Dimensionality reduction in the Geostatistical approach for Hydraulic Tomography

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Outline

1 Introduction

2 Karhunen-Loève Expansion

3 Inverse Modeling

4 Numerical Experiments
Context of our work

Motivation:

- Hydraulic tomography (HT) is a technique to estimate parameters such as \textit{hydraulic conductivity, storativity} etc.
- HT can be mathematically posed as an Inverse problem.
- Inverse problems are challenging because they are
  - under-determined
  - ill-posed, and
  - computationally expensive
- Use Quasi-Linear Geostatistical approach\(^1\)

\(^1\)Kitanidis, Quasi-linear geostatistical theory of inverting, WRR 1995.
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Our contributions:

- A computationally scalable approach to solving Hydraulic Tomography.
- Reduced dimensional modeling - via Karhunen-Loéve Expansion.
- Works on irregular spaced grids - local refinement, complex geometries.
- Extension to 3D possible.

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Previous Work:

Computing Karhunen-Loéve Expansion


Dimensionality Reduction and Inverse Problems


Using Hierarchical-matrix approach

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Random Field

Model unknowns as a Gaussian random field

\[ E[s] = \mu \quad E[(s - \mu)(s - \mu)^T] = Q \]

**Figure:** Three realizations of a Gaussian random field with exponential covariance

- Storage and computational costs for \( Q_{ij} = \kappa(x_i, x_j) \ i, j = 1, \ldots, m \) high.
- Examples of \( \kappa(\cdot, \cdot) \): Matern family, Gaussian, Exponential.
Karhunen-Loéve Expansion

Consider the Gaussian random field \( s(x) \), with mean \( \mu(x) \) and covariance \( \kappa(x, y) \), on the bounded domain \( x \in D \). The KLE can now be written as

\[
s(x) = \mu(x) + \sum_{i=1}^{\infty} \sqrt{\lambda_i} \phi_i(x) \xi_i \quad \text{with},
\]

\[
\mu(x) = E[s(x)], \quad \xi_i \sim \mathcal{N}(0, 1)
\]
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\((\lambda_i, \phi_i(x))\) are the eigenpair obtained as the solution to the Fredholm integral equation of the second kind

\[
\int_D \kappa(x, y) \phi(y) dy = \lambda \phi(x)
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\[
\int_{D} \kappa(x, y) \phi(y) dy = \lambda \phi(x)
\]

Further,

\[
C_K(x, y) = \sum_{k=1}^{K} \lambda_k \phi_k(x) \phi_k(y) \xrightarrow{K \to \infty} \kappa(x, y)
\]
Consider the integral eigenvalue problem

\[ \int_{\mathcal{D}} \kappa(x, y)\phi(y)dy = \lambda \phi(x) \]

Smother the kernel \( \kappa \) is, the faster \( \{\lambda_m\} \to 0 \).

If \( \mathcal{D} \subset \mathbb{R}^d \) and if the kernel is \(^2\)

- piecewise \( H^r \) \( \lambda_m \leq c_1 m^{-r/d} \)
- piecewise smooth \( \lambda_m \leq c_2 m^{-r} \) for any \( r > 0 \)
- piecewise analytic \( \lambda_m \leq c_3 \exp\left(-c_4 m^{1/d}\right) \)

This provides theoretical justification for truncating this series to a finite number of terms.

\(^2\text{Schwab and Todor (2006).}\)
Computing Karhunen-Loéve Expansion on irregular domains

Discretize using standard Finite Elements and perform a Galerkin projection.

\[ \int_D \kappa(x, y) \phi(y) dy = \lambda \phi(x) \]

This results in a Generalized Eigenvalue problem

\[ W \phi_l = \lambda M \phi_l \quad l = 1, 2, \ldots \]
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W \phi_l = \lambda M \phi_l \quad l = 1, 2, \ldots
\]

where,

\[
W_{ij} = \sum_{k, v} \int_{\mathcal{D}} \int_{\mathcal{D}} b_i(x) b_k(x) \kappa(x_i, y_j) b_j(y) b_v(y) dx dy \text{ over all triangles } k,v
\]

\[
M_{ij} = \int_{\mathcal{D}} b_i(x) b_j(x) dx
\]

and \( b_i \) are the Galerkin basis functions and \( M \) is the called the **mass matrix**.

This above expression can be simplified to

\[
MQM \phi_l = \lambda M \phi_l \quad l = 1, 2, \ldots
\]
Computing Karhunen-Loéve Expansion on irregular domains

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This above expression can be simplified to

\[ MQM \phi_l = \lambda M \phi_l \quad l = 1, 2, \ldots \]

Storing and computing \( Q \), the covariance matrix, is expensive.
Hierarchical matrix ($\mathcal{H}$-matrix$^3$) overview

- Storage and matrix-vector product approximately in $O(N \log N)$, as compared to $O(N^2)$.
- Relies on a hierarchy of low-rank representations of sub-blocks.
- Works on irregularly spaced points for various covariance kernels.

Figure: left: A typical $\mathcal{H}$-matrix rank structure and right: Time for matrix vector product for exponential covariance function. Each subblock is approximated with relative error in Frobenius norm as $\epsilon = 10^{-6}$

On irregular domains

Implementation Details

- $\kappa(x, y) = (1 + \alpha r) \exp(-\alpha r)$, $r = \|x - y\|$ with 10201 points
- Eigenvalue solver - Kylov-Schur algorithm. (SLEPc/PETSc).

**Figure**: Eigenvalue decay and Eigenfunctions of 2, 14, 23, 40.
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Geostatistical approach

Measurement Equation

\[ y = h(s) + v \quad v \sim \mathcal{N}(0, R) \]

- \( y \) := observations or measurements - given.
- \( s \) := model parameters, we want to estimate.
- \( h(s) \) := parameter-to-observation map - given.

Using Bayes’ rule,

\[
p(s|y) \propto p(y|s)p(s) \propto p(s) \exp \left( -\frac{1}{2} \| y - h(s) \|_R^{-1} \right)
\]

After appropriate discretization, represent \( s(\cdot) \) by a truncated KLE

\[ s_K = \mu + \Phi \xi \]

where, columns of \( \Phi \) are the eigenfunctions scaled by square root of eigenvalues.
Geostatistical approach contd.

Dimension reduced posterior pdf

\[ p(\xi | y) \propto p(s_K(\xi) | y)p(\xi) \]
\[ \propto \exp\left(-\frac{1}{2} \|y - h(\xi)\|_{R^{-1}}\right) \exp\left(-\frac{1}{2} \xi^T \xi\right) \]
Geostatistical approach contd.

Dimension reduced posterior pdf

\[ p(\xi|y) \propto p(s_K(\xi)|y)p(\xi) \]
\[ \propto \exp \left( -\frac{1}{2} \|y - h(\xi)\|_{R^{-1}} \right) \exp \left( -\frac{1}{2} \xi^T \xi \right) \]

Maximum A Posteriori estimate

\[ \arg \min_\xi \frac{1}{2} \|y - h_K(\xi)\|_{R^{-1}} + \frac{\beta}{2} \xi^T \xi \]
Geostatistical approach contd.

Dimension reduced posterior pdf

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Inexact Gauss-Newton-Krylov Iteration

\[ (J^T R^{-1} J + \beta I) \delta \xi = -J^T R^{-1} (h(\xi) - y) - \beta \xi \]

where, \( J = \frac{\partial h}{\partial s_K} \frac{\partial s_K}{\partial \xi} \) is the Jacobian at the current iteration.

This also includes a backtracking line search that satisfies Strong Wolfe’s condition.
Hydraulic Tomography

Goal: Estimate log K from discrete measurements of $u_i$.

Figure: (left) Location of sensors and pumping wells and (right) “True” field as a realization of a random field with exponential covariance.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length [m]</td>
<td>500</td>
</tr>
<tr>
<td>Mean log K m²/s</td>
<td>$-5.9220$</td>
</tr>
<tr>
<td>Var log K</td>
<td>0.3475</td>
</tr>
<tr>
<td>Q m³/s</td>
<td>$4 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Governing Equations

$$-\nabla (K(x) \nabla u_i(x)) = q_i \delta(x - x_i)$$

$$u = 0 \quad x \in \partial D_D$$

$$\frac{\partial u}{\partial n} = 0 \quad x \in \partial D_N$$
Reconstruction

**Figure:** (left) Reconstruction using KLE + GNK (400 terms) (right) “True” field as a realization of a random field with exponential covariance. The relative $L^2$ error is 0.2964

<table>
<thead>
<tr>
<th>Parameter</th>
<th>True Field</th>
<th>Reconstructed field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean log K m$^2$/s</td>
<td>$-5.9220$</td>
<td>$-5.9720$</td>
</tr>
<tr>
<td>Var log K</td>
<td>$0.3475$</td>
<td>$0.3158$</td>
</tr>
</tbody>
</table>

$$\kappa(x, y) = (1 + \alpha r) \exp(-\alpha r) \quad r = \|x - y\|$$
Performance of Gauss-Newton solver

With problem size - Fixed \# terms in KLE 100

<table>
<thead>
<tr>
<th>Problem Size</th>
<th>GN Iterations</th>
<th>Av. Inner iterations</th>
<th>Time [s]</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$26 \times 26$</td>
<td>6</td>
<td>46</td>
<td>142.78</td>
<td>0.3369</td>
</tr>
<tr>
<td>$51 \times 51$</td>
<td>5</td>
<td>56</td>
<td>619.20</td>
<td>0.3546</td>
</tr>
<tr>
<td>$101 \times 101$</td>
<td>6</td>
<td>76</td>
<td>5042.4</td>
<td>0.3968</td>
</tr>
</tbody>
</table>

With increasing terms in KLE - Fixed grid size $51 \times 51$

![Eigenvalue decay](image)

<table>
<thead>
<tr>
<th>KLE</th>
<th>Av. Inner iter.</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>12</td>
<td>0.4751</td>
</tr>
<tr>
<td>50</td>
<td>25</td>
<td>0.3561</td>
</tr>
<tr>
<td>100</td>
<td>35</td>
<td>0.3546</td>
</tr>
<tr>
<td>150</td>
<td>35</td>
<td>0.3545</td>
</tr>
</tbody>
</table>