$ is odd, the sums in (65) and (66) are exactly zero. A similar argument applied to the derivatives of $K_{Rh}(\xi)$ will lead to the result that $K_{Rh}'(0) = K_{Rh}''(±\xi/2) = 0$ when $n$ is even, and $n$ stands for the $n$th derivative. In Figure 4 the value of $K_{Rh}(\xi)$ at $\xi = 0$ and $±\xi$ are indeed zero, as are the second derivatives at those points.

The differences at large separation distances between the finite domain spectral solution and the infinite domain analytical solutions are due to different assumptions about the behavior of the covariance beyond where data are available. In the finite domain spectral method the assumption is that the log permeability repeats itself as a periodic function when the separation distances are greater than the maximum available from the data. In the unbounded-domain case, the assumption is that the log permeability repeats itself as a stationary function. The former case uses a discrete spectrum while the latter uses a continuous one. Neither assumption is verifiable, and both are, to a degree, mathematical conveniences rather than physically justifiable assumptions. Therefore deciding which assumption is “correct” involves making an assumption about the behavior of the covariance in the region where data are not available.

Flexibility can be demonstrated by applying the method to more complex problems. Mizell et al. (1982) examined two-dimensional isotropic aquifers using various log transmissivity covariance functions. As a demonstration of the numerical spectral method, we choose the log transmissivity associated with their “spectrum B”

$$R_{ff}(\xi) = \sigma_{ff}^2 \left[ 1 + \frac{1}{2}(\alpha \xi)^2 \right] K_0(\alpha \xi) - (\alpha \xi)^2 K_1(\alpha \xi)$$

$$\alpha = 3\pi/16\lambda$$

(67)

where $\xi$ is the separation distance, $K_i$ is a modified Bessel function of the second kind, $i$th order, and where $\lambda$ is the integral scale. Figure 5 compares the infinite domain solution using (67) as the covariance function. The near-field and far-field behavior of the variogram is similar to the one-dimensional case. The solutions are nearly identical at small separation distances and diverge for separation distances approaching the size of the bounded domain. The numerical spectral method reproduces the anisotropy in the head field; the head variogram varies with the angle to the principal flow direction.

In three dimensions, a commonly used log permeability covariance is the exponential model,

$$R_{ff}(\xi) = \sigma_{ff}^2 e^{-|\xi/\lambda|^\lambda}$$

(68)

where $|\xi|^2 = \xi_1^2 + \xi_2^2 + \xi_3^2$ is the squared modulus of the separation vector, and $\lambda$ is the integral scale. Bakr et al.
variograms from field data suggests that this difference would be largely lost in the uncertainty of the variogram estimation. Only at large distances, where variogram uncertainty is the greatest, do the bounded and unbounded domain solutions significantly differ. However, this far-field portion of the variogram contributes the least to point estimation.

We have demonstrated how the numerical spectral method can reproduce the currently available analytical solutions. The difficulty in using these infinite domain analytical solutions is that so few of them exist, and practitioners may be unwilling to invest the necessary effort to derive additional relations. Thus the real usefulness of the numerical spectral method is that it can be easily applied to log permeability covariances where no solution exists. The log permeability need not even be given in functional form; an

[1978] presented the analytical solution for the head covariance, and Figure 6 compares their result to that obtained from the numerical spectral method. The three-dimensional case behaves similarly to the two- and one-dimensional cases.

The solutions in the one-, two-, and three-dimensional problems share the characteristic of similar head variogram behavior at large and small separation distances. This behavior has important implications in linear estimation. Even in cases where the log permeability has an integral scale of the order of the size of the area of interest, the head variograms for both bounded and unbounded domains are nearly identical for separation distances of the order of half the size of the area of interest. Although the two solutions are mathematically distinct, our experience with developing

Fig. 6. Head fluctuation variograms in a three-dimensional domain. Log permeability fluctuations covariance given by (68). (a) Angle to flow 0 radians and (b) angle to flow π/2 radians.

Fig. 7. Head fluctuation variograms in a two-dimensional domain. Log permeability fluctuations covariance given by (69). Parametrized by the anisotropy ratio, α. (a) Angle to flow 0 radians and (b) angle to flow π/2 radians.
experimental variogram estimated from the measurements would be acceptable. Consider this log permeability covariance in a two-dimensional domain:

\[ R_{gf}(\xi) = \sigma_f^2 e^{-\omega} \]  \hspace{1cm} (69)

where

\[ \omega = \left[ \left( \frac{\xi_1}{\lambda_1} \right)^2 + \left( \frac{\xi_2}{\lambda_2} \right)^2 \right]^{1/2} \]  \hspace{1cm} (70)

The function is of common exponential form but with an anisotropy ratio \( a = \lambda_1/\lambda_2 \). No analytical solution currently exists. Unbounded-domain analytical techniques are difficult to apply because (69) is not separable into a function of \( \xi_1 \) multiplied by a function of \( \xi_2 \). Figure 7 shows the head variogram for the case where \( \lambda_1 = 0.1 \) and for various values of the anisotropy ratio. The cross covariance can be obtained with no additional effort and is plotted in Figure 8. Thus the numerical spectral method can be applied to cases where analytical solutions are not readily available.

7. Concluding Remarks

This work has presented a method for the numerical evaluation of piezometric head covariances given the log permeability covariance. The developed algorithm can be seen at the numerical analog of the analytical methods of Gelhar, Gutjahr, Dagan, and others. Consequently, it seems appropriate to conclude with some comments on the relative merits of each approach. As a general rule, closed-form analytical solutions, if available, have advantages over numerically obtained results. The problem is that there are very few cases for which analytical solutions are available. Deriving an analytical solution to a new case is a major undertaking. However, for the problem at hand, these analytical expressions usually involve specialized functions which require computer programming and numerical approximations. The proposed method is much more general and powerful because it can provide solutions for any appropriate covariance function within minutes or seconds using widely available microcomputers. When incorporated into kriging and cokriging programs, the algorithm will provide a low-cost procedure for finding the necessary covariance and cross-covariance functions.

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