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Parameter Estimation in Groundwater: Classical, Bayesian, and Deterministic Assumptions and Their Impact on Management Policies

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This work deals with a theoretical analysis of parameter uncertainty in groundwater management models. The importance of adopting classical, Bayesian, or deterministic distribution assumptions on parameters is examined from a mathematical standpoint. In the classical case, the parameters (e.g., hydraulic conductivities or storativities) are assumed fixed (i.e., nonrandom) but unknown. The Bayesian assumption considers the parameters as random entities with some probability distribution. The deterministic case, also called certainty equivalence, assumes that the parameters are fixed and known. Previous work on the inverse problem has emphasized the numerical solution for parameter estimates with the subsequent aim to use them in the simulation of field variables. In this paper, the role of parameter uncertainty (measured by their statistical variability) in groundwater management decisions is investigated. It is shown that the classical, Bayesian, and deterministic assumptions lead to analytically different management solutions. Numerically, the difference between such solutions depends upon the covariance of the parameter estimates. The theoretical analyses of this work show the importance of specifying the proper distributional assumption on groundwater parameters, as well as the need for using efficient and statistically consistent methods to solve the inverse problem. The distributional assumptions on groundwater parameters and the covariance of their sample estimators are shown to be the dominant parameter uncertainty factors affecting groundwater management solutions. An example illustrates the conceptual findings of this work.

1. INTRODUCTION

There has been a substantial number of research papers dealing with the inverse problem in the last two decades. *Yeh* [1986] summarized many of the contributions reported in the literature. The main goal of the various approaches to the inverse problem is to obtain unbiased and consistent estimators of groundwater parameters based on measured values of the pertinent field variable. The computed estimates are then available for use in simulation models that predict the response of aquifers to natural or anthropogenic inputs. Such simulation models are commonly integrated within more general management schemes to yield various decision variables that optimize specified objectives (see, for example, *Danskin and Gorelick* [1985]). The statistical properties of parameter estimators (in particular their covariances) affect the simulated field variable (see, for example, *Freeze* [1975]) and consequently should have an influence on the output resulting from any management scheme that includes the groundwater model as a subunit. The theoretical analysis of the dependence of management decisions on groundwater parameter uncertainty is the main focus of this study.

Parallel to the development of stable and reliable algorithms for the solution of the inverse problem, groundwater management modeling has received substantial attention (see, for example, *Gorelick* [1983]). However, the authors are not aware of research devoted to the analysis of the relationship between the solution to the inverse problem and the quality of groundwater management decisions, except for a few case-specific studies based on sensitivity analyses (see, for example, *Young and Bredehoeft* [1972] or *Maddock* [1974]) or the chance-constrained analysis by *Tung* [1986]. A review of the literature indicates that it is customary to solve the inverse problem first and then use the parameter estimators into management models, treating such estimators as if they were nonrandom variables. It is shown below that treating parameter estimators as deterministic entities leads to management solutions that are different from the true ones consistent with more realistic assumptions about the parameters. It is also shown in this work that if parameter estimators are treated as stochastic entities (as they should be treated), then the solutions to the management problem are functions of the statistical variability of those estimators. In fact, such management solutions are also dependent on whether the parameters are treated as fixed but unknown (i.e., the classical approach) or as random variables with some probability distribution (i.e., the Bayesian approach).

The purpose of this study is to present a theoretical analysis of groundwater parameter uncertainty and its relationship with management solutions. An analytical functional relationship between control solutions for groundwater management and the statistical properties of parameters is derived. The difference among management solutions based on the classical, Bayesian, or certainty equivalence assumptions imposed on groundwater parameters is then established. The theoretical developments are illustrated for open-loop and closed-loop versions of a management model. The former version is popular among researchers who prefer nonlinear programming

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methods, whereas the latter is appealing to those who are more inclined toward dynamic programming. The findings of this work are identically applicable to either the open-loop or the closed-loop versions of the groundwater management problem. An example provides a numerical interpretation of the theoretical results developed in this study.

2. Problem Statement

Suppose that the continuity equation for an isotropic and inhomogeneous medium is given by

$$\frac{\partial}{\partial x}\left(K^* \frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K^* \frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial z}\left(K^* \frac{\partial \phi}{\partial z}\right) - F = S\frac{\partial \phi}{\partial t} \qquad (1)$$

in which $K^* = K^*(x, y, z)$ denotes hydraulic conductivity; $S = S(x, y, z)$ denotes specific storativity; F is a time-dependent sink term (e.g., pumping); and $\phi = \phi(x, y, z, t)$ denotes piezometric head. Equation (1) is coupled with proper initial and boundary conditions that fully specify the time and space distribution of the field variable ϕ. It is assumed that K and S are distributed parameters, and under the classical approach, they are treated as unknown but fixed (i.e., nonrandom), whereas the Bayesian approach specifies them as being random coefficients following some probability distribution. The deterministic (or certainty equivalence) assumption consists of treating K and S as known and fixed parameters.

Loaiciga and Mariño [1987] have shown that by discretizing (1) by finite element or finite difference methods and solving for the field variable at time t, one obtains the linear discrete expression

$$\boldsymbol{\phi}_t = \Pi_0 \boldsymbol{\phi}_{t-1} + \Pi_1 \mathbf{x}_t + \mathbf{u}_t \qquad t = 1, 2, \cdots, T \qquad (2)$$

in which $\boldsymbol{\phi}_t$ is an $N \times 1$ vector containing piezometric heads at time t; Π_0 is an $N \times N$ matrix whose elements are functions of the vector of parameters (i.e., hydraulic conductivities and specific storativities); Π_1 is an $N \times K$ matrix whose elements are functions of the parameter vector; $\mathbf{x}_t$ is a $K \times 1$ vector of inputs or decision variables (depends on sink terms); and $\mathbf{u}_t$ is an $N \times 1$ vector error term that accounts for modeling and/or measurement errors. The error term $\mathbf{u}_t$ may have an arbitrary covariance structure, and without loss of generality, it is assumed to have an expected value equal to zero. The choice of time indexes in (2) implies that the state of the system at time t is a function of the state at time $t - 1$, of the decision implemented in the interval $[t - 1, t]$, and of the disturbance occurred in this same time interval. Notice that if physical parameters (e.g., hydraulic conductivities and/or specific storativities) are estimated by a consistent method (say, maximum likelihood), then by letting $\boldsymbol{\xi}$ be the estimated parameter vector, $\Pi_0(\boldsymbol{\xi}) = \hat{\Pi}_0$ and $\Pi_1(\boldsymbol{\xi}) = \hat{\Pi}_1$ are the corresponding matrix estimators. In the case of maximum likelihood estimation, $\hat{\Pi}_0$ and $\hat{\Pi}_1$ are also consistent. Recall that an estimator is consistent if its limiting probability distribution converges to the true but unknown parameter being estimated (see, for example, *Bickel and Doksum* [1977, pp. 132–133]).

In general, an additional (additive) term should be present on the right-hand side of (2) to account for known but essentially uncontrollable variables (i.e., boundary conditions). For the sake of simplifications in the mathematical developments, such a term has been dropped without affecting the conceptual validity of the results. The example in section 5 provides details for a case in which this term, which depends on boundary conditions, is included.

The groundwater management model consists of minimizing with respect to the decision variables $\mathbf{x}_t$, $t = 1, 2, \cdots, T$, the quadratic loss function

$$L_1 = E \sum_{t=1}^{T} \boldsymbol{\phi}_t' Q_t \boldsymbol{\phi}_t \qquad (3)$$

over the T periods in the control horizon, in which E denotes expectation, subject to the model (2); the primed notation denotes the transpose of a vector. The policymaker's preferences are embodied in the symmetric matrix Q_t (notice that since equation (3) is quadratic, symmetry is purely an assumption of convenience). Equation (3) is more general than it may seem at first hand. Costs on inputs can be handled by augmenting (2) with $\mathbf{x}_t = I\mathbf{x}_t$ (I is an identity matrix) and including their penalties in a suitably enlarged matrix Q_t. Desired paths of heads can be incorporated by subtracting them from both sides of the model equation (2). Thus (3) represents a general quadratic criterion and is quite frequently found in groundwater management models (see, for example, *Maddock* [1972], *California Department of Water Resources* [1982], and *Casola et al.* [1986]). In addition, the quadratic criterion (3) allows an analytical treatment, both in the open-loop and closed-loop formulations of the management problem, of the relationship between parameter uncertainty and the optimal solutions. An example is given in section 5.

To clarify what is at issue with regard to the three different possible assumptions (i.e., classical, Bayesian, and deterministic) on the parameters, let us consider an univariate problem involving one time period, a single head ϕ_t, and a single input x_t, with anything else relegated to an error term u_t. Under the Bayesian assumption, the parameters are random. Thus it is the sum of the mean (say, γ) and a stochastic deviation (say, δ_t) that links the input and the field variable; i.e.,

$$\phi_t = (\gamma + \delta_t)x_t + u_t \qquad (4)$$

It is important to note that it is the evolution of the parameter $\gamma + \delta_t$ and not the parameter mean γ that multiples the input variable x_t.

In the classical approach, the parameters are unknown but fixed, leading to

$$\phi_t = \gamma x_t + u_t \qquad (5)$$

in which the fixed but unknown true parameter γ links the input term to the field variable. Randomness exists because the parameter is unknown and must be estimated, not because the parameter is fundamentally stochastic, as in the Bayesian case. Given that the true parameter γ is unknown, decisions must be based on an estimate $\hat{\gamma}$ that includes sampling error η, i.e., $\hat{\gamma} = \gamma + \eta$. The model in terms of estimated variables is

$$\phi_t = (\hat{\gamma} + \eta)x_t + (u_t - \eta x_t) \qquad (6)$$

to be contrasted with the true model (5) and the Bayesian model (4). Since estimation is based on n prior observations, so that the estimation and control periods are disjoint, the unknown sampling error η (a function of the first n observations) has already occurred and will not vary through the control horizon. In contrast, the stochastic component δ_t of the parameter (see equation (4)) is yet to be realized within the control horizon under the Bayesian (random-parameter) assumption. Since the classical and Bayesian models are so different, it is not surprising that their corresponding solutions to the management problems are also distinct. A primary objective of this study is to derive the management solutions consistent with the classical, Bayesian, and deterministic assumptions, and to compare them.

3. OPEN-LOOP STOCHASTIC CONTROL

An open-loop solution to the minimization of (3) subject to (2) is more easily derived if (2) is expressed in terms of the known initial conditions $\boldsymbol{\phi}_0$; i.e.,

$$\boldsymbol{\phi}_t = \Pi_0{}^t\boldsymbol{\phi}_0 + \sum_{k=0}^{t-1} \Pi_0{}^k\Pi_1\mathbf{x}_{t-k} + \sum_{k=0}^{t-1} \Pi_0{}^k\mathbf{u}_{t-k} \qquad (7)$$

for $t = 1, 2, \cdots, T$. In (7), $\Pi_0{}^t$ means $\Pi_0\Pi_0 \cdots \Pi_0$ t times. Time stacking (7) yields

$$\underset{(TN\times 1)}{\begin{bmatrix}\boldsymbol{\phi}_1\\ \boldsymbol{\phi}_2\\ \vdots\\ \boldsymbol{\phi}_T\end{bmatrix}} = \underset{(TN\times N)}{\begin{bmatrix}\Pi_0\\ \Pi_0{}^2\\ \vdots\\ \Pi_0{}^T\end{bmatrix}} \underset{(N\times 1)}{\boldsymbol{\phi}_0} + \underset{(TN\times TK)}{\begin{bmatrix}\Pi_1 & & & \\ \Pi_0\Pi_1 & \Pi_1 & & \\ \vdots & \vdots & & \\ \Pi_0{}^{T-1}\Pi_1 & \Pi_0{}^{T-2}\Pi_1 & \cdots & \Pi_1\end{bmatrix}} \underset{(TK\times 1)}{\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\\ \vdots\\ \mathbf{x}_T\end{bmatrix}}$$

$$+ \underset{(TN\times TN)}{\begin{bmatrix}I & & & \\ \Pi_0 & I & & \\ \vdots & \vdots & & \\ \Pi_0{}^{T-1} & \Pi_0{}^{T-2} & \cdots & I\end{bmatrix}} \underset{(TN\times 1)}{\begin{bmatrix}\mathbf{u}_1\\ \mathbf{u}_2\\ \vdots\\ \mathbf{u}_T\end{bmatrix}} \qquad (8)$$

or in shorthand notation,

$$\boldsymbol{\phi} = \Theta\boldsymbol{\phi}_0 + \Psi\mathbf{x} + \mathbf{u} \qquad (9)$$

In (9), the vector $\mathbf{u}$ equals the product of the matrix and vector in the third term of the right-hand side. Notice that by expressing (8) and (9) in terms of the initial conditions, any subset of the piezometric heads can be decoupled so that only those heads that are actually targets on the management model need be carried in the algebraic developments. Equation (9) can be viewed as a response function, where the dependent variable is explicitly (and linearly) expressed in terms of the initial conditions and the control variables. Therefore (9) is a generalization of the technological function introduced by *Maddock* [1972], since it applies to irregular, finite domains, and linear processes with nonhomogeneous boundary conditions. Furthermore, groundwater quality models dealing with linear transport processes (see, for example, *Willis* [1979], *Gorelick and Remson* [1982]) would lead to system model equations identical to (9) with proper redefinition of variables (e.g., piezometric heads would be replaced by concentrations, etc.).

Applying the rule vec $(ABC) = (C' \otimes A)$ vec (B) to (9), where vec is an operator that stacks successive columns of a matrix below one another and $\otimes$ denotes Kronecker's product (see the appendix), yields

$$\boldsymbol{\phi} = (\boldsymbol{\phi}_0{}' \otimes I_{TN}) \text{ vec } (\Theta) + (\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi) + \mathbf{u} \qquad (10)$$

in which I_{TN} denotes the $TN \times TN$ identity matrix. The objective function (3) is rewritten in shorthand notation as

$$L_1 = E\boldsymbol{\phi}'Q\boldsymbol{\phi} \qquad (11)$$

in which Q is a block diagonal matrix containing $Q_1, Q_2, \cdots, Q_T$ along the diagonal.

Substituting (10) into (11) and expanding the resulting expressions gives

$$\begin{aligned} L_1 = E\{&\text{vec } (\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\boldsymbol{\phi}_0{}' \otimes I_{TN}) \text{ vec } (\Theta) \\ &+ \text{vec } (\Psi)'(\mathbf{x}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi) \\ &+ \mathbf{u}'Q\mathbf{u} + 2 \text{ vec } (\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi) \\ &+ 2 \text{ vec } (\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q\mathbf{u} \\ &+ 2 \text{ vec } (\Psi)'(\mathbf{x}' \otimes I_{TN})'Q\mathbf{u}\} \end{aligned} \qquad (12)$$

Noting that the cross-product terms in a single error (e.g., 2 vec $(\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q\mathbf{u}$) have zero expected values and regrouping the expectation of the terms that do not involve the decision vector $\mathbf{x}$ into a separate term L^* that is irrelevant to the optimization gives

$$\begin{aligned} L_1 = L^* &+ E[\text{vec } (\Psi)'(\mathbf{x}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi)] \\ &+ 2E[\text{vec } (\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi)] \end{aligned} \qquad (13)$$

The last two terms in (13) have the same structure, so it suffices to examine only one. Consider

$$l_1 = 2E[\text{vec } (\Theta)'(\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN}) \text{ vec } (\Psi)] \qquad (14)$$

By using the property of a trace operator that states that for arbitrary conformable vectors $\mathbf{a}$, $\mathbf{b}$, and matrix A, Tr $(\mathbf{a}'A\mathbf{b})$ = Tr $(\mathbf{b}\mathbf{a}'A)$ (see the appendix) permits (14) to be rewritten as

$$l_1 = 2 \text{ Tr } \{E[\text{vec } (\Psi) \text{ vec } (\Theta)'](\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})\} \qquad (15)$$

Next, in order to express (15) in terms of observables, the classical assumption on the parameters Θ and Ψ is used; i.e., they are assumed as fixed and unknown. The Bayesian and deterministic solutions are readily obtained once the classical solution is available.

3.1. *The Classical Approach*

First, notice that

$$E[\text{vec } (\Psi) \text{ vec } (\Theta)'] = E[\text{vec } (\Psi)]E[\text{vec } (\Theta)'] \qquad (16)$$

since, under the classical assumption, Ψ and Θ are nonrandom. Ψ and Θ are estimated by $\hat{\Psi}$ and $\hat{\Theta}$, and these estimators are assumed unbiased, e.g., E vec$(\hat{\Psi})$ = vec (Ψ). From the well-known expression for the covariance Σ of two arbitrary random vectors $\mathbf{w}$ and $\mathbf{z}$, i.e., $\Sigma_{\mathbf{wz}} = E\mathbf{wz}' - E\mathbf{w}E\mathbf{z}'$, it follows that

$$\begin{aligned} E[\text{vec } (\Psi) \text{ vec } (\Theta)'] &= E[\text{vec } (\Psi)]E[\text{vec } (\Theta)'] \\ &= E \text{ vec } (\hat{\Psi})E \text{ vec } (\hat{\Theta})' \\ &= E[\text{vec } (\hat{\Psi}) \text{ vec } (\hat{\Theta})'] - \Sigma_{\Psi\Theta} \end{aligned} \qquad (17)$$

The second equality in (17) follows from the fact that E[vec (Ψ)] = vec (Ψ) = E[vec $(\hat{\Psi})$], since Ψ is fixed and its estimator $\hat{\Psi}$ is unbiased. The same arguments hold true for Θ. In (17), $\Sigma_{\Psi\Theta}$ is the $TKTN \times NTN$ covariance matrix of vec $(\hat{\Psi})$ with vec $(\hat{\Theta})$. Using (17) in (15) yields

$$\begin{aligned} l_1 = 2 \text{ Tr } \{&[E[\text{vec } (\hat{\Psi}) \text{ vec } (\hat{\Theta})'] - \Sigma_{\Psi\Theta}] \\ &\cdot (\boldsymbol{\phi}_0{}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})\} \end{aligned} \qquad (18)$$

By using the identity

$$\text{Tr } (ABCDE) = \text{vec } (B')'[A'E' \otimes C] \text{ vec } (D) \qquad (19)$$

for arbitrarily conformable matrices A, B, C, D, and E (see, for example, *Neudecker* [1969]) (18) can be rewritten as

$$l_1 = 2[\text{vec}\,(\boldsymbol{\phi}_0' \otimes I_{TN})]' \cdot \{[E[\text{vec}\,(\hat{\Theta})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Theta}'] \otimes Q\}\,\text{vec}\,(\mathbf{x}' \otimes I_{TN}) \quad (20)$$

The outer factors in (20) are simplified by noting that

$$\text{vec}\,(\mathbf{x}' \otimes I_{TN}) = \Gamma_x \mathbf{x} \quad (21)$$

in which Γ_x is a $TNTKTN \times TK$ matrix aggregator whose elements are either zero or one and are suitably arranged through rows and columns to make (21) valid (see the appendix). Similarly, a $TNNTN \times N$ matrix aggregator $\boldsymbol{\Gamma}_\phi$ is also introduced to simplify the outer product on $\boldsymbol{\phi}_0$; i.e., Γ_ϕ is such that

$$\text{vec}\,(\boldsymbol{\phi}_0' \otimes I_{TN}) = \boldsymbol{\Gamma}_\phi \boldsymbol{\phi}_0 \quad (22)$$

By using (21) and (22), the term l_1 in (20) becomes

$$l_1 = 2\boldsymbol{\phi}_0'\Gamma_\phi'\{[E[\text{vec}\,(\hat{\Theta})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Theta}'] \otimes Q\}\Gamma_x\mathbf{x} \quad (23)$$

A similar treatment is applicable to the other term involving Kronecker products in (13), leading to the following equation:

$$E[\text{vec}\,(\Psi)'(\mathbf{x}' \otimes I_{TN})'Q(\mathbf{x}' \otimes I_{TN})\,\text{vec}\,(\Psi)] = \mathbf{x}'\Gamma_x'\{[E[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Psi}] \otimes Q\}\Gamma_x\mathbf{x} \quad (24)$$

in which $\Sigma_{\Psi\Psi}$ is the $TNTK \times TNTK$ symmetric covariance matrix of vec $(\hat{\Psi})$. Substitution of (23) and (24) into (13) gives

$$L_1 = L^* + \mathbf{x}'\Gamma_x'\{[E[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Psi}] \otimes Q\}\Gamma_x\mathbf{x} + 2\boldsymbol{\phi}_0'\Gamma_\phi'\{[E[\text{vec}\,(\hat{\Theta})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Theta}'] \otimes Q\}\Gamma_x\mathbf{x} \quad (25)$$

Define

$$L_{xx} = \Gamma_x'\{[E[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Psi})'] - \Sigma_{\Psi\Psi}] \otimes Q\}\Gamma_x \quad (26)$$

$$\mathbf{L}_x = \Gamma_x'\{[E[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Theta})'] - \Sigma_{\Psi\Theta}] \otimes Q\}\Gamma_\phi\boldsymbol{\phi}_0 \quad (27)$$

The first-order condition for a minimum applied to (25) and the use of (26) and (27) in the resulting expression yield the optimal vector $\mathbf{x}^*$ decisions for the entire control horizon; i.e.,

$$\mathbf{x}^* = -L_{xx}^{-1}\mathbf{L}_x \quad (28)$$

Actual implementation of a management policy requires substitution in (26) and (27) of the population moments with their sample estimates. Therefore let

$$\hat{L}_{xx} = \Gamma_x'\{[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Psi})' - \hat{\Sigma}_{\Psi\Psi}] \otimes Q\}\Gamma_x \quad (29)$$

$$\hat{\mathbf{L}}_x = \Gamma_x'\{[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Theta})' - \hat{\Sigma}_{\Psi\Theta}] \otimes Q\}\Gamma_\phi\boldsymbol{\phi}_0 \quad (30)$$

leading to the optimal solution,

$$\hat{\mathbf{x}} = -\hat{L}_{xx}^{-1}\hat{\mathbf{L}}_x \quad (31)$$

In (29) and (30), $\hat{\Sigma}_{\Psi\Psi}$ and $\hat{\Sigma}_{\Psi\Theta}$ are the covariance matrices of the parameter estimators that are available from the solution of the inverse problem. Equations (29) and (31) characterize in a general form the dependence of the management policy on the parameter estimates obtained from the solution of the inverse problem. The reader may realize that for arbitrary nonlinear objective functions, (31) represents the Newton equations that yield consecutive approximations to the solution. Even under the condition of (nonquadratic) nonlinear objective function, the dependence of the Hessian $\hat{L}_{xx}$ and gradient $\hat{\mathbf{L}}_x$ on $\hat{\Psi}$, $\hat{\Theta}$, $\hat{\Sigma}_{\Psi\Psi}$, and $\hat{\Sigma}_{\Psi\Theta}$ as specified in (29) and (30) is well-approximated. Thus $\hat{L}_{xx}$ and $\hat{\mathbf{L}}_x$ as defined in (29) and (30) are quite useful in characterizing the nature of the solution under the classical assumption. Furthermore, the usual approach, popular in the groundwater management literature, of using the parameter estimates obtained from the solution of the inverse problem in the management model and then assuming them constant is equivalent to setting $\hat{\Sigma}_{\Psi\Psi}$ and $\hat{\Sigma}_{\Psi\Theta}$ equal to zero in (29) and (30). Therefore the deterministic or certainty equivalence policies disregard the statistical variability of estimators and do not include their covariances. The certainty equivalence solution approaches the classical result as long as the covariances of estimators tend to zero. This will occur for consistent estimators $\hat{\Psi}$ and $\hat{\Theta}$ only when the sample size used in the solution of the inverse is very large, an improbable situation in applied groundwater management where data scarcity is more of the rule rather than the exception. It is emphasized that usually the inverse problem solutions are in terms of physical parameters, e.g., hydraulic conductivities and/or storativities. If such parameter set, call it $\boldsymbol{\xi}$, is estimated via a consistent method, like maximum likelihood, the matrices $\Psi(\hat{\boldsymbol{\xi}}) = \hat{\Psi}$ and $\Theta(\hat{\boldsymbol{\xi}}) = \hat{\Theta}$ are also consistent maximum likelihood estimators.

3.2. *The Bayesian Approach*

The Bayesian, random-parameter assumption leads to a solution that resembles the classical result, except for an important sign inversion. Suppose that the groundwater parameters are random, with expected values $E(\Psi) = \bar{\Psi}$ and $E(\Theta) = \bar{\Theta}$, and covariance $\Sigma_{\Psi\Psi}$ and cross-covariance $\Sigma_{\Psi\Theta}$. Thus

$$E[\text{vec}\,(\Psi)\,\text{vec}\,(\Theta)'] = \text{vec}\,(\bar{\Psi})\,\text{vec}\,(\bar{\Theta})' + \Sigma_{\Psi\Theta} \quad (32)$$

Next, the factor $E[\text{vec}\,(\Psi)\,\text{vec}\,(\Theta)']$ in (15) is substituted by the right-hand side of (32). This is in contrast to the expression used in the classical approach (i.e., equation (17)), where a minus sign appears in its right-hand side, indicating a subtraction of the covariance matrix. Notice that in (32) the correct sign is positive and the covariance matrix is added. The remaining developments leading to the Bayesian control are analogous to those shown above for the classical case. After sample estimates replace the unknown means and covariances in the appropriate expressions, the Bayesian policy can be shown to be

$$\tilde{\mathbf{x}} = -\tilde{L}_{xx}^{-1}\tilde{\mathbf{L}}_x \quad (33)$$

in which

$$\tilde{L}_{xx} = \Gamma_x'\{[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Psi})' + \hat{\Sigma}_{\Psi\Psi}] \otimes Q\}\Gamma_x \quad (34)$$

$$\tilde{\mathbf{L}}_x = \Gamma_x'\{[\text{vec}\,(\hat{\Psi})\,\text{vec}\,(\hat{\Theta})' + \hat{\Sigma}_{\Psi\Theta}] \otimes Q\}\Gamma_\phi\boldsymbol{\phi}_0 \quad (35)$$

Equations (34) and (35) are identical to the classical equations (29) and (30) except for the plus sign appearing in the factors involving second moments in the Bayesian equations (34) and (35). Notice that a minus sign is required in those factors in (29) and (30). Clearly, the classical and Bayesian management solutions differ more between themselves than each of them does with respect to the deterministic solution, where parameter covariances are ignored altogether. For consistent estimators, $\hat{\Sigma}_{\Psi\Psi}$ and $\hat{\Sigma}_{\Psi\Theta}$ vanish in the limit (i.e., for large sample sizes), and the classical and Bayesian results are asymptotically equivalent and equal to the deterministic solution. However, from a practical standpoint, field data samples are commonly quite limited and the classical and Bayesian solutions are dominated by the small sample properties of parameter estimators, rendering the asymptotic convergence only marginally significant from an utilitarian viewpoint.

4. Closed-Loop Stochastic Control

4.1. *The Classical Approach*

In some cases, the optimal feedback rule (i.e., the closed-loop solution) may be preferred to the simple knowledge of the optimal policy values over the entire horizon (i.e., the open-loop solution as shown in section 3). This section considers the closed-loop solution based on the classical assumption, i.e., fixed but unknown parameters. The Bayesian result follows readily from the classical solution. The algebra parallels the open-loop development, except for the fact that only one period is treated at a time. We will use the classical backward recursion approach of dynamic programming.

The problem is, as before, to minimize the objective function (3) subject to the model constraint in the form of (2), since a feedback rule based on $\boldsymbol{\phi}_{t-1}$ is desired, for any period t. To incorporate again the computationally expedient aggregators (see, for example, equations (21) and (22)) the model equation (2) is rewritten by applying the vec operator; i.e.,

$$\boldsymbol{\phi}_t = (\boldsymbol{\phi}_{t-1}' \otimes I_N) \operatorname{vec}(\Pi_0) + (\mathbf{x}_t' \otimes I_N) \operatorname{vec}(\Pi_1) + \mathbf{u}_t \tag{36}$$

Beginning in the terminal period T in an attempt to develop the backward dynamic programming recursion, the problem of minimizing

$$M_T = E\boldsymbol{\phi}_T' Q_T \boldsymbol{\phi}_T \tag{37}$$

is directly analogous to the open-loop solution. Substitution of the constraint equation (36) with $t = T$ into (37), dropping terms that involve a single $\mathbf{u}_t$ whose expectation is zero, and collecting terms that do not involve $\mathbf{x}_T$ and are irrelevant to the minimization into M_T^* yields

$$\begin{aligned} M_T = {} & M_T^* + \operatorname{Tr} \\ & \cdot \{E[\operatorname{vec}(\Pi_1) \operatorname{vec}(\Pi_1)'](\mathbf{x}_T' \otimes I_N)' H_T (\mathbf{x}_T' \otimes I_N)\} \\ & + 2 \operatorname{Tr} \{E[\operatorname{vec}(\Pi_1) \operatorname{vec}(\Pi_0)'](\boldsymbol{\phi}_{T-1}' \otimes I_N)' H_T (\mathbf{x}_T' \otimes I_N)\} \end{aligned} \tag{38}$$

in which $H_t \equiv Q_T$, and the trace operator has been used to reorder the factors as before (see equations (14) and (15)). As done previously, the square of the parameters is replaced by the expectation of the square of their estimates less their covariance matrix under the classical assumption, the trace rule equation (19) is used, and the matrix aggregators are substituted (the dimensions are now $NKN \times K$ for Γ_x and $NNN \times N$ for Γ_ϕ) to give

$$\begin{aligned} M_T = {} & M_T^* + \mathbf{x}_T' \Gamma_x' \{[E[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_1)'] - \Sigma_{\Pi_1\Pi_1}] \otimes H_T\} \Gamma_x \mathbf{x}_T \\ & + 2\boldsymbol{\phi}_{T-1}' \Gamma_\phi' \{[E[\operatorname{vec}(\hat{\Pi}_0) \operatorname{vec}(\hat{\Pi}_1)'] \\ & - \Sigma_{\Pi_1\Pi_0}'] \otimes H_T\} \Gamma_x \mathbf{x}_T \end{aligned} \tag{39}$$

in which $\Sigma_{\Pi_1\Pi_1}$ is the $NK \times NK$ covariance of vec $(\hat{\Pi}_1)$, and $\Sigma_{\Pi_1\Pi_0}$ denotes the $NK \times NN$ covariance of vec $(\hat{\Pi}_1)$ with vec $(\hat{\Pi}_0)$. Applying the first-order condition to (39), i.e., setting $\partial M_T / \partial \mathbf{x}_T$ equal to zero and solving yields the closed-loop rule

$$\mathbf{x}_T^* = G_T \boldsymbol{\phi}_{T-1} \tag{40}$$

in which

$$\begin{aligned} G_T = {} & -\{\Gamma_x' \{[E[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_1)'] - \Sigma_{\Pi_1\Pi_1}] \otimes H_T\} \Gamma_x\}^{-1} \\ & \cdot \Gamma_x' \{[E[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_0)'] - \Sigma_{\Pi_1\Pi_0}] \otimes H_T\} \Gamma_\phi \end{aligned} \tag{41}$$

(recall $H_T \equiv Q_T$).

For period $T-1$, the principle of optimality [*Bellman*, 1957] permits reduction of the two-period problem to a one-period problem with

$$M_{T-1} = E[\boldsymbol{\phi}_{T-1}' Q_{T-1} \boldsymbol{\phi}_{T-1} + \tilde{M}_T] \tag{42}$$

in which $\tilde{M}_T$ is the minimum cost to go obtained by substituting the optimal rule or policy equation (40) into the terminal loss equation (39). Applying the same steps used to derive (39), but now replacing population moments by their sample estimates to make the results computationally feasible, gives the required recursion in H that characterizes the closed-loop solution; i.e.,

$$\begin{aligned} H_{T-1} = {} & Q_{T-1} + \Gamma_\phi' \{[\operatorname{vec}(\hat{\Pi}_0) \operatorname{vec}(\hat{\Pi}_0)' - \hat{\Sigma}_{\Pi_0\Pi_0}] \otimes H_T\} \Gamma_\phi \\ & + G_T' \Gamma_x' \{[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_0)' - \hat{\Sigma}_{\Pi_1\Pi_0}] \otimes H_T\} \Gamma_\phi \end{aligned} \tag{43}$$

which is in general form. Thus the optimal management policy or control is generated for any period t by simply replacing T with t in (40), (41), and (43) and with the understanding that population moments are replaced with sample estimates in those equations.

4.2. *The Bayesian Approach*

By analogy with the open-loop solutions of section 3, it is straightforward to see that the Bayesian assumption of random parameters leads to equations similar to the classical closed-loop solution embodied by (40), (41), and (43), except for a sign inversion in the factors involving sample second moments in those equations. Explicitly, the Bayesian analogs of (41) and (43) are given by

$$\begin{aligned} \tilde{G}_T = {} & -\{\Gamma_x' \{[E[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_1)'] + \Sigma_{\Pi_1\Pi_1}] \otimes \tilde{H}_T\} \Gamma_x\}^{-1} \\ & \cdot \Gamma_x' \{[E[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_0)'] + \Sigma_{\Pi_1\Pi_0}] \otimes \tilde{H}_T\} \Gamma_\phi \end{aligned} \tag{44}$$

$$\tilde{H}_T \equiv Q_T$$

$$\begin{aligned} \tilde{H}_{T-1} = {} & Q_{T-1} + \Gamma_\phi' \{[\operatorname{vec}(\hat{\Pi}_0) \operatorname{vec}(\hat{\Pi}_0)' + \hat{\Sigma}_{\Pi_0\Pi_0}] \otimes \tilde{H}_T\} \Gamma_\phi \\ & + \tilde{G}_T' \Gamma_x' \{[\operatorname{vec}(\hat{\Pi}_1) \operatorname{vec}(\hat{\Pi}_0)' + \hat{\Sigma}_{\Pi_1\Pi_0}] \otimes \tilde{H}_T\} \Gamma_\phi \end{aligned} \tag{45}$$

respectively. Notice that in (45) all second population moments were replaced by their sample estimates. The deterministic approach of substituting parameter estimators in the groundwater management model and neglecting their statistical variability is equivalent to setting all the covariances appearing in (41) and (43)–(45) equal to zero.

It has been shown in sections 3 and 4 that both in the open-loop and closed-loop solutions to the management problem, the different assumptions (i.e., classical and Bayesian) lead to a fundamental sign inversion in their respective control solutions. In contrast, the deterministic approach sets all covariances equal to zero, neglecting the statistical variability of parameters. The impact of parameter uncertainty on management solutions in the classical and Bayesian cases is measurable in terms of the covariances of parameter estimators. The following application example illustrates numerically the meaning of the analytical results obtained previously.

5. APPLICATION EXAMPLE

Consider the aquifer shown in Figure 1. Groundwater flow takes place under time-varying boundary conditions and pumping at $x = L/2$ ($L = 2000$ m). The boundary conditions at $x = 0$ and $x = L$ are given by $\phi_A = 80 + t$ and $\phi_B = 100 - t$, respectively. The time index t takes the values $t = 0, 1, 2 \cdots, T$ and the heads are expressed in meters. The initial distribution of heads is linear between the two boundaries of the aquifer. *Loaiciga and Mariño* [1987] applied the method of maximum likelihood based on a set of head values at nodes 1, 2, and 3 to derive groundwater parameter estimators and their covariances (Table 1 of their paper contains the pertinent data) under the classical assumption. Assuming constant transmissivity and storativity throughout the flow domain, their values were estimated as $\hat{T} = 462$ m^2/day and $\hat{S} = 0.0110$, with standard errors of 47.8 m^2/day and 0.00390, respectively. Due to the presence of nonhomogeneous boundary conditions, the flow equation (see equation (9)) was expressed as

$$\boldsymbol{\phi} = \Theta\boldsymbol{\phi}_0 + \Psi\mathbf{x} + \Lambda\mathbf{z} + \mathbf{u} \tag{46}$$

in which the $TM \times 1$ ($M = 4$) vector $\mathbf{z}$ is a function of the boundary conditions and thus known and deterministic [see *Loaiciga and Mariño*, 1987], and Λ is a $TN \times TM$ parameter matrix. The estimates $\hat{T}$ and $\hat{S}$ quoted above and their covariances were used to compute the matrix and covariance estimates (i.e., $\hat{\Psi}$, $\hat{\Sigma}_{\Psi\Psi}$, etc.) needed in the open-loop control expressions. From the developments of section 3 it is straightforward to show that the addition of the vector $\mathbf{z}$ in (46) modifies the control solution only through the gradient, leaving the Hessian matrix unchanged. For completeness, the open-loop control expressions used in this application are

$$\mathbf{x} = -L_{xx}^{-1}\mathbf{L}_x \tag{47}$$

in which

$$L_{xx} = \Gamma_x'\{[\mathrm{vec}\,(\hat{\Psi})\,\mathrm{vec}\,(\hat{\Psi})' \pm \hat{\Sigma}_{\Psi\Psi}] \otimes Q\}\Gamma_x \tag{48}$$

$$\mathbf{L}_x = \Gamma_x'\{[\mathrm{vec}\,(\hat{\Psi})\,\mathrm{vec}\,(\hat{\Theta})' \pm \hat{\Sigma}_{\Psi\Theta}] \otimes Q\}\Gamma_\phi\boldsymbol{\phi}_0 + \Gamma_x'\{[\mathrm{vec}\,(\hat{\Psi})\,\mathrm{vec}\,(\hat{\Lambda})' \pm \hat{\Sigma}_{\Psi\Lambda}] \otimes Q\}\Gamma_z\mathbf{z} \tag{49}$$

where the plus and minus signs in the factors involving sample second moments in (48) and (49) indicate Bayesian and classical solutions, respectively. In (49), $\hat{\Sigma}_{\Psi\Lambda}$ is the estimate of the covariance of vec ($\hat{\Psi}$) with vec ($\hat{\Lambda}$). Notice that the Hessian in (48) has not been modified (compare with equations (29) and (34)), whereas the gradient in (49) includes an additional term accounting for the uncontrollable, known vector $\mathbf{z}$ (the aggregator Γ_z is of size $TNTMTN \times TM$). Since the open-loop and closed-loop solutions are numerically identical, only the former is referred to in this application. The objective is to minimize the sum of squared deviations of the piezometric head at node 2 (where pumping takes place) about a reference value of $\phi_2 = 85$ m. Since there is only one target value, it is possible to decouple and operate only with the heads at node 2 for $t = 1, 2, \cdots, T$ in (46). Hence only rows 2, 5, 8, $\cdots$, $3T - 1$ of (46) are used. The vectors $\boldsymbol{\phi}_0$, $\mathbf{x}$, and $\mathbf{z}$ are not affected by the decoupling processes. Using a time horizon of 20 periods, i.e., $t = 1, 2, \ldots, 20$, the dimensions of the vectors $\boldsymbol{\phi}$, $\boldsymbol{\phi}_0$, $\mathbf{x}$, $\mathbf{z}$, and $\mathbf{u}$ in the decoupled flow equation used in the application are 20×1, 3×1, 20×1, 80×1, and $20 \times$ ∴′ respectively. Notice that there is only one decision variable for each time period. The dimensions of the matrices Θ, Ψ, and Λ are 20×3, 20×20, and 20×80, respectively, in the decoupled equation. Only the 20 rows corresponding to the head values at node 2 have been kept in these matrices, while their column dimensions were not affected by the decoupling procedure. In order to express the objective function in the quadratic form given in (11), one must subtract the 20×1 vector of target heads whose elements are equal to 85 m from both sides of the (decoupled) flow equation. Because of the short time horizon, the weighting matrix Q in (11) was set equal to the identity matrix (of dimensions 20×20), giving equal weight to each squared deviation through the control horizon.

The decision policies were computed for the classical, Bayesian, and deterministic cases and are shown in Figure 2, along with their corresponding temporal head distributions at node 2. Notice that the classical decision policy specified higher pumping rates at early times, driving the head closer to the target than the Bayesian and deterministic policies. However, for $t \geq 10$, the classical decision policy (i.e., pumping) levels off at values lower than the Bayesian and deterministic solutions, and hence its rate of approach to the target head becomes smaller than that exhibited by the other two solutions. The Bayesian solution shows a pattern almost symmetrically opposite to the classical results, i.e., lowest pumping rates at early times and highest rates for $t \geq 10$, thus exhibiting the lowest and highest rates of approach to the target head value for $t < 10$ and $t \geq 10$, respectively, relative to the classical and deterministic policies. The deterministic pumping rates and head distribution lie in between the classical and Bayesian results throughout the entire control horizon. In terms of the total loss associated with each solution, their values were 105.6, 125.8, and 145.3 for the classical, Bayesian, and deterministic policies, respectively. Since the inverse problem was solved under the classical assumption, the classical solution should be viewed as the correct answer in this case. This example illustrates in a clear manner the conceptual findings of sections 3 and 4. Parameter variability and the assumption imposed on the structure of the parameters produce different management solutions and therefore may have an impact on management policies.

6. SUMMARY AND CONCLUSIONS

Closed-loop and open-loop groundwater management solutions have been analytically derived for the optimization of a quadratic objective function subject to the linear system of constraints imposed by the groundwater flow equations. The solutions are of a stochastic nature, in the sense that groundwater parameters are modeled as statistical quantities, both under classical and Bayesian assumptions imposed upon them. The groundwater parameters can be estimated by any method suitable to solve the inverse problem, and even though the estimates and covariance matrices may vary from method to method, one form of the control solutions remains unchanged. It has been shown that classical and Bayesian solutions differ by a sign inversion in those factors involving sample second moment estimates, e.g., Hessian and gradients, whereas the deterministic solution sets the covariances of estimators equal to zero.

One important practical implication of our findings is relevant to actual groundwater management model applications. The classical approach, i.e., groundwater parameters assumed nonrandom and unknown, is widely adopted in the solution of the inverse problem. Typically, the inverse problem is first

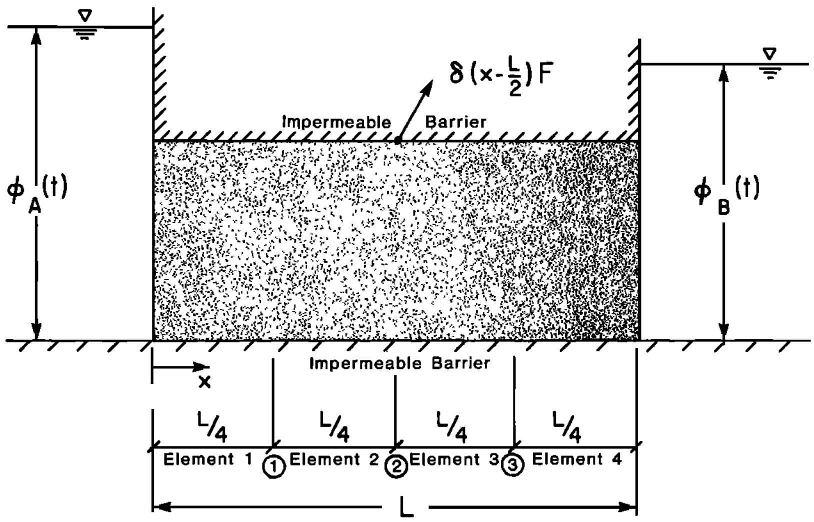

Fig. 1. Confined aquifer subject to time-dependent boundary conditions and a discharge (of units $L^3T^{-1}L^{-1}$) at $x = L/2$.

solved, and subsequently the calibrated parameters are introduced in the management model as deterministic quantities, producing management solutions that are compatible with a deterministic assumption on the parameters, but inconsistent with their original classical interpretation in the solution of the inverse problem. From a practical viewpoint, the consequences of mixing two worlds, i.e., adopting a classical standpoint when solving the inverse problem, but using their values deterministically in a management model, depend upon the covariance of estimators and on the relative importance of various variables that enter in the management model as shown above. In particular, when the covariance of estimators is large, the classical, Bayesian, and deterministic solutions are bound to be significantly different. If the parameter estimates from the solution of the inverse problem are consistent, then their covariances monotonically decrease with the sample size and the classical, Bayesian, and deterministic solutions converge to the same results.

The Bayesian approach is often found in the literature too, and for example, it is frequently assumed that the logarithm of transmissivities follows a Gaussian distribution. If such parameters are used in a groundwater management problem, the results of sections 3 and 4 indicate the role of the Bayesian assumption on groundwater management policies. It was

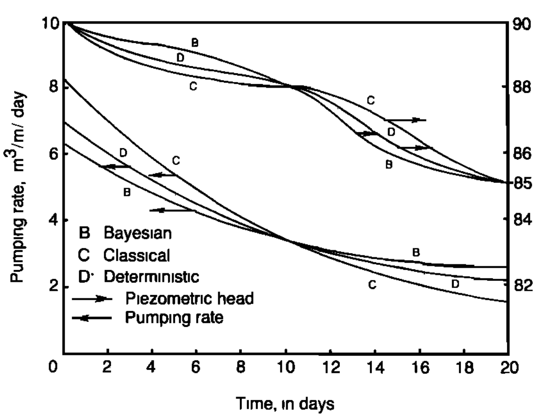

Fig. 2. Classical, Bayesian, and deterministic policies (pumping rates) and head distributions at node 2.

shown that the Bayesian solution leads to a sign inversion in the closed-loop and open-loop solutions to the groundwater management problem when compared to the classical results. Solving the inverse problem under a Bayesian framework and then using parameter estimators deterministically in a management model results in biased policies. The magnitude of such bias is a function of the covariance of parameter estimators.

A numerical example has shown the differences in pumping schedules that are obtained for the same groundwater management problem under the classical, Bayesian, and deterministic assumptions on the parameters. In the example, the inverse problem was solved under the classical assumption, and therefore the corresponding classical solution should be viewed as the correct answer that incidentally produced the minimum loss amongst the three alternative solutions. In complex management problems it is not possible to assess beforehand, i.e., prior to the solution of the problem, which of the three alternative solutions will produce a minimum (under minimization) of the objective function. It is conceivable that the answer obtained by mixing assumptions, e.g., taking a classical viewpoint when solving the inverse problem but adopting a deterministic stance in the management model, could produce values of the objective function that are lower (assuming minimization), for example, than those obtained from a classical solution of the inverse and the groundwater management problems. However, one must realize that mixing worlds, obtaining a classical solution to the inverse problem and then computing deterministic groundwater management solutions, may be computationally expeditious but it is tantamount to solving a management problem (i.e., the deterministic case) that is inherently different from the one conceived prior to the solution of the inverse problem. Further research is needed to fully assess the implications of the classical, Bayesian, and deterministic assumptions within the context of complex management problems. This paper provides a first contribution in that direction.

When parameters are treated deterministically in a groundwater management model, perhaps because of extreme mathematical complexity, the developments of this work indicate the need for using consistent methods to solve the inverse problem and collecting reasonably large samples of field data. In such cases, parameter covariances usually approach small values quickly as the sample sizes increase, yielding management solutions that are likely to be numerically similar to those that would be obtained if groundwater parameters were truly deterministic, i.e., fixed and known. Last, but not least, a recent simulation study by *Tung* [1986], where a Bayesian assumption on the parameters is used, appears to further confirm our theoretical results, indicating the importance of explicitly including the statistical variability of certain parameters (e.g., transmissivity) in groundwater management studies.

APPENDIX: VECTOR-MATRIX OPERATORS

The trace of an $n \times n$ square matrix A is defined as follows:

$$\mathrm{Tr}\,(A) = \sum_{i=1}^{n} a_{ii} \quad \text{(A1)}$$

in which a_{ii} denotes the ith diagonal element of A.

The vec operator stacks successive columns of an $n \times m$ matrix B below one another, i.e.,

$$\mathrm{vec}\,(B) = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_m \end{bmatrix}_{nm \times 1} \quad \text{(A2)}$$

in which $\mathbf{b}_i$ denotes the ith column of B.

The Kronecker or (right) direct product of an $l \times s$ matrix C and an $n \times m$ matrix B is defined as follows:

$$C \otimes B = \begin{bmatrix} c_{11}B \cdots c_{1s}B \\ \vdots \\ c_{l1}B \cdots c_{ls}B \end{bmatrix}_{ln \times sm} \quad \text{(A3)}$$

Several useful identities used throughout the paper are given next. Suppose that C and D are conformable and square matrices, then

$$\mathrm{Tr}\,(CD) = \mathrm{Tr}\,(DC) \quad \text{(A4)}$$

For a square matrix A,

$$\mathrm{Tr}\,(A) = \mathrm{Tr}\,(A') \quad \text{(A5)}$$

For conformable vectors $\mathbf{a}$, $\mathbf{b}$ and matrix A,

$$\mathrm{Tr}\,(\mathbf{a}'A\mathbf{b}) = \mathrm{Tr}\,(\mathbf{b}\mathbf{a}'A) \quad \text{(A6)}$$

$$(d/d\mathbf{b})(\mathbf{a}'A\mathbf{b}) = A'\mathbf{a} \quad \text{(A7)}$$

Let A, B, C, D, F, and I be suitably dimensioned matrices in which I denotes the identify matrix; let $\mathbf{a}$ be a suitably dimensioned vector, then

$$\mathrm{vec}\,(ABC) = (C' \otimes A)\,\mathrm{vec}\,(B) \quad \text{(A8)}$$

$$\mathrm{Tr}\,(ABCDF) = [\mathrm{vec}\,(B')]'[A'F' \otimes C]\,\mathrm{vec}\,(D) \quad \text{(A9)}$$

$$\mathrm{vec}\,(a' \otimes I) = \Gamma_a \mathbf{a} \quad \text{(A10)}$$

In (A10), Γ_a is a matrix aggregator with elements equal to either zero or one, e.g., let $\mathbf{a}' = (a_1, a_2)$ and I be the 2×2 identity matrix, then

$$\mathrm{vec}\,(a' \otimes I) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad \text{(A11)}$$

NOTATION

H_t $N \times N$ recursive matrix in the classical closed-loop solution.
$\tilde{H}_t$ $N \times N$ recursive matrix in the Bayesian closed-loop solution.
I_n $n \times n$ identity matrix.
K dimension of the decision vector for period t.
K^* hydraulic conductivity.
L length of aquifer (m).
L_1 objective function of the management problem.
L^* term of the objective function independent of decision variables.
$\mathbf{L}_x$ $TK \times 1$ gradient vector.
$\tilde{\mathbf{L}}_x$ gradient in the Bayesian solution.
$\hat{\mathbf{L}}_x$ gradient in the classical solution.
L_{xx} $TK \times TK$ Hessian matrix of second derivatives.
$\tilde{L}_{xx}$ Hessian in the Bayesian solution.
$\hat{L}_{xx}$ Hessian in the classical solution.
M_t cost-to-go function in the closed-loop solution.
M_t^* term in the cost-to-go function independent of decision variables.
$\tilde{M}_t$ minimum cost to go at time t.
N dimension of the field variable vector.
Q $TN \times TN$ matrix in the objective function in the open-loop formulation.
Q_t $N \times N$ penalty matrix.
S specific storativity.
T number of periods in the control horizon.
$\mathbf{u}$ $TN \times 1$ error vector.
$\mathbf{u}_t$ $N \times 1$ error vector.
$\mathbf{x}$ $TK \times 1$ decision vector.
$\mathbf{x}_t$ $K \times 1$ decision vector.
$\hat{\mathbf{x}}$ $TK \times 1$ classical decision vector.
$\tilde{\mathbf{x}}$ $TK \times 1$ Bayesian decision vector.
$\mathbf{x}_t^*$ $K \times 1$ optimal closed-loop decision vector.
γ mean of a random parameter.
δ stochastic deviation about the mean of a random parameter.
η sampling error of a parameter estimator.
Γ matrix aggregator.
Θ $TN \times N$ parameter matrix in the open-loop formulation.
$\hat{\Theta}$ estimator of Θ.
$\bar{\Theta}$ expected value of Θ.
Λ $TN \times TM$ parameter matrix.
ξ vector of parameters (unspecified dimension).
Π_0 $N \times N$ parameter matrix.
$\hat{\Pi}_0$ estimator of Π_0.
Π_1 $N \times K$ parameter matrix.
$\hat{\Pi}_1$ estimator of Π_1.

$\Sigma_{\Pi_0\Pi_0}$ $NN \times NN$ covariance matrix of vec ($\hat{\Pi}_0$).
$\hat{\Sigma}_{\Pi_0\Pi_0}$ estimator of $\Sigma_{\Pi_0\Pi_0}$.
$\Sigma_{\Pi_1\Pi_0}$ $NK \times NN$ covariance matrix of vec ($\hat{\Pi}_1$) with vec ($\hat{\Pi}_0$).
$\hat{\Sigma}_{\Pi_1\Pi_0}$ estimator of $\Sigma_{\Pi_1\Pi_0}$.
$\Sigma_{\Psi\Psi}$ $TNTK \times TNTK$ covariance matrix of vec ($\hat{\Psi}$).
$\hat{\Sigma}_{\Psi\Psi}$ estimator of $\Sigma_{\Psi\Psi}$.
$\Sigma_{\Psi\Theta}$ $TNTK \times TNN$ covariance matrix of vec ($\hat{\Psi}$) with vec ($\hat{\Theta}$).
$\hat{\Sigma}_{\Psi\Theta}$ estimator of $\Sigma_{\Psi\Theta}$.
$\Sigma_{\Psi\Lambda}$ $TN \times TM$ covariance matrix of vec ($\hat{\Psi}$) with vec ($\hat{\Lambda}$).
$\hat{\Sigma}_{\Psi\Lambda}$ estimator of $\Sigma_{\Psi\Lambda}$.
$\boldsymbol{\phi}_t$ $N \times 1$ vector of piezometric heads for period t.
$\boldsymbol{\phi}$ $TN \times 1$ vector of piezometric heads.
Ψ $TN \times TK$ parameter matrix in the open-loop formulation.
$\bar{\Psi}$ expected value of Ψ.
$(\ )'$ transpose of a vector or matrix.

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