Technical Note

Some aspects of head-variance evaluation

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We compare two methods of evaluating head covariance for two-dimensional steady-state flow in mildly heterogeneous bounded rectangular aquifers. The quasi-analytical approach, widely used in stochastic subsurface hydrology, is based on the Green's function representation, and involves numerical four-fold integration. We compare this approach with a numerical solution of the two-dimensional boundary-value problem for head covariance. We show that the finite differences integration of this problem is computationally less expensive than numerical four-fold integration of slowly-convergent infinite series.

Keywords: head variance, moment equations, stochastic hydrology

Stochastic analysis has emerged as a powerful tool for coping with uncertainties associated with flow through heterogeneous formations. While first ensemble moments of system states predict the average behavior of a system, the corresponding second moments quantify the errors introduced by such predictions. A deterministic alternative to computationally demanding Monte Carlo simulations allows predicting flow through randomly heterogeneous porous media without having to generate random fields of permeability or hydraulic conductivity. For such an alternative to be viable, it must be efficient. In order to find an optimal way for evaluating hydraulic head variance, we consider two methods. The first method utilizes Green's functions and involves many-fold numerical integration. The second method solves the two-dimensional (2D) boundary-value problem for head-covariance by finite differences.

We consider steady-state saturated flow in a rectangular domain Ω. Flow is driven by a uniform mean hydraulic head gradient J induced by the presence of two constant head boundaries and two no-flow boundaries. The hydraulic head distribution $h(x_1, x_2)$ is described by

$$\nabla \cdot \left[K(\mathbf{x})\nabla h(\mathbf{x})\right] = 0, \quad \mathbf{x} \in \Omega, \tag{1}$$

subject to boundary conditions

$$h(x_1 = 0, x_2) = H_1, \quad h(x_1 = a, x_2) = H_2, \quad H_1 > H_2, \tag{2}$$

$$\frac{\partial h(x_1, x_2 = 0)}{\partial x_2} = \frac{\partial h(x_1, x_2 = b)}{\partial x_2} = 0, \tag{3}$$

where H_1 and H_2 are prescribed constant heads such that $J = (H_2 - H_1)/a$.

Let $\langle K(\mathbf{x})\rangle$ be a relatively smooth and unbiased estimate of $K(\mathbf{x})$ obtained from the available data. Then the unknown $K(\mathbf{x})$ differs from the known (deterministic) $\langle K(\mathbf{x})\rangle$ by a random error $K'(\mathbf{x})$, such that $K'(\mathbf{x}) = K(\mathbf{x}) - \langle K(\mathbf{x})\rangle$ and $\langle K'(\mathbf{x})\rangle \equiv 0$. It is customary in subsurface hydrology to assume that the K-field is second-order stationary and log-normally distributed, i.e., $Y = \ln K$ has constant mean $\langle Y\rangle$ and variance σ_Y^2, and its covariance function $C_Y(\mathbf{x}, \mathbf{y}) = \langle Y'(\mathbf{x})Y'(\mathbf{y})\rangle = C_Y(r)$, where $r = |\mathbf{x} - \mathbf{y}|$, has an exponential form,

$$C_Y(r) = \sigma_Y^2 \exp\left(-\frac{r}{l_Y}\right), \quad r = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}, \tag{4}$$

where l_Y is the correlation length of Y.

Under given conditions, the mean head distribution can be easily obtained [2] as $\langle h(x_1)\rangle = Jx_1 + H_1$. Thus, one can concentrate on determining a prediction error $\sigma_h^2(\mathbf{x}) = \langle h'(\mathbf{x})h'(\mathbf{x})\rangle$, where $h'(\mathbf{x})$ is a deviation of an "actual" random hydraulic head $h(\mathbf{x})$ from its predicted value $\langle h(\mathbf{x})\rangle$. A first-order (in σ_Y^2) approximation of $\sigma_h^2(\mathbf{x})$ is given by [1,3,7]

$$\frac{\sigma_h^2(\mathbf{x})}{J^2} = K_G^2 \int_\Omega \int_\Omega C_Y\big(|\xi - \zeta|\big) \frac{\partial G(\mathbf{x}, \xi)}{\partial \xi_1} \frac{\partial G(\mathbf{y}, \zeta)}{\partial \zeta_1} \, \mathrm{d}\xi \, \mathrm{d}\zeta, \tag{5}$$

where $K_G = \exp(\langle Y\rangle)$ is the geometric mean of K, and $G(\mathbf{x}, \mathbf{y})$ is the Green's function associated with the problem (1)–(3) wherein $K(\mathbf{x})$ is replaced by K_G. This Green's function has the form [4]

$$G(\mathbf{x}, \mathbf{y}) = \frac{2}{\pi K_G} \sum_{n=1}^{\infty} \frac{\gamma_n(x_2, y_2)}{n} \frac{\sin(n\pi x_1/a)\sin(n\pi y_1/a)}{\sinh(n\pi\varepsilon)}, \tag{6}$$

where $\varepsilon = b/a$ and

$$\gamma_n(x_2, y_2) = \begin{cases} \cosh(n\pi[y_2 - b]/a)\cosh(n\pi x_2/b), & 0 \leqslant x_2 \leqslant y_2, \\ \cosh(n\pi y_2/b)\cosh(n\pi[x_2 - b]/a), & y_2 \leqslant x_2 \leqslant 1. \end{cases} \tag{7}$$

To facilitate analytical integrability of (5), a separated exponential function $C_Y(\mathbf{x}, \mathbf{y}) = \sigma_Y^2 \exp\left[-(|x_1 - y_1| + |x_2 - y_2|)/l_Y\right]$ is often used in place of (4) [4–7]. To justify this substitution, references [5,6] state that the difference between the two correlation functions has a negligible effect upon the statistical moments of $h(\mathbf{x})$. Figure 1 shows that, although using the separated exponential function instead of the exponential covariance function captures correctly the qualitative behavior of $\sigma_h^2(\mathbf{x})$, it can underestimate head variance by as much as 41%. Thus for 2D domains, a numerical evaluation of the four-fold integrals in (5) is required.

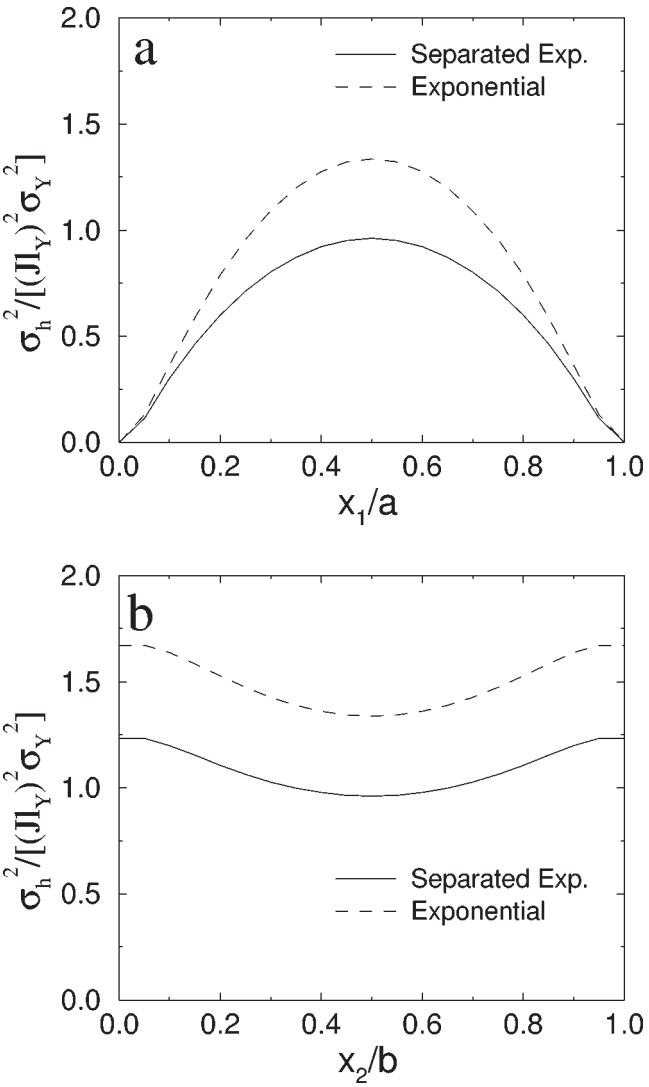

Figure 1. Head variance (normalized by $J^2 l_Y^2 \sigma_Y^2$) for exponential and separated exponential covariance functions of log hydraulic conductivity. **a** – horizontal direction; **b** – vertical direction.

An alternative approach is to find numerically the head-variance $\sigma_h^2(\mathbf{x})$ as the solution to a boundary-value problem

$$K_G \nabla_{\mathbf{x}}^2 C_h(\mathbf{x},\mathbf{y}) = -J \frac{\partial C_{Kh}(\mathbf{x},\mathbf{y})}{\partial x_1}, \quad \mathbf{x},\mathbf{y} \in \Omega, \tag{8}$$

$$C_h(\mathbf{x},\mathbf{y}) = 0, \quad x_1 = 0, a, \qquad \frac{\partial C_h(\mathbf{x},\mathbf{y})}{\partial x_2} = 0, \quad x_2 = 0, b, \tag{9}$$

where $C_h(\mathbf{x},\mathbf{y})$ and $C_{Kh}(\mathbf{x},\mathbf{y})$ are the first-order approximations of the head covariance

$\langle h'(\mathbf{x})h'(\mathbf{y})\rangle$ and cross-covariance $\langle K'(\mathbf{x})h'(\mathbf{y})\rangle$, respectively. The latter is found as the solution to

$$\nabla^2_{\mathbf{y}} C_{Kh}(\mathbf{x},\mathbf{y}) = -JK_G \frac{\partial C_Y(\mathbf{x},\mathbf{y})}{\partial y_1}, \quad \mathbf{y},\mathbf{x}\in\Omega, \tag{10}$$

$$C_{Kh}(\mathbf{x},\mathbf{y}) = 0, \quad y_1 = 0, a, \qquad \frac{\partial C_{Kh}(\mathbf{x},\mathbf{y})}{\partial y_2} = 0, \quad y_2 = 0, b. \tag{11}$$

The variance $\sigma^2_h(\mathbf{x})$ can be found by taking the limit $\mathbf{y}\to\mathbf{x}$ in $C_h(\mathbf{x},\mathbf{y})$.

Four-fold numerical integration in (5) was performed by using an adaptive grid integration of the *NAG* numerical library. While for the domain size of 1 correlation length it typically takes 5 terms for the series (6) to converge, for the domain size of 15 correlation lengths the convergence requires about 100 terms. This gives rise to an enormous increase in computational time.

The boundary-value problems (8)–(9) and (10)–(11) were solved numerically by finite differences [8]. It is clear that the two methods yield identical results. However, an exceedingly small convergence criterion for the direct numerical integration of (5) must be chosen to obtain non-oscillatory results. This makes the latter approach substantially time and memory consuming. Typically the numerical solution of the boundary-value problems took 1.5–2 times less CPU time than the numerical integration of (5). In conclusion, we would like to point out the importance of the proper choice of a correlation function as well as an optimal numerical algorithm.

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