THE KALMAN SMOOTHER APPROACH TO THE STOCHASTIC INVERSE PROBLEM OF GROUNDWATER HYDROLOGY

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ABSTRACT

In this paper we are concerned with the estimation of the hydraulic conductivity profile on the basis of noisy observations of hydraulic heads. An augmented Kalman smoother is applied to the stochastic flow equation. The implementation of the smoother requires the solution of a Riccati type partial differential equation for the smoother covariance and a stochastic partial differential equation to obtain the optimal estimate of the augmented state. We discuss finite dimensional approximations of the smoothing problem and propose an EM algorithm for the estimation of the conductivity parameters.

1. INTRODUCTION

We consider a groundwater flow through a porous, heterogenous, isotropic medium which is modeled by the continuity equation

$$S\frac{\partial h}{\partial t} + \nabla \cdot \mathbf{q} = s(t,\mathbf{x}) + \xi(t,\mathbf{x}) \tag{1}$$

and Darcy's law

$$\mathbf{q} = -K\nabla h$$

where $h=$ hydraulic head, $\mathbf{q}=$ fluid velocity vector, $S=$ specific storage coefficient, $K=$ hydraulic conductivity, $s=$ deterministic source term and $\xi=$ stochastic forcing term. Equations (1) and (2) can be combined to give a stochastic partial differential equation (SPDE) for the hydraulic head

$$S\frac{\partial h}{\partial t} = \nabla \cdot (K\nabla h) + s(t,x) + \xi(t,x). \tag{2}$$

The equation may be adapted to 1D, 2D or 3D-flow, subject to some initial and boundary conditions.

The hydraulic conductivity K is a measure how freely the fluid is flowing in the medium. Since the medium is heterogenous, the hydraulic conductivity depends on the position $\mathbf{x}$. The lack of information about $K(\mathbf{x})$ makes it natural to represent it as a *random field.* Freeze [1975] discovered that $Y(\mathbf{x}) = \log K(\mathbf{x})$ is close to a Gaussian field. This observation was supported by the work of Hoeksema and Kitanidis [1985]. In the simplest case the log-conductivity is a stochastically homogeneous and isotropic Gaussian random field, which can be written as

$$Y(\mathbf{x}) = \mu_{\mathbf{Y}} + \widetilde{\mathbf{Y}}(\mathbf{x}), \tag{3}$$

where $\mu_Y = E[Y(\mathbf{x})]$ and $\widetilde{Y}(\mathbf{x})$ is the fluctuation part with $E[\widetilde{Y}(\mathbf{x})] = 0$. In the literature, the following covariance function is often used to represent the spatial variability of hydraulic conductivity:

$$R(\mathbf{x},\mathbf{x}') = \sigma_Y^2 \exp\left[-\frac{|\mathbf{x}-\mathbf{x}'|}{l_Y}\right]. \tag{4}$$

σ_Y^2 is the variance of Y and l_Y the correlation length.

We assume the stochastic forcing term $\xi(t,\mathbf{x})$ representing the modeling error is a distributed Gaussian white noise process with the following properties:

$$\begin{aligned} E[\xi(t,\mathbf{x})] &= 0 \\ E[\xi(t,\mathbf{x})\,\xi(t',\mathbf{x})] &= Q(t,\mathbf{x},\mathbf{x}')\delta(t-t'). \end{aligned} \tag{4}$$

Then the hydraulic heads $h(t,\mathbf{x})$ are also random. We define $\bar{h}(t,\mathbf{x}) = E[h(t,\mathbf{x})]$ and $\widetilde{h}(t,\mathbf{x}) = h(t,\mathbf{x}) - \bar{h}(t,\mathbf{x})$. Neclecting nonlinear terms Dagan [1] obtained the following equation

$$S\frac{\partial \bar{h}}{\partial t} = k_G \nabla^2 \bar{h} + s(t,\mathbf{x}) \tag{5}$$

with $k_G = e^{\mu_Y}$ subject to the same initial and boundary conditions as equation (3). The linearized evolution equation for the head fluctuations is

$$S\frac{\partial \widetilde{h}}{\partial t} = k_G(\nabla^2 \widetilde{h} + \nabla \cdot (\bar{h}(t,\mathbf{x})\widetilde{Y}(\mathbf{x})) + \xi(t,\mathbf{x}) \tag{6}$$

with the homogenous boundary condition

$$\widetilde{h}(t,\mathbf{x}) = 0, \qquad \mathbf{x} \in \partial D, \tag{7}$$

and the initial condition

$$\widetilde{h}(0,\mathbf{x}) = \zeta(\mathbf{x}), \tag{8}$$

where $\zeta(x)$ also is Gaussian noise with $E[\zeta(x)] = 0$ and the covariance function $P_0(\mathbf{x},\mathbf{x}') = E[\zeta(\mathbf{x})\zeta(\mathbf{x}')]$.

An important task is the estimation of the unknown values of μ_Y, σ_Y^2 and l_Y. Usually only few measured values of the conductivity are available, which cannot provide reliable estimates of the unknown parameters. Therefore estimation has to be based on the measurements of the heads. For this task we augment the state space by adjunction of the auxiliar equation

$$\frac{\partial f}{\partial t} = 0 \tag{9}$$

with the initial condition

$$f(0,\mathbf{x}) = \check{Y}(\mathbf{x}) := \widetilde{Y}(\mathbf{x})/\sigma_Y. \tag{10}$$

We rewrite eqs. (6) and (9) using the augmented state vector $\mathbf{u} = (\widetilde{h}, f)^T$

$$\frac{\partial \mathbf{u}}{\partial t} = A(t,\mathbf{x})\mathbf{u}(t,\mathbf{x}) + \frac{1}{S}\xi_{\mathbf{u}}(t,x), \tag{11}$$

where $\xi_{\mathbf{u}} = (\xi, 0)^T$ and

$$A(t,\mathbf{x}) = \frac{k_G}{S}\begin{pmatrix} \nabla^2 & \sigma_Y \nabla \cdot \nabla \bar{h}(t,\mathbf{x}) \\ 0 & 0 \end{pmatrix}.$$

Let us assume that the head measurements are taken at fixed points $\mathbf{x}_1^*, ..., \mathbf{x}_m^*$. If the measurement times are fast relative to the characteristic groundwater flow evolution time and are well modeled by a *continuous measurement* process. We define a m-vector $\mathbf{h}_m(t) = (h(t,\mathbf{x}_1^*), ..., h(t,\mathbf{x}_m^*))^T$. Then, the measurement process is given by

$$\mathbf{z}(t) = \mathbf{h}_m(t) + \eta(t), \tag{12}$$

where $\eta(t)$ is the measurement noise, a m-dimensional Gaussian white noise stochastically independent of $\xi(t,\mathbf{x})$ and $\zeta(\mathbf{x})$. Since we have a linear state equation and Gaussian system-and measurement noise, we are in the realm of the Kalman filter. Since we are concerned with an off-line problem, we shall use fixed interval Kalman smoother. The augmented Kalman smoother is applied to the state equation (11). The implementation of the smoother requires the solution of a Riccati differential equation for the smoother covariance and a stochastic linear differential equation to obtain the optimal estimate of the augmented state. For the details we refer to the paper of Riedel [1994] and the monography of Omatu and Seinfeld [1989].

2. NUMERICAL IMPLEMENTATION

Since the state space of a SPDE is an infinite-dimensional function space a finite-dimensional approximation is required. Following Seinfeld and Koda [1978] two ways are possible. The d.p.s. can be approximated by a lumped parameter system at the very beginning of the problem. Then we use the conventional estimation theory for finite-dimensional systems. Seinfeld and Koda called this approach *approximation at the beginning*. On the other hand, the distributed character of the problem can be retained throughout the analysis, and only at the point where numerical implementation of the p.d.e.s is necessary, a discretization is introduced. This approach was termed *approximation at the end*. Since no fundamental advantage exist for either approach, we use the first one.

We construct a *Galerkin approximation* to (6) and (9) as follows. An approximation $\widetilde{h}_N$ is sought in the form

$$\widetilde{h}_N(t,\mathbf{x}) = \sum_{n=1}^{N} H_n(t)\phi_n(\mathbf{x}), \tag{13}$$

where $\{\phi_n(\mathbf{x})\}$ is a set of basis functions, satisfying the boundary conditions (7). If the domain is subdivided into triangular elements and ϕ_n is taken as a shaping function, the procedure is the finite element method.

The random field $\check{Y}(\mathbf{x})$ may be approximated by a truncated Karhunen-Loeve expansion

$$\check{Y}_P(\mathbf{x}) = \sum_{n=1}^{P} \sqrt{\lambda_n}\psi_n(\mathbf{x})\,\varepsilon_n$$

(see the Appendix). Since $f(0,\mathbf{x}) = \check{Y}(\mathbf{x})$ we get the Galerkin approximation

$$f_P(t,\mathbf{x}) = \sum_{n=1}^{P} F_n(t)\psi_n(\mathbf{x}), \tag{14}$$

where $F_n(0) = \sqrt{\lambda_n}\,\varepsilon_n$.

We use the inner product notation of functions

$$(f|g) = \int_D f(\mathbf{x})g(\mathbf{x})\,d\mathbf{x}.$$

We set $\theta_1 = k_G$ and $\theta_2 = \sigma_Y k_G$. The third parameter, which appears only in (4) is set to $\theta_3 = 1/l_Y$. The expansions coefficients $H_n(t)$ and $F_n(t)$ are determined by the Galerkin equations (Seinfeld and Koda [9])

$$\begin{aligned}\sum_{m=1}^{N}(\phi_n|\phi_m)\frac{dH_m(t)}{dt} = \frac{\theta_1}{S}\sum_{m=1}^{N}(\phi_n|\phi_m'')H_m(t)+&\\ +\frac{\theta_2}{S}\sum_{m=1}^{P}[(\phi_n|\psi_m'\bar{h}_x(t)) + (\phi_n|\psi_m\bar{h}_{xx}(t))]F_m(t)+&\\ +\frac{1}{S}(\phi_n|\xi(t))&\end{aligned} \tag{15}$$

and

$$\sum_{m=1}^{P}(\psi_p|\psi_m)\frac{dF_m(t)}{dt} = 0, \tag{16}$$

$n = 1,\dots,N$, $p = 1,\dots,P$.

When the basis functions (ϕ_n) and (ψ_p) are orthogonal, (15) and (16) reduces to a linear system of ordinary differential equations of the form:

$$\begin{aligned}\frac{dH_m}{dt} &= \theta_1 a_m H_m(t) + \theta_2\sum_{n=1}^{P} b_{mn}F_n(t) + c_n\dot{W}_m(t)\\ \frac{dF_p}{dt} &= 0\end{aligned} \tag{17}$$

where $\dot{W}_1(t), \ldots, \dot{W}_N(t)$ denotes N-dimensional standard white noise. The coefficients in (17) are

$$\begin{aligned} a_n &= (\phi_n|\phi_n'')/S \\ b_{mn} &= ((\phi_n|\psi_m'\bar{h}_x(t)) + (\phi_n|\psi_m\bar{h}_{xx}(t))/S \\ c_n &= \sqrt{(\phi_n|\xi(t))}/S \end{aligned}$$

Using vector-matrix notation the augmented state

$$\mathbf{U} = (H_1, \ldots, H_N, F_1, \ldots, F_P)^T$$

satisfy a state equation of the form

$$\frac{d\mathbf{U}}{dt} = \widetilde{A}\mathbf{U}(t) + \widetilde{C}\widetilde{\mathbf{W}}(t) \tag{18}$$

The system matrices $\widetilde{A}$ and $\widetilde{C}$ are easily identified from (15) and (16). Assuming the availability of measurements given by equation (12), the conventional Kalman filter and Kalman smoother may be applied to (18).

3. ESTIMATION OF THE CONDUCTIVITY PARAMETERS - THE EM ALGORITHM

For the calibration of a groundwater model the conductivity parameters are to be estimated indirectly from the head measurements. So we are faced with a parameter estimation problem with partial observations. In this situation two approaches are possible:

i. The direct approach, where the likelihood function itself is computed and maximized
ii. the EM algorithm combined with Kalman smoothing as investigated by Dembo and Zeitouni [1986].

The first approach uses analytic expressions for the likelihood ratio of the measurement process with respect to a Wiener measure (the measure of some Brownian motion), which can be found e.g. in Liptser and Shiryayev [1978,chap. 7]. The evaluation of the likelihood ratio and its maximization with respect to the unknown parameters is somewhat difficult. This difficulties can be circumvented by the *Expectation Maximation algorithm* (EM algorithm), which generates a maximizing sequence of estimates in the sense that the corresponding sequence of likelihood function values is monotone increasing. We give now a short description of the estimation algorithm in the case of continuous-time measurements.

Let $L(t_f;\theta)$ denote the *full* likelihood and $l(Z_0^{t_f};\theta)$ the log-likelihood based on observations $Z_0^{t_f} = (\mathbf{z}(t); 0 \leq t \leq t_f)$ only. For two admissible parameter values θ and θ' we obtain by Jensen's inequality

$$l(Z_0^{t_f};\theta) - l(Z_0^{t_f};\theta') = \log E_{\theta'}\left[\frac{L(t_f;\theta)}{L(t_f;\theta')}|Z_0^{t_f}\right] \geq E_{\theta'}\left[\log\frac{L(t_f;\theta)}{L(t_f;\theta')}|Z_0^{t_f}\right].$$

The quantity

$$\mathcal{Q}(\theta,\theta') := E_{\theta'}\left[\log\frac{L(t_f;\theta)}{L(t_f;\theta')}|Z_0^{t_f}\right],$$

called *pseudo-likelihood*. We have

$$l(t_f;\theta) - l(t_f;\theta') \geq \mathcal{Q}(\theta,\theta')$$

with $\mathcal{Q}(\theta,\theta) = 0$.

Setting $\theta' = \widehat{\theta}_k$ as the current of θ after k iteration cycles, we have the inequality

$$l(Z_0^{t_f};\widehat{\theta}_{k+1}) \geq l(Z_0^{t_f};\widehat{\theta}_k) + \mathcal{Q}(\widehat{\theta}_{k+1},\widehat{\theta}_k) \geq l(Z_0^{t_f};\widehat{\theta}_k)$$

where $\widehat{\theta}_{k+1} = \mathrm{argmax}_\theta\, \mathcal{Q}(\theta,\widehat{\theta}_k)$ is the maximizer of the pseudo-likelihood. This defines the EM algorithm, whose iterations are described by the following steps

1. Set k=0, choose an initial guess $\widehat{\theta}_0$
2. set $\theta' = \widehat{\theta}_k$,
3. (E-step) compute $\mathcal{Q}(.,\theta')$,
4. (M-step) find $\widehat{\theta}_{k+1} = \arg\max_\theta \mathcal{Q}(\theta,\theta')$
5. if a stopping rule is satisfied, then set final estimate $\widehat{\theta} = \widehat{\theta}_{k+1}$, else repeat from step 2 with $k <= k+1$.

Using eq.(17) and general formulae from Liptser, Shiryayev [1978, chap. 7] we get an expression for the likelihood ratio of the Galerkin approximation $\mathbf{u}_{N,P}(t,x) := (\widetilde{h}_N(t,x), f_P(t,x))^T$

$$
\begin{aligned}
L(t_f;\theta) = \exp \sum_{m=1}^{N} \frac{1}{c_m^2} \Bigg[& \int_0^{t_f} \left(\theta_1 a_m H_m(t) + \theta_2 \sum_{n=1}^{P} b_{mn} F_n(t) \right) dH_m(t) \\
& - \frac{1}{2} \int_0^{t_f} \left(\theta_1 a_m H_m(t) + \theta_2 \sum_{n=1}^{P} b_{mn} F_n(t) \right)^2 dt \Bigg] .
\end{aligned} \tag{21}
$$

Since the initial state $h_0(x)$ is independent of θ the log density ratio of the initial state vector $\mathbf{u}_{N,P}(0)$ reduces to the log density ratio of $F_1(0),\ldots,F_P(0)$, which depends on θ_3 only. Using the notations of the appendix it takes the form

$$
\frac{1}{2} \sum_{n=1}^{P} \log \frac{\lambda_n(\theta')}{\lambda_n(\theta)} - F_n(0)^2 [\lambda_n(\theta)^{-1} - \lambda_n(\theta')^{-1}], \tag{22}
$$

where terms independent of θ were discarded.

Summing up (21) and (22) and taking the conditional expectation $E_{\theta'}[.|Z_0^{t_f}]$ we obtain the pseudo-likelihood

$$
\begin{aligned}
\mathcal{Q}(\theta,\theta') = {} & \theta_1 E_1(\theta') + \theta_2 E_2(\theta') - \frac{1}{2}\theta_1^2 E_3(\theta') - \frac{1}{2}\theta_2^2 E_4(\theta') - \theta_1\theta_2 E_5(\theta') \\
& + \mathcal{Q}_{IC}(\theta_3,\theta_3')
\end{aligned} \tag{23}
$$

where

$$
\begin{aligned}
E_1(\theta') &= \sum_{m=1}^{N} \frac{a_m}{c_m^2} E_{\theta'}[\int_0^{t_f} H_m(t)\, dH_m(t) | Z_0^{t_f}] \\
E_2(\theta') &= \sum_{m=1}^{N} \sum_{n=1}^{P} \frac{b_{mn}}{c_m^2} E_{\theta'}[\int_0^{t_f} F_n(t)\, dH_m(t) | Z_0^{t_f}] \\
E_3(\theta') &= \sum_{m=1}^{N} \frac{a_m^2}{c_m^2} \int_0^{t_f} E_{\theta'}[H_m^2(t) | Z_0^{t_f}]\, dt \\
E_4(\theta') &= \sum_{m=1}^{N} \frac{1}{c_m^2} \int_0^{t_f} E_{\theta'} \left[\left(\sum_{m=1}^{P} b_{mn} F_n(t) \right)^2 | Z_0^{t_f} \right] dt \\
E_5(\theta') &= \sum_{m=1}^{N} \sum_{n=1}^{P} \frac{a_m b_{mn}}{c_m^2} \int_0^{t_f} E_{\theta'} \left[H_m(t) F_n(t) | Z_0^{t_f} \right] dt
\end{aligned}
$$

and

$$
\mathcal{Q}_{IC}(\theta_3,\theta_3') = \frac{1}{2} \sum_{n=1}^{P} \log \frac{\lambda_n(\theta_3')}{\lambda_n(\theta_3)} - E_{\theta'} \left[F_n(0)^2 | Z_0^{t_f} \right] [\lambda_n(\theta_3)^{-1} - \lambda_n(\theta_3')^{-1}].
$$

The pseudo-likelihood (101) is a modification of the expressions (3.5-6) in [*Dembo, Zeitouni*,1986] to our context. It is quadratic in θ_1 and θ_2, but the dependence of θ_3 is quite complicated. With respect to θ_1,θ_2 the execution of the M step is trivial (a linear equation system in θ_1,θ_2), maximation with respect to θ_3 involves a (one-dimensional) search procedure. The evaluation of the expressions $E_i(\theta'), i = 4,5,6$ involves smoothed first and second moments, to be obtained by *Kalman smooothing*. Because of the appearence of the stochastic integrals (Ito integrals) the evaluation of $E_i(\theta'), i = 1,2$ is more cumbersome. E.g. for $E_1(\theta')$ we use a Riemann sum approximation

$$\int_0^{t_f} H_m(t)\, dH_m(t) \simeq \sum_k H_m(t_k)[H_m(t_{k+1} - H_m(t_k)]$$

Taking the conditional expectation we obtain

$$\begin{aligned} &E_{\theta'}[\int_0^{t_f} H_m(t)\, dH_m(t)|Z_0^{t_f}] \\ &\simeq \sum_k \Big(E_{\theta'}[H_m(t_k)H_m(t_{k+1})|Z_0^{t_f}] - E_{\theta'}[H_m(t_k)^2|Z_0^{t_f}]\Big) \end{aligned}$$

To compute the conditional expectation

$$E_{\theta'}[H_m(t_k)[H_m(t_{k+1})|Z_0^{t_f}]$$

we introduce an augmented state vector $\Xi_{m,k} = (H_m(t_k), H_m(t_{k+1}))^T$ and by use of the formula

$$\begin{aligned} &E_{\theta'}[H_m(t_k)[H_m(t_{k+1})|Z_0^{t_f}] \\ &= \mathrm{Cov}(H_m(t_k), H_m(t_{k+1})|Z_0^{t_f}) + E_{\theta'}[H_m(t_k)|Z_0^{t_f}]E_{\theta'}[H_m(t_{k+1})|Z_0^{t_f}] \end{aligned}$$

it is sufficient to implement this augmented Kalman smoother for the conditional covariance only. This device appears in Singer [1993].

4. CONCLUSION

In this paper, we have presented an application of the augmented Kalman smoother to the stochastic inverse problem in groundwater hydrology. It has been applied to a linearized form of the flow equation augmented by a stochastic forcing term representing the model error. We have outlined the estimation of the conductivity parameters by an extension of the EM algorithm.

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APPENDIX: KARHUNEN-LOEVE EXPANSION

We consider a random function (r.f.) $Y(\mathbf{x},\omega)$ defined on a probability space $(\Omega,\mathbf{F},P)$ and indexed by a bounded domain D, $D\subset \mathrm{I\!R}^d$. Thus for each $\mathbf{x}\in D$, $Y(\mathbf{x},.)$ is a random variable and for each $\omega\in\Omega$, $Y(.,\omega)$ is a realization of the r.f. We shall assume that the r.f. has a zero mean and a finite variance, i.e. $E[Y(\mathbf{x})]=0$, and $E[Y^2(\mathbf{x})]<\infty$.

The Karhunen-Loeve expansion of $Y(\mathbf{x})$ is a representation of form

$$Y(x,\omega)=\sum_{n=1}^{\infty}\sqrt{\lambda_n}\psi_n(x)\varepsilon_n(\omega) \qquad (A.1)$$

where (ε_n) is an orthonormal sequence of r.v., λ_n and ψ_n refer to the eigenvalues and eigenfunctions of the covariance operator of the r.f.

Let $R(\mathbf{x},\mathbf{x}')$ denote the covariance function of $Y(x)$, i.e.

$$R(\mathbf{x},\mathbf{x}')=E[Y(\mathbf{x})Y(\mathbf{x}')].$$

It has the spectral decomposition

$$R(x,x')=\sum_{n=1}^{\infty}\lambda_n\psi_n(x)\psi_n(x'),\quad \lambda_n>0, \qquad (A.2)$$

where λ_n and ψ_n denote the the eigenvalues and normalized eigenfunctions of the Fredholm integral equation

$$\int C(x,x')\psi_n(x')\,dx'=\lambda_n\psi_n(x),\qquad \int\psi_m(x)\psi_n(x)\,dx=\delta_{mn},$$

respectively. Many terms in (A.2) may be required,to reproduce the covariance function accurately. On the other hand the physical system to be modelled may act as a bandpass filter, eliminating the effect of the discarded terms. Therefore, in many cases, a good approximation may be achieved, even for

$$Y_P(x,\omega)=\sum_{n=1}^{P}\sqrt{\lambda_n}\psi_n(x)\varepsilon_n(\omega),$$

with a relatively small truncation number P.

In the main text we are concerned with a homogenous zero-mean r.f. $\check{Y}$ having the covariance function (4). In the one-dimensional case $D=[0,L]$ we have

$$\psi_n(x)=(2/(L++\lambda_n)^{1/2}\sin[\omega_n(x-L/2)+n\pi/2],$$
$$\lambda_n=2\theta/(\theta^2+\omega_n^2),\quad n=1,2,\ldots$$

where $\theta=1/l_Y$ and ω_n is a positive root of the equation

$$\tan\omega L=-2\theta\omega/(\theta^2-\omega^2).$$