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An iterative stochastic inverse method: Conditional effective transmissivity and hydraulic head fields

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Abstract. An iterative stochastic approach is developed to estimate transmissivity and head distributions in heterogeneous aquifers. This approach is similar to the classical cokriging technique; it uses a linear estimator that depends on the covariances of transmissivity and hydraulic head and their cross covariance. The linear estimator is, however, improved successively by solving the governing flow equation and by updating the covariances and cross-covariance function of transmissivity and hydraulic head fields in an iterative manner. As a result the nonlinear relationship between transmissivity and head is incorporated in the estimation, and the estimated fields are approximate conditional means. The ability of the iterative approach is tested with some deterministic and stochastic inverse problems. The results show that the estimated transmissivity and hydraulic head fields have smaller mean square errors than those obtained by classical cokriging even in the aquifer with variance of transmissivity up to 3.

Introduction

During the past few decades, numerous mathematical models have been developed to solve the inverse problem associated with groundwater systems given scattered hydraulic head, ϕ, and conductivity or transmissivity, T, measurements (see *Yeh* [1986] and *Carrera and Neuman* [1986a] for a detailed review). One popular method is the minimum-output-error based approach [e.g., *Yeh and Tauxe*, 1971; *Gavalas et al.*, 1976; *Willis and Yeh*, 1987; *Cooley*, 1982; *Neuman and Yakowitz*, 1979; *Neuman*, 1980; *Clifton and Neuman*, 1982; *Carrera and Neuman*, 1986a, b]. A shortcoming of this approach is that the identity of the estimate is often undefined. In other words, it is unclear what the transmissivity and head fields derived from these methods represent in the case in which only scattered head and transmissivity measurements are given. Are they the mean fields conditioned on the measurements or one possible realization of the ensemble transmissivity and head fields? Being unable to ascertain their identities, this approach suffers from the same difficulty as any manual model calibration approaches [e.g., *Yeh and Mock*, 1996] because the uncertainty associated with the output cannot be addressed.

The geostatistically based approaches [*Kitanidis and Vomvoris*, 1983; *Hoeksema and Kitanidis*, 1984; *Dagan*, 1985; *Rubin and Dagan*, 1987; *Gutjahr and Wilson*, 1989] have received increasing attention recently. The geostatistical approach to the inverse problem relies on the use of cokriging estimation technique. It is based explicitly on the statistical characterization of the spatial variability of natural log transmissivity, $\ln T$. The idea is to take advantage of the spatial continuity of the $\ln T$ field implied by a covariance function or variogram and to make use of the linearized relationship between $\ln T$ and ϕ implied by the stochastic flow equation. In cokriging, the unknown f (mean removed $\ln T$) value at a point of interest is estimated by a weighted linear combination of the observed f and h (mean removed ϕ). The weights are determined by requiring that the estimator be unbiased and have minimum variance. By casting the problem in a probability framework, *Dagan* [1982, 1985] and *Rubin and Dagan* [1987] show that when the random transmissivity f and head h fields are jointly Gaussian (or multivariate normal) with known mean and covariance, the cokriging estimate and cokriging covariance are equivalent to the conditional mean and conditional covariance of the new joint probability distribution function conditioned on the measurements.

Classical cokriging is a linear predictor. In addition, the cross-covariance function between f and h and the covariance of h required in cokriging are derived from a first-order linearized version of the governing flow equation [*Mizell et al.*, 1982; *Kitanidis and Vomvoris*, 1983; *Hoeksema and Kitanidis*, 1984, 1989], while the relation between T and ϕ is nonlinear. Even if the log transformation of T is adopted, the nonlinear nature between f and h still remains. The linearized relations, being based on small perturbation theory, are valid only if the unconditional variance of f is less than 1.0. The nonlinearity in the flow equation implies that in general, h will not be normal, and f and h will not be jointly normal, even if f is normal. As a result the use of classical geostatistical techniques is not justified. This inconsistency is bound to be larger if the nonlinearity of the flow equation is stronger, as in the case of nonuniform flow, or if the variance of the log transmissivity is large. To overcome these problems described above, *Yeh et al.* [1995] proposed an iterative cokriging-like method that combines the cokriging and numerical flow model. *Gutjahr et al.* [1994] developed an iterative coconditional simulation approach.

Cokriging also suffers from the numerical stability problem as in the classical inverse models. *Dietrich and Newsam* [1989] showed that as the quantity of available data increases and the discretization of the system is refined, both a numerically ill-conditioned parameter estimation problem and an ill-conditioned cokriging equation may appear. Subsequently, the cokriged transmissivity field may contain some anomalies. To avoid this problem, addition of an error term to the cokriging equation is suggested for stabilizing the numerical solution in

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the method. But they pointed out that addition of such an error term may result in the loss of information.

Carrera and Glorioso [1991] compared the classical cokriging approach with an iterative statistical inverse approach. They concluded that basic hypotheses are similar for the two formulations and the main differences stem from the fact that linearization is performed around the estimated mean in cokriging methods and around the estimated log T in the iterative statistical approach. As a result the latter is less constrained by linearity than the former and leads to better estimates and to more consistent estimation covariance matrices. However, the identity of the estimate remains unknown.

The purpose of this paper is to illustrate problems associated with the assumption of the linear relationship between f and h embedded in the classical cokriging technique for estimating transmissivity values based on f and h data sets. To improve the classical cokriging approach and the minimum-output-error based approach, an iterative stochastic inverse method is presented. This iterative approach uses an unbiased linear estimator that depends on the covariances of transmissivity and hydraulic head and their cross covariance. This linear estimator is then improved successively by solving the governing flow equation and by updating the covariances and cross covariances of transmissivity and hydraulic head fields in an iterative manner. Therefore the estimated transmissivity and head fields from our approach become the coconditional mean fields, at least in an approximate sense.

The Inverse Algorithm

Consider the natural log of transmissivity, ln $T(x)$, of an aquifer to be a stationary stochastic process with a constant unconditional mean, E [ln T] = f, and the unconditional perturbation, f. The corresponding hydraulic head is given by $\phi(x) = H(x) + h(x)$, where $H = E[\phi]$ and h is the unconditional head perturbation. Suppose a limited number of transmissivity and head measurements in the aquifer are available: n_f observed transmissivity values, $f_i^* = (\ln T_i^* - F)$, and n_h observed head values, ϕ_j^*, where $i = 1, \cdots, n_f$ and $j = n_f + 1, \cdots, n_f + n_h$. One possible solution that an inverse model can produce is head and transmissivity fields that preserve the observed head and transmissivity values at sample locations and satisfy their underlying statistical properties (i.e., mean and covariance and so on) and the governing flow equation. In the conditional probability concept, such a head or transmissivity field is a conditioned realization of ϕ or ln T field in the ensemble. Many possible realizations of such conditioned ϕ or ln T fields exist. Instead of each individual conditional realization, our stochastic inverse model intends to derive the expected value of all the possible conditioned realizations.

To accomplish our goal, our inverse approach starts with the classical cokriging technique, using observed f_i^* and h_j^* to construct a cokriged, mean removed log transmissivity map, which is an approximate coconditional mean. That is,

$$f_k(x_o) = \sum_{i=1}^{n_f} \lambda_{io} f_i^*(x_i) + \sum_{j=n_f+1}^{n_f+n_h} \mu_{jo} h_j^*(x_j) \tag{1}$$

where $f_k(x_o)$ is the cokriged f value at location x_o. Then transmissivity $T_k(x_o)$ becomes exp $[F + f_k(x_o)]$; λ_{io} and μ_{jo} are the cokriging weights associated with x_o, which can be evaluated as follows:

$$\sum_{i=1}^{n_f} \lambda_{io} R_{ff}(x_i, x_l) + \sum_{j=n_f+1}^{n_f+n_h} \mu_{jo} R_{hf}(x_j, x_l) = R_{ff}(x_o, x_l) \qquad l = 1, 2, \cdots, n_f$$

$$\sum_{i=1}^{n_f} \lambda_{io} R_{fh}(x_i, x_l) + \sum_{j=n_f+1}^{n_f+n_h} \mu_{jo} R_{hh}(x_j, x_l) = R_{fh}(x_o, x_l) \qquad l = n_f + 1, n_f + 2, \cdots, n_f + n_h \tag{2}$$

where R^{ff}, R_{hh}, and R_{fh} are covariances of f and h and cross covariance of f and h, respectively. Equations similar to (1) and (2) were also derived to construct a cokriged hydraulic head map. The covariances R_{hh} and R_{fh} in (2) are derived from the first-order numerical approximation (see equations (10)–(14)) because of its flexibility for bounded domains and nonstationary problems.

Once the cokriged $T_k(x)$ field is obtained, it is used to solve the governing groundwater flow equation,

$$\nabla[T_k(x) \cdot \nabla\phi(x)] = 0 \tag{3}$$

with specified boundary conditions to derive a new head field, ϕ. The new head field is guaranteed to satisfy the given flow equation and boundary conditions. This head field, however, is an approximate mean head conditioned on the f and h measurements, and it is not necessarily equal to the coconditional mean head, $\langle\phi_c\rangle$ (subscript c denotes conditioned, and angle brackets stand for expectation). To show this, we can express a conditional random transmissivity field as the sum of conditional mean transmissivity and its conditional perturbation, $T_c(x) = \langle T_c(x)\rangle + t_c(x)$. Similarly, we can write the conditional head as $\phi_c = \langle\phi_c(x)\rangle + h_c(x)$. Then the exact conditional mean flow equation becomes

$$\nabla[\langle T_c(x)\rangle \cdot \nabla\langle\phi_c(x)\rangle] + \langle\nabla[t_c(x) \cdot \nabla h_c(x)]\rangle = 0 \tag{4}$$

As shown in (4), true conditioned mean T and ϕ fields do not satisfy the continuity equation (3), and $\langle\phi_c\rangle$ is not necessarily equivalent to the ϕ in (3) unless the second term in (4) is zero. The second term becomes zero only under two conditions: (1) all the transmissivity values in the aquifer are specified (i.e., $t_c(x) = 0$), or (2) all the head values in the domain are known (measured) so that $h_c(x)$ is zero everywhere. Suppose that the head field is known everywhere (i.e., a conditioned mean field, $\langle\phi_c\rangle$) but our information about the transmissivity field is incomplete. The cokriged transmissivity field, $T_k(x)$, in (3) will be the coconditioned mean T field if and only if the divergence of the product of $T_k(x)$ and the gradient of the known head field is zero. More specifically, if T_k is obtained from classical cokriging by using all the head values and the incomplete transmissivity data set, the head field, ϕ, derived from (3) by using this T_k should not equal $\langle\phi_c\rangle$ or the observed head field. This is attributed to the fact that T_k is an approximated coconditioned mean field based on classical cokriging, which assumes a linear relationship between f and h. In order to derive the true conditional mean head field a conditional mean transmissivity estimator that uses head information must consider the nonlinearity between f and h. For cases in which information about both head and transmissivity distributions is incomplete the exact conditional mean flow equation (4) and the exact coconditional mean transmissivity field, $\langle T_c \rangle$, must be used.

Since we do not have a way to evaluate the term, $\langle \nabla(t_c \cdot \nabla h_c) \rangle$, in (4) at this moment, we have to ignore its existence but focus on the development of the method for tackling the nonlinear relationship between f and h. To accomplish this goal, we adopt a successive linear estimator to modify the $T_k(x)$ field in (3). That is,

$$\hat{Y}_c^{(r+1)}(x_o) = \hat{Y}_c^{(r)}(x_o) + \sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)}[\phi_j^*(x_j) - \phi_j^{(r)}(x_j)] \qquad (5)$$

where ω_{jo} is the weighting coefficient for the estimate at location x_o with respect to the head measurement at location x_j and r is the iteration index. $\hat{Y}_c$ is an estimate of the conditional mean of ln T, which is equal to the cokriged log transmissivity field, $f_k + F$, at $r = 0$. The residual about the mean estimate is y, (i.e., $y = \ln T - \hat{Y}_c$). Note that $\hat{Y}_c$ and y are different from F and f previously defined; $\phi_j^{(r)}$ is the head at the jth location of the solution to (3) at iteration r, and ϕ_j^* is the observed head at location j (i.e., $\phi_j^* = H_j + h_j^*$). The successive linear estimator is unbiased, since

$$E[\hat{Y}_c^{(r+1)}] = E[\hat{Y}_c^{(r)}] + \sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)}\{E[\phi_j^*] - E[\phi^{(r)}_j]\} = F \qquad (6)$$

To ensure the estimator having minimal variance, the mean square error (MSE) criterion is used to select the optimal coefficient, ω,

$$E[(\ln T - \hat{Y}_c^{(r+1)})^2] = \min \qquad (7)$$

The mean square error for our estimator can be expanded as

$$E[(\ln T - \hat{Y}_c^{(r+1)})^2]$$

$$= E\left\{\left[(\ln T - \hat{Y}_c^{(r)}) - \sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)}(\phi_j^* - \phi_j^{(r)})\right]^2\right\}$$

$$= E\left[\left(y^{(r)} - \sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)} h_j^{(r)}\right)^2\right]$$

$$= \varepsilon_{yy}^{(r)} - 2 \sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)} \varepsilon_{yh}^{(r)} + \sum_{j=n_f+1}^{n_f+n_h} \sum_{k=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)} \omega_{ko}^{(r)} \varepsilon_{hh}^{(r)} \qquad (8)$$

where ε_{yy}, ε_{yh}, and ε_{hh} are error covariances and cross covariance at each iteration. To minimize (8), we differentiate it with respect to ω and set the resultant to zero. Thus we have

$$\sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)} \varepsilon_{hh}^{(r)}(x_j, x_l) = \varepsilon_{yh}^{(r)}(x_o, x_l) \qquad (9)$$

$$l = n_f + 1, \cdots, n_f + n_h$$

The ω values are determined by solving (9) with given ε_{yh} and ε_{hh}. With new ω values, (5) can be employed to update our estimate, $\hat{Y}_c$. However, the solution to (9) requires the knowledge of ε_{yh} and ε_{hh} which can be evaluated at each iteration as follows.

On the basis of the first-order analysis for a finite element groundwater flow model [e.g., *Dettinger and Wilson*, 1981], hydraulic head at the rth iteration can be written as a first-order Taylor series:

$$\phi = \hat{\phi}_c^{(r)} + h^{(r)} = \mathcal{F}[\hat{Y}_c^{(r)} + y] \approx \mathcal{F}[\hat{Y}_c^{(r)}] + \left.\frac{\partial \mathcal{F}}{\partial \ln T}\right|_{\hat{Y}_c^{(r)}} y^{(r)} \qquad (10)$$

where $\mathcal{F}$ represents (3). The first-order approximation of the residual $h^{(r)}$ can be written as

$$h^{(r)} \approx \left.\frac{\partial \mathcal{F}}{\partial \ln T}\right|_{\hat{Y}_c^{(r)}} y^{(r)} = J^{(r)} y^{(r)} \qquad (11)$$

where J can be evaluated by using an adjoint state sensitivity method [e.g., *Sykes et al.*, 1985; *Sun and Yeh*, 1992] subject to boundary conditions. Using (11), we then derive the approximate covariance of $h^{(r)}$ and cross covariances between $y^{(r)}$ and $h^{(r)}$,

$$\begin{aligned} \varepsilon_{hh}^{(r)}(x_i, x_j) &= J^{(r)} \varepsilon_{yy}^{(r)}(x_l, x_m) J^{t^{(r)}} \\ \varepsilon_{yh}^{(r)}(x_i, x_j) &= J^{(r)} \varepsilon_{yy}^{(r)}(x_l, x_m) \end{aligned} \qquad (12)$$

where i and $j = n_f + 1$ to $n_f + n_h$; l and $m = 1, 2, \cdots, N$ (total number of nodes); J is the sensitivity matrix of $n_h \times N$, and superscript t stands for the transpose. Here, ε_{yy} is the covariance of y, which is given by

$$\varepsilon_{yy}^{(1)}(x_o, x_k) = R_{ff}(x_o, x_k) - \sum_{i=1}^{n_f} \lambda_{io} R_{ff}(x_o, x_i)$$

$$- \sum_{j=n_f+1}^{n_f+n_h} \mu_{jo} R_{fh}(x_k, x_j) \qquad (13)$$

at iteration $r = 0$, where $k = 1, 2, \cdots, N$ and λ and μ are cokriging coefficients. Equation (13) is the cokriging variance if $x_o = x_k$. For $r \geq 1$ the covariances are evaluated according to

$$\varepsilon_{yy}^{(r+1)}(x_o, x_k) = \varepsilon_{yy}^{(r)}(x_o, x_k) - \sum_{i=n_f+1}^{n_f+n_h} \omega_{io}^{(r)} \varepsilon_{yh}^{(r)}(x_k, x_i) \qquad (14)$$

After updating $\hat{Y}_c(x)$ the flow equation (3) is solved again with the newly updated $\hat{Y}_c(x)$ for a new head field, ϕ. Then the absolute difference in σ_f^2 (the variance of the estimated transmissivity field) between two successive iterations is evaluated. If the difference is smaller than a prescribed tolerance, the iteration stops. If not, new ε_{yh} and ε_{hh} are evaluated by using (12). Then (9) is solved to obtain a new set of weights which are used in (5) with $(\phi_j^* - \phi_j^{(r)})$ to obtain a new estimate of $\hat{Y}_c(x)$.

The condition numbers of the cokriging matrix equation (2) and the matrix equation (9) of our iterative inverse method can be extremely large if the number of head measurements is large. Truncation errors thus may be amplified and may affect the interpolation of transmissivity values by cokriging (1) and our iterative method. To avoid such a problem, addition of an error term to the head covariance matrix in (2) was employed. In addition, a relaxation term, Θ, was added to the diagonal of the matrix in (9) during each iteration:

$$\sum_{j=n_f+1}^{n_f+n_h} \omega_{jo}^{(r)} \varepsilon_{hh}^{(r)}(x_j, x_l) + \Theta^{(r)} \delta_{li} = \varepsilon_{yh}^{(r)}(x_o, x_l) \qquad (15)$$

$$l = n_f + 1, \cdots, n_f + n_h$$

where δ_{li} is the identity matrix. In general, a large value of Θ slows down the convergence rate, and a small value may lead to numerical instability. In our approach, the Θ value is assigned dynamically; the value of the relaxation term is determined as the product of a constant weighting factor and the maximum value of $\varepsilon_{hh}(x_i, x_i)$ at each iteration. Since the value of ε_{hh} will decrease as iteration proceeds, the Θ value will decrease accordingly. This term represents not a measurement error, as discussed by *Dietrich and Newsam* [1989] and *Carrera and Glorioso* [1991], but merely a numerical technique to condition the matrix. In fact, this approach is analogous to the pseudo transient technique employed for nonlinear numerical problems described by *Fletcher* [1988].

Examples

Assessment of an inverse method under any field condition is difficult unless a large number of transmissivity and head data sets are available. Such detailed data sets rarely exist. Even if these data sets are available, it is difficult to determine the number of measurement errors in the data sets. Therefore validation of a model for field condition is inconclusive [see *Gelhar*, 1993, p. 347]. More important, verification of an inverse model against a perfectly known scenario is always a first step toward the model application. For this reason the performance of our stochastic inverse approach is demonstrated by using hypothetical heterogeneous aquifers with the assumption that all the statistical parameters characterizing the spatial variability of ln T are known exactly and measurements are considered to be error free. The domain size of the two-dimensional hypothetical aquifers is specified as 21 m long and 11 m wide and is discretized with uniform elements of 1 m × 1 m. Each element was assigned a constant mean transmissivity value (ln T = 0.0). The perturbation f field was generated from a random field generator [*Gutjahr*, 1989] by using an exponential covariance function with anisotropic correlation scales (3 m in the x direction and 1 m in the y direction). These transmissivity values will be called the true transmissivity values. The upper and lower sides of the aquifer are assigned as no flux boundaries and the left- and right-hand sides are prescribed head boundaries with prescribed head values of 0.95 m and 0.85 m, respectively. In addition, a pumping well with a constant discharge Q is placed at a given high-transmissivity location. The steady state groundwater flow equation (3) was solved with the true transmissivity field to obtain the corresponding true head field. Samples were then taken from these true fields. Note that a finite element model was used to solve (3) for the head at each node. The head values at the four nodes of an element were then averaged to represent the head at the center of the element.

Two different types of inverse problems (deterministic and stochastic, as explained below) are examined. Results of our approach are compared with those derived from the classical cokriging approach. The performance of these methods is evaluated quantitatively by using the following criteria:

$$P_1 = \frac{1}{N}\sum_{i=1}^{N}(y_{oi} - y_{ei})$$
$$P_2 = \frac{1}{N}\sum_{i=1}^{N}(y_{oi} - y_{ei})^2 \qquad (16)$$

where y_{oi} and y_{ei} are the observed and estimated transmissivity values at ith location, respectively. N is the total number of elements for f. P_1 is a measure of the bias, and P_2 is the mean square error of our estimates.

Deterministic Inverse Problems

Assuming the Darcy law is valid, the Darcy velocity can be written in terms of conditional means and perturbations:

$$\langle q_c\rangle + q_c = -[(\langle T_c\rangle + t_c)\cdot\nabla\langle H_c\rangle + \langle(\langle T_c\rangle + t_c)\cdot\nabla h_c\rangle] \qquad (17)$$

Suppose that all the head and transmissivity measurements are error free and the head values at every node of our finite element aquifer are known. Thus the second term on the right-hand side of (17) must be zero, since the conditional perturbation in h_c is zero everywhere, and (17) becomes

$$\langle q_c\rangle + q_c = -[(\langle T_c\rangle + t_c)\cdot\nabla\langle H_c\rangle] \qquad (18)$$

In order to obtain a unique transmissivity distribution, $T_c(x) = \langle T_c(x)\rangle + t_c(x)$, the Darcy velocity, $\langle q_c(x)\rangle + q_c(x)$, must be specified at every point in the aquifer. Since flow is under steady state conditions, Darcy's velocity must be constant along any given streamline. Therefore, if all the heads are known and the velocity is specified at all the boundary nodes or a column of transmissivity values crossing all the stream lines is prescribed, the solution of the inverse problem is unique. We call this type of inverse problem deterministic. Under these conditions a reliable inverse model is expected to reasonably identify all the transmissivity values in the aquifer. Problems associated with the linear cross correlation between f and h and the linear predictor embedded in cokriging as the variance of f increases can be explored. Further, our relaxation approach for alleviating numerical instability problems associated with our inverse model can be tested.

For the above reasons, two such deterministic cases were examined: case 1, $\sigma_f^2 = 0.38$, and case 2, $\sigma_f^2 = 3.01$. A well discharging $Q = 5$ m^2/m was located at point (5, 8) in these two cases. The random transmissivity fields were generated with the same seed number. We assume that the transmissivity values of the elements on the left-hand side of the boundary ($n_f = 11$) are known and all the heads in the aquifer ($n_h = 231$) are given. Since all heads were used, the condition number of the cokriging matrix is excessively large. Without the addition of a relaxation term the cokriged transmissivity map produced some anomalous values of transmissivity due to numerical instability [see *Dietrich and Newsam*, 1989]. To alleviate this problem, a small relaxation term with a value equal to 1% of the σ_h^2 was added to the head covariance matrix in the cokriging equation. Figures 1a, 1b, and 1c show the true, the cokriged, and our estimated transmissivity distributions of the hypothetical aquifer of case 1, respectively. It is evident that even when all the head information is given, cokriging tends to produce a much smoother transmissivity field than the true one, although the general patterns of the two fields are very similar. On the other hand, the transmissivity field estimated by our approach depicts all the detailed variation in transmissivity and is in excellent agreement with the true transmissivity distribution.

The true transmissivity field, the cokriged field, and our approach for case 2 are illustrated in Figures 2a, 2b, and 2c, respectively. As σ_f^2 increases to 3.01, the cokriged transmissivity field again is very smooth except near the 11 f measurements at the left-hand side boundary. In this case the spatial pattern of the cokriged transmissivity map has little resemblance to the general pattern of the true field. Similarly to case

1, the transmissivity field from our approach is in good agreement with the true one, although the discrepancy between the estimated and the true field is slightly larger than that in case 1.

The above results are expected, since the linear relationship between f and h assumed in classical cokriging is valid only for small variances in f. More specifically, consider one-dimensional steady state flow through a stochastic transmissivity field with a given flux, q. The q can be expressed as

$$q = -T\frac{d\phi}{dx} = -e^{(F+f)}\left(\frac{dH}{dx} + \frac{dh}{dx}\right) = T_g e^{f}(J + j) \qquad (19)$$

where J is the mean gradient and j is its perturbation. T_g is the geometric mean of T. The gradient perturbation can thus be expressed as

$$j = \frac{dh}{dx} = \frac{q}{T_g} e^{-f} - J \qquad (20)$$

which shows that h and f are related in a nonlinear manner. If f is small, the exponential term in (20) can be approximated by the first two terms of a series expansion. Thus (20) becomes

$$j = \frac{dh}{dx} \approx \frac{q}{T_g}(1 - f) - J \qquad (21)$$

According to (21), for small values of f or σ_f^2, h can be closely approximated as a linear function of f. This approximation

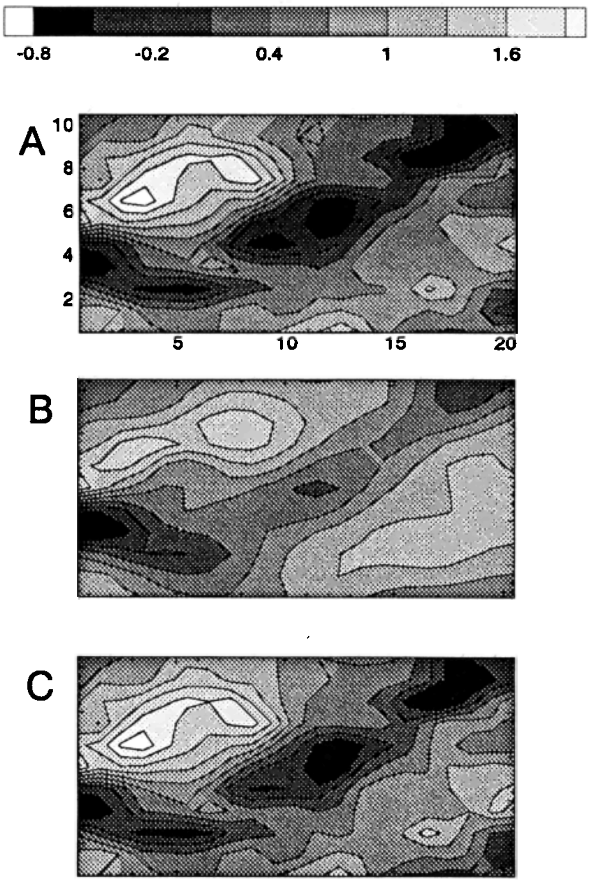

Figure 1. (a) The true ln T field, (b) the cokriged ln T field, and (c) the estimated ln T field by our iterative approach for case 1.

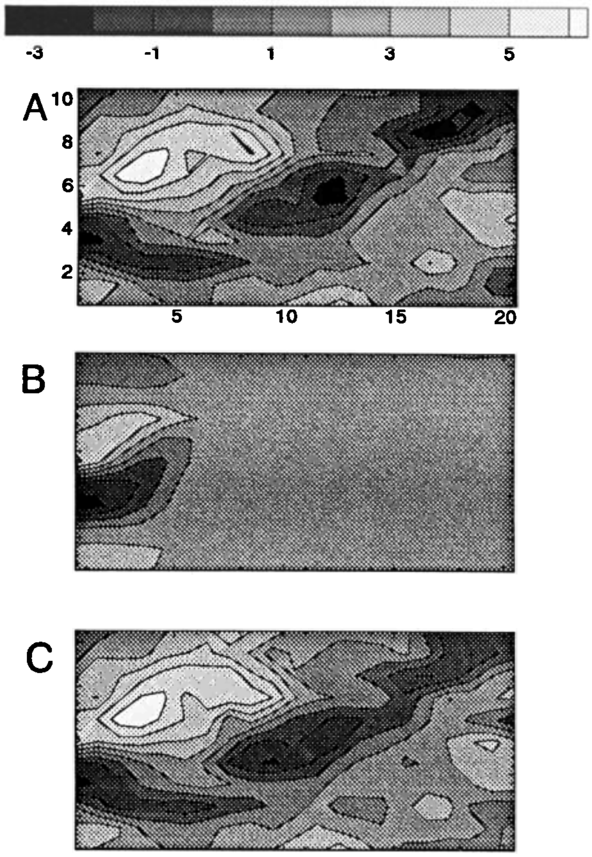

Figure 2. (a) The true ln T field, (b) the cokriged ln T field, and (c) the estimated ln T field by our iterative approach for case 2.

supports the preference of using ln T in the inverse modeling, as stated by *Carrera and Neuman* [1986b].

The convergence patterns of our iterative approach for cases 1 and 2 are illustrated in Figures 3a and 3b, where the criteria P_1, P_2, σ_f^2, max δh (the maximum head difference between the observed and estimated head at observation locations), and max ε_f (the square root of the maximum $\varepsilon_{ff}(x, x)$) are plotted as a function of iteration. For both cases our iterative approach produces estimates that are much less biased and have smaller MSE than those by cokriging, although both are unbiased estimators. The σ_f^2 of our estimated transmissivity field stabilizes rapidly in case 1 and reaches the value of 0.36. For case 2, where $\sigma_f^2 = 3.01$, our approach produces a field with $\sigma_f^2 = 2.84$ at the three hundredth iteration. The value of max ε_f for case 1 decreases rapidly with iterations, indicating improvements of the estimated f field. For case 2 this value decreases at a slower rate than that of case 1 due to the stronger nonlinearity of the problem.

Stochastic Inverse Problems

The stochastic inverse problems are referred to the case in which one or both of the perturbation terms in (4) are unknown, owing to the lack of measurements. Subsequently, no unique solution to the identification of transmissivity values can be obtained. A logical solution to these stochastic inverse problems is to derive the mean ln T and ϕ fields that are conditioned on the observed ln T and ϕ values [see *Dagan*, 1985; *Kitanidis*, 1986]. Uncertainties around the conditional

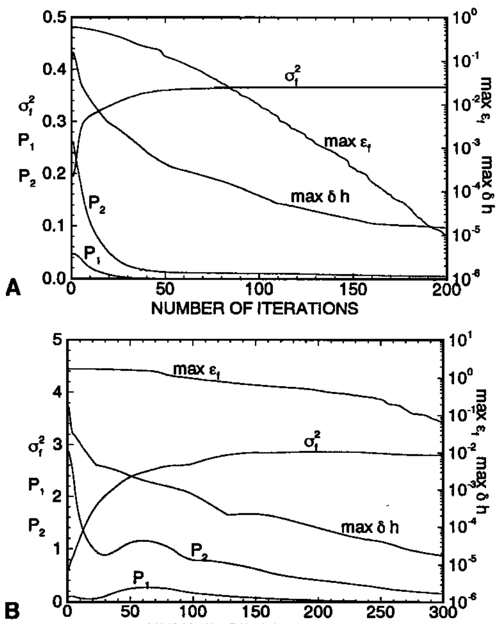

Figure 3. The convergence patterns of our iterative approach for (a) case 1 and (b) case 2.

means at the unsampled locations are then addressed by using the conditional variances of ln T and ϕ. Classical cokriging is a possible tool for this purpose. However, as demonstrated in the examples of the deterministic inverse problems, the cokriging technique is restricted by its assumption of the linear relationship between f and h. Our iterative approach alleviates the problem of linear assumption and is capable of producing ln T and ϕ fields that preserve the measured values at sample locations and satisfy the continuity equation. These ln T and ϕ fields are not necessarily the true conditional mean ln T and ϕ fields defined in (4), since the term $\langle\nabla(t_c \cdot \nabla h_c)\rangle$ is not evaluated explicitly and is excluded from the flow equation (3) in our iterative approach. As a result the contribution of this term is likely lumped into our estimates of $\langle \ln T_c\rangle$ and $\langle\phi_c\rangle$. Subsequently, ln T and ϕ fields derived from our iterative method are merely approximate coconditional means. They may be qualified as coconditional effective transmissivity and head fields in the sense that they satisfy the flow equation. Nevertheless, these approximations should be close to the exact conditional means if the magnitude of the term $\langle\nabla(t_c \cdot \nabla h_c)\rangle$ in (4) is small. One way to prove our claims is to conduct coconditional Monte Carlo simulations. This coconditioning approach will require a large number of simulations and demands a high-performance computer. More important, it requires the use of a coconditional Monte Carlo technique that is capable of producing coconditioned realizations of ln T and ϕ fields. This technique does not exist at this moment. For these reasons we can only test our results by using the following criteria: The variances of our estimated ln T and ϕ fields should be larger than the variances of the cokriged fields but smaller than the variances of the real-world analog. In addition, our mean estimates should be unbiased and have smaller MSE than that of cokriging. Using these criteria, we employ the scenario below to test our iterative approach.

The two-dimensional flow scenario in the previous cases of the deterministic inverse problems is used with the exception that the number of head and transmissivity measurements, n_h and n_f, are specified as 30 and 5, respectively. The locations of these measurements are shown in Figure 4 by the circles. In addition, a different seed number is used to generate the random f field, and the well is located at point (9, 6) with $Q = 5$ m^2/m. Also shown in Figure 4 are the resultant transmissivity and head fields from cokriging and our iterative approach. Both approaches produced head fields that closely resemble

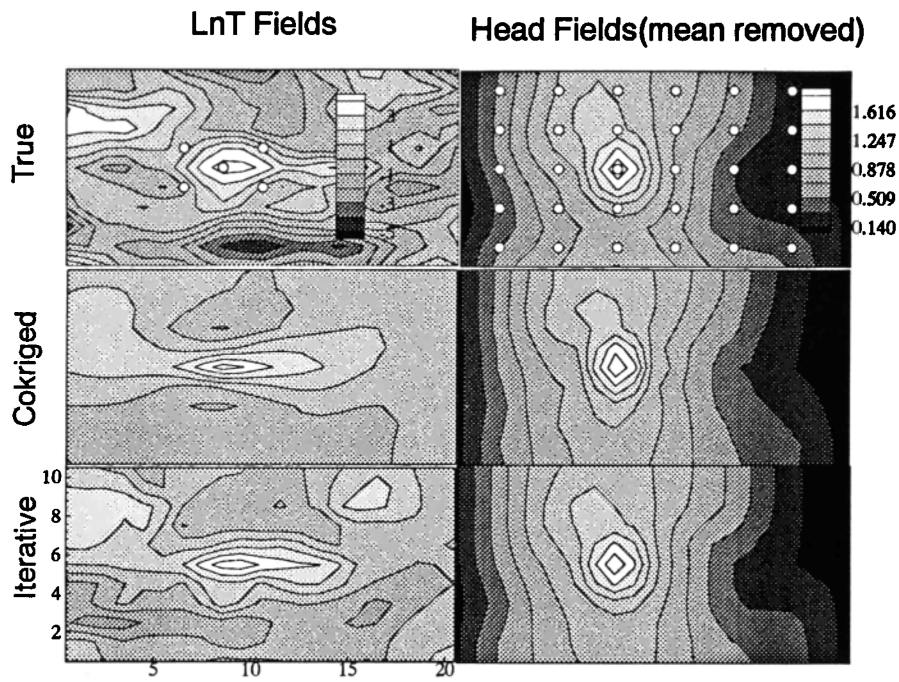

Figure 4. Illustrations of the true ln T and head perturbation fields and those by the classical cokriging method and our iterative approach for case 3.

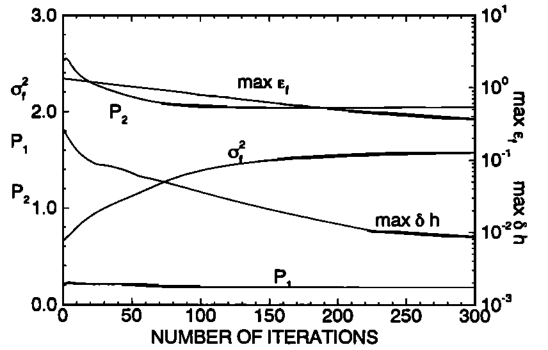

Figure 5. The convergence patterns of our iterative approach for case 3.

the true head field. Although the difference between the results of the two approaches is small, the cokriged transmissivity field is smooth, depicting the general structure of the true field. The transmissivity field from our iterative approach reveals more detailed structures.

Figure 5 shows the performance measures of our iterative approach as a function of iteration number. Again the performance of cokriging is reflected by these measures at the zeroth iteration. On the basis of this figure our transmissivity estimates are less biased, and the MSE is smaller than that of classical cokriging. The variance of our estimated transmissivity field, σ_f^2, stabilized around the three hundredth iteration and reached a value of 1.7, which is greater than that of the cokriging estimate (0.67) but smaller than the variance of the true field (2.96). The values of P_1 and P_2 for the estimated head fields by cokriging are 0.77×10^{-4} and 0.35×10^{-2}, respectively. The corresponding values by our approach are 0.25×10^{-5} and 0.13×10^{-2}. The magnitude of max ε_f decays exponentially at a slower constant rate than in the deterministic cases. The constant rate also decreases after around the two hundredth iteration, indicating further reduction in the improvement of f as the iteration continues.

Discussion

The rationale of our successive linear predictor is different from the rationales described by *Gavalas et al.* [1976] and *Carrera and Glorioso* [1991], although (5) is similar in form to their equations. Our approach uses a linear estimator and the governing flow equation successively to update the error covariances ε_{yy}, ε_{hh} and cross covariance ε_{yh} and in turn improves the difference in estimated and observed head values. Our approach attempts not to minimize the differences between the observed and estimated head but to minimize the mean square error in our ln T estimates. In our view the ln T and ϕ fields obtained by our approach are essentially approximate conditional means.

We have to point out that the covariances (R_{hh} and ε_{hh}) and the cross covariance (R_{fh} and ε_{fh}) are derived from first-order approximations (see (11) and (12)). In addition, the exact conditional mean flow equation was not used to derive the sensitivity matrix. The quality of the approximations, especially for the large variance problems, is unknown. Subsequently, the conditional covariances of f, ε_{ff}, updated by these linear approximations may be affected. The continuous decline of max ε_f value with iterations, although at a slow rate in the stochastic inverse problem, appears to reflect this problem.

The addition of the relaxation term is necessary. It is capable of controlling the instability of the numerical solution in the case in which a large number of observed head values are used. If a relaxation term of an extremely small value (or zero) is used, our iterative method may diverge as in the case of solving steady state nonlinear equation (e.g., Richards' equation). A large value stabilizes the solution but decreases the rate of convergence.

The CPU time for case 2 of the deterministic inverse problem was about 30 min on an IBM RISC/6000/590 with 512-Mbit memory for the 300 iterations, since it used all the 231 head information. On the other hand, it only required approximately 1.2 min of CPU time for the stochastic inverse problem.

Conclusion

Our proposed iterative approach attempts to circumvent the nonlinear relationship between f and h through successive linear approximations. Two deterministic inverse problems with different degrees of nonlinearity were used to demonstrate the ability of our model. We show that our inverse approach is undoubtedly superior to classical cokriging, which relies on the linear assumption of the relationship between f and h. Our approach is able to reproduce transmissivity and head fields that are in close agreement with the true fields even for aquifers with variance of f up to 3 under nonuniform flow conditions. These estimated fields thus represent the conditional mean fields. However, our approach requires more computational effort than the cokriging.

For stochastic inverse problems the estimated transmissivity patterns by the cokriging technique and our approach are very similar. Nevertheless, our approach is better than the classical cokriging method, since it produces smaller bias and MSE of the estimates. In addition, it reveals a more detailed spatial pattern of the true transmissivity field. We have to emphasize the fact that the estimates of ln T and ϕ fields by our method are merely approximate mean fields conditioned on the observed f and h values. They may be best called the conditional effective transmissivity and head fields.

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