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Comments on "Comparison of Gaussian Conditional Mean and Kriging Estimation in the Geostatistical Solution of the Inverse Problem" by R. J. Hoeksema and P. K. Kitanidis

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Hoeksema and Kitanidis [1985*b*] have presented a small-perturbation approach to geostatistical estimation. It is shown herein that the small-perturbation approach leads in many realistic instances to an ill-posed cokriging system. The purpose of this comment is to exmine the validity of the small-perturbation approach for the estimation of regionalized variables and indicate its limitations.

Following *Hoeksema and Kitanidis* [1985*b*], the differential equation relating the piezometric head ϕ to the log-transmissivity Y is given by

$$\frac{\partial Y}{\partial x}\frac{\partial \phi}{\partial x}+\frac{\partial^2 \phi}{\partial x^2}+\frac{\partial Y}{\partial y}\frac{\partial \phi}{\partial y}+\frac{\partial^2 \phi}{\partial y^2}=0 \tag{1}$$

Without loss of generality, source terms have been omitted in (1). The small-perturbation approach replaces the piezometric head and log transmissivity with the following expressions:

$$\phi = H + h \tag{2}$$

$$Y = F + f \tag{3}$$

in which $H = E(\phi)$; $F = E(Y)$; and h and f are zero mean perturbations. Substitution of (2) and (3) into (1) and a subsequent numerical discretization of the resulting differential equation over the flow domain yields the approximate expression

$$\mathbf{h} = Z\mathbf{f} \tag{4}$$

in which $\mathbf{h}$ and $\mathbf{f}$ are vectors of head and log-transmissivity perturbations, respectively, associated with the numerical scheme (e.g., finite differences or finite elements), and Z is a matrix that depends on the numerical discretization scheme. The use of geostatistical methods requires further transformation of (4) so that it can be expressed in terms of measurement point perturbations. *Hoeksema and Kitanidis* [1984] have shown that the vector of measurement point head perturbations $\mathbf{h}_p$ is given by

$$\mathbf{h}_p = T\mathbf{h} = T(Z\mathbf{f}) = W\mathbf{f} \tag{5}$$

in which the matrix T is a function of the geometry of the measurement point locations relative to the position of the nodal or block-centered head perturbation values associated with the numerical discretization method.

The following covariances are of foremost importance in the geostatistical method:

$$Q_{\phi\phi} = E(\mathbf{h}_p\mathbf{h}_p{}^T) \tag{6}$$

$$Q_{\phi Y} = E(\mathbf{h}_p\mathbf{f}_p{}^T) \tag{7}$$

$$Q_{YY} = E(\mathbf{f}_p\mathbf{f}_p{}^T) \tag{8}$$

in which $\mathbf{f}_p$ is the vector of measurement point log-transmissivity perturbations. If $Q_{\phi\phi}$, $Q_{\phi Y}$, and Q_{YY} are known one can estimate the value of a regionalized variable Y_0 (say, log transmissivity) at a location x_0 by means of cokriging. The resulting cokriging system is

$$\begin{array}{c} \\ n \\ m \\ 1 \end{array}\begin{array}{c} \begin{array}{ccc} n & m & 1 \end{array} \\ \begin{bmatrix} Q_{\phi\phi} & Q_{\phi Y} & \mathbf{0} \\ Q_{\phi Y}{}^T & Q_{YY} & \mathbf{1} \\ \mathbf{0}^T & \mathbf{1} & 0 \end{bmatrix} \end{array} \begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\lambda} \\ \nu \end{bmatrix} = \begin{bmatrix} \mathbf{C}(\boldsymbol{\phi}, Y_0) \\ \mathbf{C}(\mathbf{Y}, Y_0) \\ 1 \end{bmatrix} \tag{9}$$

in which $\mathbf{C}(\boldsymbol{\phi}, Y_0)$ and $\mathbf{C}(\mathbf{Y}, Y_0)$ are the covariances of the measurement vectors $\boldsymbol{\phi}$ (for piezometric head) and $\mathbf{Y}$ (for log transmissivity), respectively, with the regionalized log-transmissivity Y_0 at location x_0; $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$ are vectors that define the linear combination of measured variables expressing the cokriged estimate $\hat{Y}_0$ of Y_0 (i.e., $\hat{Y}_0 = \boldsymbol{\lambda}^T\mathbf{Y} + \boldsymbol{\mu}\cdot[\boldsymbol{\phi} - E(\boldsymbol{\phi})]$); ν is a Lagrange multiplier; $\mathbf{1}$ is a vector of ones; and m, n, and 1 in the left-hand side of (9) express the dimensions of matrices and vectors.

It is known (see, for example, *Journel and Huijbregts* [1978, pp. 326]) that a necessary condition for the existence of a unique solution to the cokriging system of (9) is that the cokriging covariance matrix

$$\begin{bmatrix} Q_{\phi\phi} & Q_{\phi Y} \\ Q_{\phi Y}{}^T & Q_{YY} \end{bmatrix}$$

be positive definite. It is shown next that as a result of the small-perturbation approach presented by *Hoeksema and Kitanidis* [1985*b*], the positive definiteness condition does not hold. Substitution of (5) into (7) yields

$$Q_{\phi Y} = E[(W\mathbf{f})\mathbf{f}_p{}^T] \tag{10}$$

In (10) the vector of measurement point log-transmissivity perturbations $\mathbf{f}_p$ can be expressed as a linear combination of the vector of head perturbations $\mathbf{f}$ association with the numerical discretization scheme, just as it is done with the head perturbations (see equation (5)). Thus

$$\mathbf{f}_p = L\mathbf{f} \tag{11}$$

in which the matrix L depends on the geometry of the system. Letting $M = L^{-1}$, it follows from (11) that

$$\mathbf{f} = M\mathbf{f}_p \tag{12}$$

substitution of (12) into (10) yields

$$Q_{\phi Y} = (WM)E(\mathbf{f}_p\mathbf{f}_p{}^T) = RQ_{YY} \tag{13}$$

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Similarly, the use of (5) and (12) in (6) leads to

$$Q_{\phi\phi} = E(\mathbf{h}_p\mathbf{h}_p{}^T) = E[(R\mathbf{f}_p)(R\mathbf{f}_p)^T$$
$$= RQ_{YY}R^T \qquad (14)$$

so that

$$\begin{bmatrix} Q_{\phi\phi} & Q_{\phi Y} \\ Q_{\phi Y}{}^T & Q_{YY} \end{bmatrix} = \begin{bmatrix} RQ_{YY}R^T & RQ_{YY} \\ Q_{YY}R^T & Q_{YY} \end{bmatrix} \qquad (15)$$

The determinant of a partitioned positive definite matrix A can be expressed as follows [*Anderson*, 1958, p. 42]:

$$A = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix} = |A_{11} - A_{12}A_{22}{}^{-1}A_{21}| \quad |A_{22}| \qquad (16)$$

Suppose that the cokriging covariance matrix of (15) is positive definite. Then, by virtue of (16) its determinant is

$$|RQ_{YY}R^T - (RQ_{YY})Q_{YY}{}^{-1}(Q_{YY}R^T)| \quad |Q_{YY}|$$
$$= |RQ_{YY}R^T - RQ_{YY}R^T| \quad |Q_{YY}| = 0$$

thus implying that the cokriging matrix is singular, which contradicts the positive definiteness assumption. Thus by contradiction, it has been shown that the cokriging matrix is not positive definite when it is derived from the small-perturbation approach as presented by *Hoeksema and Kitanidis* [1985*b*]. This implies that the cokriging system of (9) does not have a unique solution.

The previous developments indicate that in deriving the cokriging matrix via small-perturbation analysis, it is essential that the linear relationship linking head and transmissivity embodied in (4) be replaced by

$$\mathbf{h} = Z\mathbf{f} + \boldsymbol{\eta} \qquad (17)$$

in which $\boldsymbol{\eta}$ is an stochastic term that could account for measurement errors, for example, and has a nonsingular covariance matrix. An expression similar to (17) was used by *Hoeksema and Kitanidis* [1984], where $\boldsymbol{\eta}$ represented boundary perturbations. In general, however, adding the error term $\boldsymbol{\eta}$ may not be justified by the physical features of the flow system, say, because boundary conditions are well defined and known with sufficient accuracy as *Hoeksema and Kitanidis* [1984, p. 1005] have acknowledged.

In conclusion, unless there is a physical justification for the use of an expression such as that given in (17), the small perturbation approach is not suitable for the solution of the inverse problem via geostatistical methods such as cokriging. It has been shown that the cokriging matrix is not positive definite, and, in fact, it is singular, leading to an ill-posed cokriging system. Fortunately, there are simpler methods, such as maximum likelihood, that have been successfully and convincingly used to estimate regionalized variables [*Hoeksema and Kitanidis*, 1985*a*].

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