Conditioning steady-state mean stochastic flow equations on head and hydraulic conductivity measurements

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Abstract Non-local moment equations allow one to obtain deterministically optimum predictions of flow in randomly heterogeneous media and to assess predictive uncertainty conditional on measured values of medium properties. We present a geostatistical inverse algorithm for steady-state flow that makes it possible to further condition such predictions and assessments on measured values of hydraulic head (and/or flux). Our algorithm is based on recursive finite-element approximations of exact first and second conditional moment equations. Hydraulic conductivity is parameterized via universal kriging based on unknown values at pilot points and (optionally) measured values at other discrete locations. We illustrate the method for superimposed mean uniform and convergent flows in a bounded two-dimensional domain. Our examples illustrate how conductivity and head data act separately or jointly to reduce parameter estimation errors and model predictive uncertainty.

Key words aquifer characteristics; geostatistics; groundwater flow; inverse problem; regression analysis; steady-state conditions; stochastic processes; uncertainty

INTRODUCTION

We consider steady-state flow of groundwater in a randomly non-uniform domain, $\Omega$. The flux $q(x)$ and the hydraulic head $h(x)$ obey the continuity equation and Darcy’s law, subject to appropriate boundary conditions. All parameters and state variables are defined on a consistent non-zero support volume, $\Omega$, which is small in comparison to $\Omega$ but sufficiently large for Darcy’s law to be locally valid. It has been shown that it is theoretically possible (Neuman & Orr, 1993; Neuman et al., 1996) and computationally feasible (Guadagnini & Neuman, 1999a,b) to render optimum unbiased predictions of $h(x)$ and $q(x)$ under ubiquitously non-uniform and uncertain field conditions by means of their first ensemble (statistical) moments (expected or mean values), $\langle h(x) \rangle_c$ and $\langle q(x) \rangle_c$, conditioned on measurements of $K(x)$. The predictors $\langle h(x) \rangle_c$ and $\langle q(x) \rangle_c$ satisfy the equations:

$$ - \nabla \langle q(x) \rangle_c + \langle f(x) \rangle = 0 $$

(1)
\[ \langle q(x) \rangle_c = - \langle K(x) \rangle_c \nabla \langle h(x) \rangle_c + r_c \] (2)
in \Omega subject to the boundary conditions:
\[ \langle h(x) \rangle_c = \langle H(x) \rangle \text{ on } \Gamma_D, \quad - \nabla \langle q(x) \rangle_c \cdot n(x) = \langle Q(x) \rangle \text{ on } \Gamma_N \] (3)
where the subscript \(c\) implies “conditional”; primed quantities represent random fluctuations about (conditional) mean values; \(K(x)\) is a random field of scalar hydraulic conductivities; \(r_c(x)\) is a residual flux; \(\langle f(x) \rangle, \langle H(x) \rangle, \langle Q(x) \rangle\) are prescribed unconditional first moments of the statistically independent random source and boundary forcing terms \(f(x), H(x), Q(x)\); and \(n(x)\) is a unit outward normal to \(\Gamma = \Gamma_D \cup \Gamma_N\) where \(\Gamma_D\) and \(\Gamma_N\) are Dirichlet and Neumann boundaries, respectively.

The residual flux \(r_c(x)\) is given implicitly by Neuman et al. (1996):
\[ r_c(x) = \int a_c(y, x) \nabla \langle h(y) \rangle_c \, dy + \int d_c(y, x) r_c(y) \, dy \] (4)
where the kernels:
\[ a_c(y, x) = \langle K'(x) K'(y) \nabla x \nabla y \rangle \] (5)
\[ d_c(y, x) = \langle K'(x) \nabla x \rangle \] (6)
form a symmetric and a non-symmetric tensor, respectively. Here \(G\) is a random Green’s function, or solution of the random flow equations for the case where \(f(x)\) is a point source of unit strength at point \(y\) subject to homogeneous boundary conditions \(H(x) = Q(x) = 0\).

Due to the integro-differential nature of \(r_c(x)\), the conditional moment equations include non-local parameters that depend on more than one point in space (hence the equations are referred to as non-local). The traditional concept of an REV (representative elementary volume) is neither necessary nor relevant for their validity or application. The corresponding parameters are inherently non-unique in that they depend not only on medium properties but also on the information one has about these properties (scale, location, type, quantity, and quality of data). The flux predictor is generally non-local and non-Darcian, depending on the residual flux \(r_c(x)\). The traditional notion of effective conductivity looses meaning in the context of flow prediction by means of conditional ensemble mean quantities.

Guadagnini & Neuman (1999a,b) have developed corresponding integro-differential equations for the conditional variance-covariance of associated prediction errors in head and flux, and have shown how to solve both sets of equations by finite elements. Their solution entails expansion of the exact non-local moment equations in terms of a small parameter, \(\sigma_Y\), representing a measure of the standard deviation of natural logconductivity, \(Y(x) = \ln K(x)\).

**CONDITIONING ON STATE VARIABLES THROUGH MODEL CALIBRATION**

The recursive finite element algorithm of Guadagnini & Neuman (1999a,b) is valid to second order in \(\sigma_Y\). It assumes that one has at his/her disposal two functional parameters: a conditional unbiased estimate, \(\langle Y(x) \rangle_c\), of the randomly varying logconductivity function and the second conditional moment of associated estimation errors, \(C_{Yc}(x, y) = \langle Y'(x) Y'(y) \rangle_c\). When conditioning is performed on the basis of existing \(\omega-\)
scale measurements of \( Y \) at a set of discrete points, \( \langle Y(x) \rangle_c \) and \( C_{Y}(x, y) \) can be obtained (in principle) by means of geostatistical methods (e.g. Deutsch & Journel, 1998; Chiles & Delfiner, 1999).

In this paper, we describe an inverse algorithm that allows one to estimate \( \langle Y(x) \rangle_c \) and \( C_{Y}(x, y) \) not only (or not at all) on the basis of measured logconductivity values, but also (or only) on the basis of measured state variables such as head and flux. This is tantamount to conditioning the non-local mean flow equations not only (or not at all) on logconductivity measurements but also (or only) on measurements of head and flux. Estimates of \( \langle Y(x) \rangle_c \) and \( C_{Y}(x, y) \) based on logconductivity measurements (if available) are treated as prior information in the manner of Carrera & Neuman (1986).

To parameterize \( \langle Y(x) \rangle_c \), we express it as the weighted sum of precisely or imprecisely known values at discrete measurement points and unknown values at discrete "pilot points" (de Marsily, 1978, 1984). Both sets of values are treated (the first optionally) as unknown parameters to be estimated by inversion. The weights of the sum are evaluated through universal kriging considering the variance of measurement errors at actual data points (assumed to be uncorrelated) and the covariance of estimation errors at pilot points (set equal to the inverse Fisher information matrix of the most recent iterate). At least one measured conductivity or flux value is needed to obtain a unique set of parameter estimates.

Parameters are estimated by minimizing the generalized sum of squared residuals:

\[
F = J_h + J_y = (\hat{h} - h^*)^T S_h^{-1} ((\hat{h} - h^*) + (\hat{Y} - Y^*)^T S_Y^{-1} (\hat{Y} - Y^*)
\]  

where \( h^* \) is a vector of head measurements and \( \hat{h} \) is a corresponding vector of calculated heads; \( S_h \) is the (diagonal) covariance matrix of head measurement errors (assumed to be uncorrelated); \( Y^* \) is a vector of prior logconductivity values consisting of imprecise measurements and corresponding kriged values at pilot points; \( \hat{Y} \) is a corresponding vector of inverse estimates; and \( S_Y \) is the covariance matrix of associated prior (measurement and kriging) errors. If \( S_h \) and/or \( S_Y \) are known only up to a constant of multiplication, then one can estimate these statistical constants jointly with \( \hat{Y} \) by the maximum likelihood method of Carrera & Neuman (1986). The same is true about other statistical parameters entering into \( S_h \) and/or \( S_Y \), such as those defining the spatial correlation of the data. We minimize \( F \) using the Levenberg-Marquardt algorithm (Doherty, 2002).
Conditioning steady-state mean stochastic flow equations

Fig. 2 Contours of reference (true) head compared with: (a) Monte Carlo results conditioned on measured log conductivity, and (b) inverse results conditioned additionally on measured head.

The inverse procedure yields optimum unbiased posterior estimates of logconductivity, their covariance matrix, as well as head and flux conditioned on all available data used for this purpose. We then use these estimates to solve the second-order conditional moment equations for the posterior covariances of head and flux. The latter provide measures of predictive uncertainty due to the combined effects of stochastic averaging and parameter uncertainty (Neuman & Guadagnini, 2000). In general, one expects joint conditioning on reliable parameter and head measurements to yield smaller prediction errors than conditioning on only one such set of data. When reliable prior information about the parameters is not available, it may be better to ignore such information and rely exclusively on calibration against head and flux data. In this case, $J_y$ is excluded from $F$ in equation (7).

NUMERICAL EXAMPLES

We illustrate our inverse methodology for the case of superimposed mean uniform and convergent flows in a rectangular domain of width 8 and length 18, measured in arbitrary consistent units (Fig. 1(a)). The domain is subdivided into $40 \times 90$ square elements in each of which logconductivity is uniform. Deterministic head values of 10 and 0 are prescribed along the left and right boundaries, and deterministic no-flow conditions along the top and bottom boundaries, respectively. A well at the domain centre pumps at a constant deterministic rate of 1. Using the sequential Gaussian simulator SGSIM (Deutsch & Journel, 1998) we have generated a single unconditional realization of logconductivity across the grid by considering $Y$ to be multivariate Gaussian, statistically homogeneous and isotropic, with variance $\sigma_Y^2 = 1$, exponential autocovariance and spatial correlation scale $\lambda = 1$ (Fig. 1(b)). We used a standard finite element algorithm to obtain a corresponding distribution of heads and fluxes. These constitute our reference ("true") values of hydraulic conductivity, head and flux in the domain.

For purposes of conditioning, we sampled the generated $Y$ field at 16 evenly spaced "measurement" points at element centres, indicated by $x$ in Fig. 1(a). We sampled the generated $h$ field at 36 "measurement" points, indicated by plus signs, located randomly in the interiors of evenly spaced subdomains consisting of $2 \times 2$
elements each. For purposes of inversion, we designated 16 pilot points at locations indicated by PP in Fig. 1(a).

Our calibration code couples an improved (by an efficient direct solution method) version of the finite element conditional mean simulator of Guadagnini & Neuman (1999a,b), a universal kriging package we wrote for this purpose and the inverse code PEST-ASP of Doherty (2002). Though PEST-ASP is designed to run in parallel on multiple processors, we used only one processor on the University of Arizona SGI Origin 2000 supercomputer. Each calibration required between 78 and 179 min of execution time. We compare below, a forward solution of the moment equations conditioned solely on logconductivity data with inverse solutions conditioned on: (a) both logconductivity and head data, and (b) head data alone. Our forward solution is compared with corresponding conditional Monte Carlo results that were computed using 2000 conditional logconductivity realizations generated with the SGSIM simulator.

Figure 2 compares contours of reference (true) heads with those obtained by: (a) Monte Carlo simulations conditioned on measured log conductivities, and (b) inversion conditioned on both head and logconductivity data. A visual comparison of Figs 2(a) and (b) suggests that the inverse moment solution is closer to the true head field than is the forward Monte Carlo solution. This is confirmed quantitatively by the normalized root mean square (RMS) head and flux residuals (differences between computed and “true” values at all nodes) in Table 1. Figure 3 suggests visually that the inverse solution is associated with smaller head and flux prediction variances than is the forward Monte Carlo simulation. This is corroborated quantitatively by the normalized prediction variances in Table 1, in which $q_{x1}$ and $q_{x2}$ represent longitudinal and transversal fluxes, respectively.

Table 1 indicates that ignoring prior information about logconductivities leads to closer fits between computed and “true” log conductivities, heads and fluxes. This is so because absence of constraining prior information makes it possible to fit the model more closely to the available head data. Yet taking prior information into account leads to a significant reduction in the estimation variance of logconductivity and the predictive uncertainty of flux, while resulting in only an insignificant increase in the predictive uncertainty of head. This confirms that a good model fit does not necessarily insure superior predictive capabilities.

**Table 1** Comparison of Monte Carlo and inverse moment solutions. Statistics are normalized by their largest values.

<table>
<thead>
<tr>
<th></th>
<th>Forward Monte Carlo</th>
<th>Inverse without prior data</th>
<th>Inverse with prior data</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMS of $Y$ residuals in all elements</td>
<td>1.00</td>
<td>0.89</td>
<td>1.00</td>
</tr>
<tr>
<td>RMS of head residuals at all nodes</td>
<td>1.00</td>
<td>0.46</td>
<td>0.62</td>
</tr>
<tr>
<td>RMS of $q_{x1}$ residuals at all nodes</td>
<td>1.00</td>
<td>0.88</td>
<td>0.96</td>
</tr>
<tr>
<td>RMS of $q_{x2}$ residuals at all nodes</td>
<td>1.00</td>
<td>0.95</td>
<td>0.97</td>
</tr>
<tr>
<td>Average $Y$ kriging estimation variance</td>
<td>1.00</td>
<td>0.93</td>
<td>0.88</td>
</tr>
<tr>
<td>Average head prediction variance</td>
<td>1.00</td>
<td>0.59</td>
<td>0.61</td>
</tr>
<tr>
<td>Average prediction variance of $q_{x1}$</td>
<td>1.00</td>
<td>0.93</td>
<td>0.55</td>
</tr>
<tr>
<td>Average prediction variances of $q_{x2}$</td>
<td>1.00</td>
<td>0.84</td>
<td>0.49</td>
</tr>
<tr>
<td>RMS of flux cross-variances $C_{Qx1Qx2}$</td>
<td>0.88</td>
<td>1.00</td>
<td>0.58</td>
</tr>
</tbody>
</table>
Conditioning steady-state mean stochastic flow equations

Fig. 3 Variance of (a) head, (b) $q_{x1}$, (c) $q_{x2}$, and (d) cross-covariance (at zero lag) of $q_{x1}$ and $q_{x2}$ along section A–A’ in Fig. 1(a). Inverse solution is conditioned on both log-conductivity and head data.

Table 2 lists the same statistics as Table 1 except that now the forward solution is based on non-local moment equations rather than on Monte Carlo simulations. We see that conditioning the moment equations on both log-conductivity and head data is generally better than conditioning them on only one of these data sets. Conditioning on $Y$ data alone leads to better estimates of $Y$ and fluxes than conditioning only on head, while conditioning only on head data results in better estimates of $h$ than in the opposite case.

Table 2 Comparison of forward and inverse moment solutions. Statistics are normalized by their largest values.

<table>
<thead>
<tr>
<th></th>
<th>Conditioned on $Y$ only</th>
<th>Conditioned on head only</th>
<th>Conditioned on both $Y$ and head</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMS of $Y$ residuals in all elements</td>
<td>0.95</td>
<td>1.00</td>
<td>0.93</td>
</tr>
<tr>
<td>RMS of head residuals at all nodes</td>
<td>1.00</td>
<td>0.80</td>
<td>0.78</td>
</tr>
<tr>
<td>RMS of $q_{x1}$ residuals at all nodes</td>
<td>0.72</td>
<td>1.00</td>
<td>0.72</td>
</tr>
<tr>
<td>RMS of $q_{x2}$ residuals at all nodes</td>
<td>0.95</td>
<td>1.00</td>
<td>0.94</td>
</tr>
<tr>
<td>Average $Y$ kriging estimation variance</td>
<td>0.70</td>
<td>1.00</td>
<td>0.59</td>
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<tr>
<td>Average head prediction variance</td>
<td>1.00</td>
<td>0.95</td>
<td>0.59</td>
</tr>
<tr>
<td>Average prediction variance of $q_{x1}$</td>
<td>0.26</td>
<td>1.00</td>
<td>0.21</td>
</tr>
<tr>
<td>Average prediction variance of $q_{x2}$</td>
<td>0.50</td>
<td>1.00</td>
<td>0.42</td>
</tr>
<tr>
<td>RMS of flux cross-variances $C_{q_{x1}q_{x2}}$</td>
<td>0.60</td>
<td>1.00</td>
<td>0.49</td>
</tr>
</tbody>
</table>

CONCLUSIONS

It is possible and computationally feasible to condition non-local ensemble moment equations of steady-state flow jointly on measurements of log-conductivity and hydraulic head through geostatistical inversion. Our examples show that, whereas
conditioning on conductivity or head data alone may lead to a closer correspondence between these quantities and the model, conditioning on both yields improved parameter estimates and predictions of head and flux.

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