Conditioning mean steady state flow on hydraulic head and conductivity through geostatistical inversion

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Abstract. Nonlocal moment equations allow one to render 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. Optimum unbiased inverse estimates of natural log hydraulic conductivity, head and flux are obtained by minimizing a residual criterion using the Levenberg-Marquardt algorithm. 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.

Keywords: Aquifer characteristics, Groundwater flow, Inverse problem, Regression analysis, Uncertainty, Steady-state conditions, Stochastic processes, Geostatistics

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This work is supported in part by NSF/ITR Grant EAR-0110289. The first author was additionally supported by scholarships from CONACYT and Instituto de Investigaciones Electricas of Mexico. Additional support was provided by the European Commission under Contract EVK1-CT-1999-00041 (W-SAHaRA-Stochastic Analysis of Well Head Protection and Risk Assessment).

Introduction

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

$$-\nabla \cdot \langle \mathbf{q}(\mathbf{x}) \rangle_c + \langle f(\mathbf{x}) \rangle = 0 \tag{1}$$

$$\langle \mathbf{q}(\mathbf{x}) \rangle_c = -\langle K(\mathbf{x}) \rangle_c \nabla \langle h(\mathbf{x}) \rangle_c + \mathbf{r}_c(\mathbf{x}) \quad \mathbf{r}_c(\mathbf{x}) = -\langle K'(\mathbf{x}) \nabla h'(\mathbf{x}) \rangle_c \tag{2}$$

in Ω subject to the boundary conditions

$$\langle h(\mathbf{x}) \rangle_c = \langle H(\mathbf{x}) \rangle$$
 on $\Gamma_D - \nabla \cdot \langle \mathbf{q}(\mathbf{x}) \rangle_c \cdot \mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x}) \rangle$ on Γ_N (3)

where the subscript *c* implies "conditional"; primed quantities represent random fluctuations about (conditional) mean values; $K(\mathbf{x})$ is a random field of scalar hydraulic conductivities; $\mathbf{r}_c(\mathbf{x})$ is a residual flux; $\langle f(\mathbf{x}) \rangle$, $\langle H(\mathbf{x}) \rangle$, $\langle Q(\mathbf{x}) \rangle$ are prescribed unconditional first moments of the statistically independent random source and boundary forcing terms $f(\mathbf{x}), H(\mathbf{x}), Q(\mathbf{x})$; and $\mathbf{n}(\mathbf{x})$ is a unit outward normal to $\Gamma = \Gamma_D \cup \Gamma_N$ where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. The residual flux $\mathbf{r}_c(\mathbf{x})$ is given implicitly by (Neuman et al., 1996)

$$\mathbf{r}_{c}(\mathbf{x}) = \int_{\Omega} \mathbf{a}_{c}(\mathbf{y}, \mathbf{x}) \nabla_{\mathbf{y}} \langle h(\mathbf{y}) \rangle_{c} \mathrm{d}\mathbf{y} + \int_{\Omega} \mathrm{d}_{c}(\mathbf{y}, \mathbf{x}) \mathbf{r}_{c}(\mathbf{y}) \, \mathrm{d}\mathbf{y}$$
(4)

where the kernels

$$\mathbf{a}_{c}(\mathbf{y},\mathbf{x}) = \left\langle K'(\mathbf{x})K'(\mathbf{y})\nabla_{\mathbf{x}}\nabla_{\mathbf{y}}^{\mathrm{T}}G(\mathbf{y},\mathbf{x})\right\rangle_{c}$$
(5)

$$\mathbf{d}_{c}(\mathbf{y}, \mathbf{x}) = \langle K'(\mathbf{x}) \nabla_{\mathbf{x}} \nabla_{\mathbf{y}}^{\mathrm{T}} G(\mathbf{y}, \mathbf{x}) \rangle_{c}$$
(6)

form a symmetric and a non-symmetric tensor, respectively. Here $G(\mathbf{y}, \mathbf{x})$ is a random Green's function, or solution of the random flow equations for the case where $f(\mathbf{x})$ is a point source of unit strength at point \mathbf{y} subject to homogeneous boundary conditions $H(\mathbf{x}) \equiv Q(\mathbf{x}) \equiv 0$.

Due to the integro-differential nature of $\mathbf{r}_c(\mathbf{x})$, the conditional moment equations include nonlocal parameters that depend on more than one point in space (hence the equations are referred to as nonlocal). 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 nonlocal and non-Darcian, depending on the residual flux $\mathbf{r}_c(\mathbf{x})$. The traditional notion of effective conductivity looses meaning in the context of flow prediction by means of conditional ensemble mean quantities.

Guadagnini and Neuman (1999a, b) have developed corresponding integrodifferential 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 nonlocal moment equations in terms of a small parameter, σ_Y , representing a measure of the standard deviation of natural log conductivity, $Y(\mathbf{x}) = \ln K(\mathbf{x})$. The second order approximation of the conditional covariance for heads, C_{hc} , satisfies

$$\nabla_{\mathbf{x}} \cdot \left[K_{G}(\mathbf{x}) \nabla_{\mathbf{x}} C_{hc}(\mathbf{x}, \mathbf{y}) + C_{hKc}(\mathbf{x}, \mathbf{y}) \nabla_{\mathbf{x}} \langle h^{(0)}(\mathbf{x}) \rangle_{c} \right]$$

+
$$\int_{\Omega} \langle f'(\mathbf{x}) f'(\mathbf{z}) \rangle \langle G^{(0)}(\mathbf{z}, \mathbf{y}) \rangle_{c} \, \mathrm{d}\mathbf{z} = 0$$
(7)

in Ω subject to the boundary conditions

$$C_{hc}(\mathbf{x}, \mathbf{y}) = -\int_{\Gamma_D} \langle H'(\mathbf{x}) H'(\mathbf{z}) \rangle \Big[K_G(\mathbf{z}) \nabla_z \langle G^{(0)}(\mathbf{z}, \mathbf{y}) \rangle_c + 1 \Big] \cdot \mathbf{n}(\mathbf{z}) \, \mathrm{d}\mathbf{z} \quad \mathbf{x} \in \Gamma_D$$
(8)

$$\begin{bmatrix} K_G(\mathbf{x})\nabla_{\mathbf{x}}C_{hc}(\mathbf{x},\mathbf{y}) + C_{hKc}(\mathbf{x},\mathbf{y})\nabla_{\mathbf{x}}\langle h^{(0)}(\mathbf{x})\rangle_c \end{bmatrix} \cdot \mathbf{n}(\mathbf{x})$$
$$= \int_{\Gamma_N} \langle Q'(\mathbf{x})Q'(\mathbf{z})\rangle \langle G^{(0)}(\mathbf{z},\mathbf{y})\rangle_c \, \mathrm{d}\mathbf{z} \quad \mathbf{x} \in \Gamma_N$$
(9)

where C_{hKc} is a second order approximation of the cross covariance between hydraulic head and conductivity,

$$C_{hKc}(\mathbf{x}, \mathbf{y}) = -K_G(\mathbf{x}) \int_{\Omega} \nabla_z^{\mathrm{T}} \langle h^{(0)}(\mathbf{z}) \rangle_c \nabla_z \langle G^{(0)}(\mathbf{z}, \mathbf{y}) \rangle_c K_G(\mathbf{z}) \langle Y'(\mathbf{z}) Y'(\mathbf{x}) \rangle_c \mathrm{d}\mathbf{z}$$
(10)

 K_G is the conditional geometric mean of K; $\langle h^{(0)} \rangle_c$ is the solution of (1)-(3) with $\mathbf{r}_c(\mathbf{x}) = 0$; $\langle G(\theta) \rangle_c$ is zero-order approximation of the conditional mean Green's function; f', H', and Q' are zero-mean fluctuations of f, H, and Q about their corresponding means; and $\langle Y'(\mathbf{z})Y'(\mathbf{x}) \rangle_c$ is second conditional moment of estimation errors of Y.

Conditioning on state variables through model calibration

The recursive finite element algorithm of Guadagnini and Neuman (1999a,b) is valid to second order in σ_Y . It assumes that one has at his/her disposal two functional parameters: a conditional unbiased estimate, $\langle Y(\mathbf{x}) \rangle_c$, of the randomly varying log conductivity function and $C_{Yc}(\mathbf{x}, \mathbf{y}) = \langle Y'(\mathbf{x})Y'(\mathbf{y}) \rangle_c$. When conditioning is performed on the basis of existing ω -scale measurements of Y at a set of

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discrete points, $\langle Y(\mathbf{x}) \rangle_c$ and $C_{Yc}(\mathbf{x}, \mathbf{y})$ can be obtained (in principle) by means of geostatistical methods (e.g., Deutsch and Journel, 1998; Chilès and Delfiner, 1999).

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

To estimate $\langle Y(\mathbf{x})\rangle_c$, we parameterize it as a weighted sum of precisely or imprecisely known values (Y_M) at discrete measurement points $\mathbf{x}_i (i = 1, ..., I)$ and unknown values (Y_P) at discrete "pilot points" \mathbf{x}_p (p = 1, ..., P) in a way reminiscent of de Marsily (1978) and de Marsily et al. (1984):

$$\langle Y(\mathbf{x}) \rangle_c = \sum_{i=1}^{I} \omega_i(\mathbf{x}) Y_M(\mathbf{x}_i) + \sum_{p=1}^{P} \omega_p(\mathbf{x}) Y_P(\mathbf{x}_p) \quad \mathbf{x} \in \Omega$$
 (11)

Both sets of values (Y_M and Y_P) are treated (the first optionally) as unknown parameters to be estimated by inversion. The weights (ω_i) of the sum are evaluated through universal kriging (to allow dealing with statistically nonhomogeneous Y fields) considering the variance of Y measurement and/or interpretive errors at actual data points (assumed to be uncorrelated), the covariance matrix **Q** of parameter estimation errors at pilot points (set equal to the inverse Fisher information matrix of the most recent iterate), and an estimate of the variogram or autocovariance of Y. At least one measured conductivity or flux value is needed to obtain a unique set of parameter estimates.

In our examples the number and positioning of pilot points are intuitive. Both could be optimized in a manner proposed by Hernandez (2002).

Let \mathbf{h}^* be a vector of head measurements at discrete space locations; \mathbf{h} and \mathbf{h} the corresponding vectors of (unknown) true and conditional mean heads calculated through (1)–(6), respectively; \mathbf{S}_h a (diagonal) covariance matrix of head measurement errors (assumed to be uncorrelated); \mathbf{Y}^* a vector of prior log conductivity values consisting of imprecise measurements and corresponding kriged values at pilot points; \mathbf{Y} and $\hat{\mathbf{Y}}$ the corresponding vectors of true values and inverse estimates of $\langle Y(\mathbf{x}) \rangle c$, respectively; and \mathbf{S}_Y the covariance matrix of associated prior (measurement and kriging) errors. If (a) the true measurement errors ($\mathbf{h}^* - \mathbf{h}$) and ($\mathbf{Y}^* - \mathbf{\hat{Y}}$), respectively; (b) each set of residuals is reasonably unbiased and Gaussian; (c) head residuals are uncorrelated with Y residuals, Y, h, and themselves; and (d) \mathbf{S}_h and/or \mathbf{S}_Y are known up to a constant of multiplication; then the parameters Y_P and, optionally, Y_M can be estimated jointly with these statistical constants by the maximum likelihood method of Carrera and Neuman (1986). This is accomplished by minimizing the generalized sum of squared residuals

$$F = \left(\hat{\mathbf{h}} - \mathbf{h}^*\right)^T \mathbf{S}_h^{-1} \left(\hat{\mathbf{h}} - \mathbf{h}^*\right) + \left(\hat{\mathbf{Y}} - \mathbf{Y}^*\right)^T \mathbf{S}_Y^{-1} \left(\hat{\mathbf{Y}} - \mathbf{Y}^*\right)$$
(12)

through an iterative procedure. Other statistical parameters entering into S_h and/or S_Y , such as those defining the spatial correlation of the data, can also be estimated. When the statistical parameters are known, the maximum likelihood

approach reduces to nonlinear regression. We minimize F using the Levenberg–Marquardt algorithm (Doherty, 2002).

By virtue of the maximum likelihood approach, the (iterative) inverse procedure yields optimum unbiased posterior estimates of log conductivity, their covariance matrix Q, as well as head and flux conditioned on all available data utilized for this purpose through the nonlocal mean equations (1)-(6). Eigenanalysis of the matrix \mathbf{Q} is informative about parameter estimation uncertainty and correlation. For example, parameters associated with eigenvectors characterized by small eigenvalues are less uncertain than those associated with large eigenvalues. Linear confidence intervals can also be used to assess estimation uncertainty provided the residuals (of calibrated state variables and parameters) are reasonably close to being univariate Gaussian and the model behaves linearly near the estimates of $\langle Y(\mathbf{x}) \rangle_c$. We use the estimates to solve the second-order conditional moment equations for 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 and 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, the last term is excluded from F in (12).

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. 1a). The domain is subdivided into 40×90 square elements in each of which log conductivity 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 center pumps at a constant deterministic rate of 1. Using the sequential Gaussian simulator SGSIM (Deutsch and Journel, 1998) we have generated a single unconditional realization of log conductivity 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. 1b). 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.



Fig. 1. a Two-dimensional domain and layout of measurements and pilot points; b reference log hydraulic conductivity field

For purposes of conditioning, we sampled the generated Y field at 16 evenly spaced "measurement" points at element centers, indicated by x's in Fig. 1a. We sampled the generated head field at 36 "measurement" points, indicated by plus signs, located randomly in the interiors of evenly spaced subdomains consisting of 2×2 elements each. For purposes of inversion, we designated arbitrarily 16 pilot points at locations indicated by PP in Fig. 1a.

Our calibration code couples the finite element conditional mean flow simulator of Guadagnini and Neuman (1999a,b), a universal kriging package we wrote for this purpose and the inverse code PEST-ASP of Doherty (2002). Numerical performance of the flow simulator was significantly improved utilizing an efficient (sparse) direct linear solver (Liu, 1987) that exploits the common structure of finite element matrices at various iterations. Though PEST-ASP is designed to run in parallel on multiple processors, we utilized 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 (i.e., a single run of the moment equations (1)-(10)) conditioned solely on log conductivity data with inverse solutions conditioned on (A) head data alone and (B) both log conductivity and head data. Our forward solution is also compared with a corresponding ensemble mean of 2000 forward conditional Monte Carlo flow simulations based on 2000 conditional log conductivity realizations generated using SGSIM. It would have been desirable to compare our results with Monte Carlo simulations conditioned on both head and Y data using a method such as that of Gómez-Hernández et al. (1997) but this would have required an inordinate amount of computer time.

For example, Fig. 2 shows parameter estimates at pilot points and associated covariance eigen-analysis for inverse solution (B). Values of $Y_P(\mathbf{x}_p)$ and \mathbf{S}_Y considered in the calibration process were obtained by kriging noise-free measurements $Y_M(\mathbf{x}_i)$ at pilot points with known σ_Y^2 , λ and autocovariance of $Y(\mathbf{x})$; \mathbf{S}_h was set equal to the identity matrix. All priors in Fig. 2a are within computed confidence intervals of their corresponding parameter estimates. Eigenvalues in Fig. 2b have similar orders of magnitude and indicate that the inversion is relatively well posed. Fig. 2c shows that parameter estimates are weakly correlated.

Parameter estimates and log conductivity data are used to estimate geostatistically the field $Y(\mathbf{x})$ and associated variance $\sigma_Y^2(\mathbf{x})$ in Ω as shown in Fig. 3. The kriged field $\langle Y(\mathbf{x}) \rangle_c$ in Fig. 3a is a smooth optimum unbiased estimate of $Y(\mathbf{x})$ that is closest, in the mean, to all likely $Y(\mathbf{x})$ realizations, of which the reference field is only one. Kriging variance is zero or close to it at conductivity and pilot points, as depicted in the image (Fig. 3b) of $\sigma_Y^2(\mathbf{x})$ and its sections along (Fig. 3c) and across (Fig. 3d) the domain. In general, conditioning on both head and log



Fig. 2. a Parameter estimates at pilot points with associated linear confidence intervals and prior information. **b** Eigenvalues and **c** eigenvectors of the parameter estimation covariance matrix. Inverse solution (B) is conditioned on both log conductivity and head data



Fig. 3. Images of **a** estimated log conductivity field and **b** associated estimation variance (σ_y^2) conditioned on both head and log conductivity data, **c** longitudinal and **d** transverse sections of σ_y^2



Fig. 4. 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 (A) c-d Sections of the same contours along section A-A' in Fig. 1a, respectively

conductivity data through geostatistical inversion diminishes significantly the estimation uncertainty of $Y(\mathbf{x})$.

Figure 4 compares contours and sections of reference (true) heads with those obtained by (1) Monte Carlo simulations conditioned on measured log conductivities and (2) inversion (A). A visual comparison of Fig. 4a–d 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 residuals (differences between computed and "true" values at all nodes) in Table 1.

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	Forward Monte Carlo	Inverse (A) without prior data	Inverse (B) with prior data
RMS of Y residuals in all elements	1.00	0.89	1.00
RMS of head residuals at all nodes	1.00	0.46	0.62
RMS of q_{x1} residuals at all nodes	1.00	0.88	0.96
RMS of q_{x2} residuals at all nodes	1.00	0.95	0.97
Average <i>Y</i> kriging estimation variance	1.00	0.93	0.88
Average head prediction variance	1.00	0.59	0.61
Average prediction variance of q_{x1}	1.00	0.93	0.55
Average prediction variances of q_{x2}	1.00	0.84	0.49
RMS of flux cross-variances $C_{q_{x1}q_{x2}}$	0.88	1.00	0.58

Table 1. Comparison of Monte Carlo and inverse moment solutions

Note: Statistics are normalized by their largest values



Fig. 5. Section of **a-b** longitudinal and **c-d** transverse components of reference flux compared with corresponding components of inverse (B) and Monte Carlo solutions. Inverse solution is conditioned on both head and log conductivity measurements

Sections of flux in Fig. 5 allow comparing longitudinal and transverse components of reference flux with those of conditional Monte Carlo and inverse (B) solutions. Both mean fluxes compare equally well with the reference mean flux, although the inverse mean flux reproduces the reference flux better than the Monte Carlo mean flux near Y measurement points (see normalized RMS flux residuals in Table 1).

Figure 6 suggests visually that the inverse (B) solution is associated with smaller head and flux prediction variances than is the mean 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 log conductivities leads to closer fits between computed and "true" log conductivities, heads and



Fig. 6. 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. 1a. Inverse (B) (—) and Monte Carlo (—) solutions

	Conditioned on Y only (Forward)	Conditioned on head only (Inverse (A))	Conditioned on both Y and head (Inverse (B))
RMS of Y residuals in all elements	0.95	1.00	0.93
RMS of head residuals at all nodes	1.00	0.80	0.78
RMS of q_{x1} residuals at all nodes	0.72	1.00	0.72
RMS of q_{x2} residuals at all nodes	0.95	1.00	0.94
Average Y kriging estimation variance	0.70	1.00	0.59
Average head prediction variance	1.00	0.95	0.59
Average prediction variance of q_{x1}	0.26	1.00	0.21
Average prediction variance of q_{x2}	0.50	1.00	0.42
RMS of flux cross-variances C_{qx1qx2}	0.60	1.00	0.49

Table 2. Comparison of forward and inverse moment solutions

Note: Statistics are normalized by their largest values

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 log conductivity 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 2 lists the same statistics as Table 1 except that now the forward solution is based on nonlocal 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. Figs. 3–6 indicate that head measurements have an unnoticeable conditioning effect on the residuals and variances of log conductivity, head, and flux.

Conclusions

It is possible and computationally feasible to condition nonlocal 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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