Characterization of heterogeneous hydraulic conductivity field via Karhunen-Loève expansions and a measure-theoretic computational method

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Specification of a variety of parameters, such as hydraulic conductivity, is required in models that have been widely used to analyze groundwater systems and contaminant transport. However, it is practically impossible to characterize the model parameters exhaustively due to the complex hydrogeological environment. For this reason, inverse modeling is needed to identify input parameters by incorporating observed model responses, e.g., hydraulic conductivities are derived based on observed hydraulic head.

Given uncertain hydraulic head data from observation wells, the stochastic inverse problem is solved numerically to obtain a probability measure on the space of unknown parameters characterizing the heterogeneity of the hydraulic conductivity field.
Overview

1. Introduction

2. Parameterization
   - Karhunen-Loève expansions

3. Inverse Estimation
   - Measure-theoretic framework

4. Illustrative example
   - Synthetic problem
Groundwater flow equation

\[ S \frac{\partial h(x, t)}{\partial t} + \nabla \cdot q(x, t) = g(x, t) \]  
(1)

\[ q(x, t) = -K(x) \nabla h(x, t) \]  
(2)

subject to initial and boundary conditions

\[ h(x, 0) = H_0(x), \quad x \in D \]  
(3)

\[ h(x, t) = H(x, t), \quad x \in \Gamma_D \]  
(4)

\[ q(x, t) \cdot n(x) = Q(x, t), \quad x \in \Gamma_N \]  
(5)

where \( S \) is specific storage \((LT^{-1})\), \( h \) is hydraulic head \((L)\), and \( g \) is source or sink \((T^{-1})\).
Inverse problems are often ill-posed. Inverse estimation of permeability fields is commonly performed by reducing the number of original unknowns of a heterogeneous hydraulic conductivity field to a smaller group of unknowns. This makes the inverse problem better posed by reducing redundancy while capturing the most important features of the field. The Karhunen-Loeve Expansion (KLE) is a classical option for deriving low-dimensional parameterizations for inverse estimation applications [1]. With the knowledge of the property covariance function, the KLE can provide an accurate characterization of a complex field.

"In the theory of stochastic processes, the Karhunen-Loève theorem (named after Kari Karhunen and Michel Loève), also known as the Kosambi-Karhunen-Love theorem is a representation of a stochastic process as an infinite linear combination of orthogonal functions..." (wikipedia)
Let \( Y(x, \omega) = \ln[K(x, \omega)] \) be a random process, where \( K \) is the hydraulic conductivity, \( x \) is the position vector defined over the domain \( D \), and \( \omega \) belongs to the space of random events \( \Omega \). Let \( \bar{Y}(x) \) denote the expected value of \( Y(x, \omega) \) over all possible realizations of the process, and \( C(x_1, x_2) \) denote its covariance function. Being an autocovariance function, \( C(x_1, x_2) \) is bounded, symmetric, and positive definite. Thus, it has the spectral decomposition

\[
C(x_1, x_2) = \sum_{n=1}^{\infty} \lambda_n f_n(x_1) f_n(x_2) \quad (Mercer's Thm) \tag{6}
\]

where \( \lambda_n \) and \( f_n(x) \) are the solutions to the homogeneous Fredholm integral equation of the second kind:

\[
\int_D C(x_1, x_2) f_n(x_1) dx_1 = \lambda_n f_n(x_2). \tag{7}
\]
The eigenfunctions are orthogonal and form a complete set. They can be normalized according to the following criterion

\[ \int_{\Omega} f_n(x)f_m(x) = \delta_{nm}. \]  

(8)

Hence, \( Y(x, \omega) \) can be written as

\[ Y(x, \omega) = \bar{Y}(x) + \sum_{n=1}^{\infty} \xi_n(\omega) \sqrt{\lambda_n} f_n(x), \quad \text{(Karhunen–Loeve Thm)} \]  

(9)

where \( \{\xi_n(\omega)\} \) is a set of random variables to be determined. The KLE of a Gaussian field has the further property that \( \xi_n(\omega) \) are independent standard normal random variables (Itô-Nisio Theorem). Truncating the series in Eq (9) at the \( N^{th} \) term, gives

\[ Y(x, \omega) = \bar{Y}(x) + \sum_{n=1}^{N} \xi_n(\omega) \sqrt{\lambda_n} f_n(x). \]  

(10)
Inverse estimation

\[ Y(x, \omega) = \bar{Y}(x) + \sum_{n=1}^{N} \xi_n(\omega) \sqrt{\lambda_n} f_n(x). \]  

(11)

The KLE provides a flexible and effective method for describing a spatially distributed hydraulic conductivity field. It represents the uncertain hydraulic conductivity field as weighted sums of predefined spatially variable basis functions. The random variables \( \xi_n \) in basis function weights will be quantified with a recently developed measure-theoretic framework.

The stochastic inverse estimation in this characterization of a heterogeneous hydraulic conductivity field problem is to determine a probability measure on \( \xi_n \) (input parameters) such that mapping this probability measure through the model produces the same probability measure as the one defined on the observable hydraulic head.
Inverse problem

Figure: Illustrations of the inverse problem for a general two-to-one map. Left: The set-valued inverse of a single output value. Middle: The representation of $L$ as a transverse parameterization. Right: A probability measure described as a density on $D$ maps uniquely to a probability density on $L$. Figures adopted from [2]

\[
P_L(A) = \int_A \rho_L \, d\mu_L = \int_{Q_L(A)} \rho_D \, d\mu_D = P_D(Q_L(A))
\]
To calculate the probability of more arbitrary events in $\Lambda$, we make use of the Disintegration Theorem and a standard ansatz to compute a probability measure $P_\Lambda$ in terms of an approximate density $\rho_\Lambda$ that is consistent with $P_\mathcal{D}$. By saying $P_\Lambda$ is consistent with $P_\mathcal{D}$, we mean that if $B$ is any event in $\mathcal{D}$ (so $Q^{-1}(B)$ is a generalized contour event in $\Lambda$), then

$$\int_{Q^{-1}(B)} \rho_\Lambda(\lambda) d\mu_\Lambda = P_\Lambda(Q^{-1}(B)) = P_\mathcal{D}(B) = \int_B \rho_\mathcal{D} d\mu_\mathcal{D}. \quad (13)$$
Suppose the probability density function $\rho_\mathcal{D}$ associated with $P_\mathcal{D}$ is known. Let $\{D_k\}_{k=1}^M$ be a partition of $\mathcal{D}$, and let $p_k$ be the probability of $D_k$. Let $A$ be an event in $\Lambda$. We thus have the approximation

$$\int_{Q(A)} \rho_\mathcal{D} d\mu_\mathcal{D} \approx \sum_{D_k \subset Q(A)} p_k. \quad (14)$$

Let $\{\lambda^{(j)}\}_{j=1}^N$ be a collection of $N$ points in $\Lambda$, which implicitly defines an $n$-dimensional Voronoi tessellation $\{\mathcal{V}_j\}_{j=1}^N$ associated with the points. For example, given $\lambda \in \Lambda$, $\lambda \in \mathcal{V}_k$ if $\lambda^{(k)}$ is the closest $\lambda^{(j)}$ to $\lambda$. Using the implicitly defined Voronoi tessellation and the partitioning of $\mathcal{D}$, we can calculate the probability $p_{\Lambda,j}$ associated with the implicitly defined Voronoi cell $\mathcal{V}_j$. Then we can approximate the probability of any event $A \subset \Lambda$ using a counting measure

$$P_{\Lambda}(A) \approx P_{\Lambda,N}(A) = \sum_{\lambda^{(j)} \in A} p_{\Lambda,j}. \quad (15)$$
Algorithm:

- Choose points \( \{\lambda^{(j)}\}_{j=1}^N \in \Lambda \).
- Denote the associated Voronoi tessellation \( \{V_j\}_{j=1}^N \subset \Lambda \).
- Evaluate \( Q_j = Q(\lambda^{(j)}) \) for all \( \lambda^{(j)} \), \( j = 1, \ldots, N \).
- Choose a partitioning of \( D \), \( \{D_k\}_{k=1}^M \subset D \).
- Compute \( p_k \approx \int_{D_k} \rho_D d\mu_D \), for \( k = 1, \ldots, M \).
- Let \( C_k = \{j | Q_j \in D_k\} \) for \( k = 1, \ldots, M \).
- Let \( O_j = \{k | Q_j \in D_k\} \), for \( j = 1, \ldots, N \).
- Let \( V_j \) be the approximate measure of \( V_j \), i.e. \( V_j \approx \int_{V_j} d\mu(V_j) \) for \( j = 1, \ldots, N \).
- Set \( p_{\Lambda,j} = (V_j / \sum_{i \in O_j} V_i) p_{D,O_j} \), \( j = 1, \ldots, N \).
Figure: The domain with observation wells shown as red dots
Forward model

\[
\nabla \cdot \mathbf{q}(x) = 0 \quad (16)
\]

\[
\mathbf{q}(x) = -K(x)\nabla h(x) \quad (17)
\]

subject to boundary conditions

\[
\begin{align*}
    h(x) &= H(x), \quad x \in \Gamma_D \\
    \mathbf{q}(x) \cdot \mathbf{n}(x) &= Q(x), \quad x \in \Gamma_N
\end{align*}
\] 

\[
\begin{align*}
    h(x) &= H(x), \quad x \in \Gamma_D \\
    \mathbf{q}(x) \cdot \mathbf{n}(x) &= Q(x), \quad x \in \Gamma_N
\end{align*}
\] 

(18) 

(19)
Special types of covariance functions

\[ C(x_1, y_1) = \sigma^2 \exp\left(-\frac{|x_1 - y_1|}{\eta_1}\right) \]

Eigenvalues and eigenfunctions of a covariance function can be solved from the following Fredholm equation:

\[ \int_D C(x_1, x_2) f_n(x_1) \, dx_1 = \lambda_n f_n(x_2) \tag{20} \]

\( \lambda_n \) and \( f_n(x) \) can be found analytically:

\[ \lambda_n = \frac{2\eta\sigma^2}{\eta^2 w_n^2 + 1} \tag{21} \]

\[ f_n(x) = \frac{1}{\sqrt{(\eta^2 w_n^2 + 1)L/2 + \eta}} \left[ \eta w_n \cos(w_n x) + \sin(w_n x) \right] \tag{22} \]

where \( w_n \) are positive roots of the characteristic equation

\[ (\eta^2 w^2 - 1)\sin(wL) = 2\eta w \cos(wL). \]
For problems in multidimension, if the covariance function is separable, for example, 
\[ C(x, y) = C(x_1, x_2; y_1, y_2) = \sigma^2 \exp \left[ -\frac{|x_1-y_1|}{\eta_1} - \frac{|x_2-y_2|}{\eta_2} \right] \]
(Gaussian random field with the exponential covariance function) for a rectangular domain 
\[ D = \{(x_1, x_2) : 0 \leq x_1 \leq L_1, 0 \leq x_2 \leq L_2\} \]
Eq.(20) can be solved independently for \( x_1 \) and \( x_2 \) directions to obtain 
eigenvalues \( \lambda_n^{(1)} \) and \( \lambda_n^{(2)} \), and eigenfunctions \( f_n^{(1)}(x_1) \) and \( f_n^{(2)}(x_2) \).

\[ \lambda_n = \lambda_n^{(1)} \lambda_n^{(2)} \] (23)

\[ f_n(x) = f_n(x_1, x_2) = f_n^{(1)}(x_1) f_n^{(2)}(x_2) \] (24)
Figure: Examples of eigenfunctions $f_n$. Figures adopted from [6]
\[ Y(x, \omega) = \bar{Y}(x) + \sum_{n=1}^{7} \xi_n(\omega) \sqrt{\lambda_n} f_n(x). \] (25)

Figure: The domain and "true" lnK
Figure: 1D pdf of predicted hydraulic heads at blue dots
Figure: Log hydraulic conductivity fields generated using samples with the highest probability densities


Thank You