Solving the steady state diffusion equation with uncertainty

Mid-year presentation
Virginia Forstall
vhfors@gmail.com

Advisor: Howard Elman
elman@cs.umd.edu
Department of Computer Science

December 8, 2011
Problem

The equation to be solved is

$$- \nabla \cdot (k(x, \omega) \nabla u) = f(x), \quad (1)$$

where $k = e^{a(x, \omega)}$. 

The equation to be solved is

\[-\nabla \cdot (k(x, \omega) \nabla u) = f(x),\]  

(1)

where \( k = e^{a(x, \omega)} \).

- Assume a bounded spatial domain \( D \subset \mathbb{R}^2 \).
Problem

The equation to be solved is

$$-\nabla \cdot (k(x, \omega) \nabla u) = f(x),$$  \hspace{1cm} (1)

where $k = e^{a(x, \omega)}$.

- Assume a bounded spatial domain $D \subset \mathbb{R}^2$.
- The boundary conditions are deterministic.
Problem

The equation to be solved is

\[-\nabla \cdot (k(x, \omega) \nabla u) = f(x),\]

where \( k = e^{a(x, \omega)}. \)

- Assume a bounded spatial domain \( D \subset \mathbb{R}^2. \)
- The boundary conditions are deterministic.

\[ u(x, \omega) = g(x) \text{ on } \partial D_D \]
\[ \frac{\partial u}{\partial n} = 0 \text{ on } \partial D_n. \]
Outline of approach

Algorithm

1. Approximate the random field using the Karhunen-Loève expansion.
2. Solve the PDE using either the stochastic collocation method or stochastic Galerkin method.

Validation

Compare the moments of this solution to the moments obtained from solving the equation using the Monte-Carlo method.
Outline of approach

Algorithm

1. Approximate the random field using the Karhunen-Loéve expansion.
Outline of approach

Algorithm

1. Approximate the random field using the Karhunen-Loéve expansion.

2. Solve the PDE using either the stochastic collocation method or stochastic Galerkin method.

Validation

Compare the moments of this solution to the moments obtained from solving the equation using the Monte-Carlo method.
Outline of approach

Algorithm

1. Approximate the random field using the Karhunen-Loéve expansion.
2. Solve the PDE using either the stochastic collocation method or stochastic Galerkin method.

Validation

- Compare the moments of this solution to the moments obtained from solving the equation using the Monte-Carlo method.
Karhunen-Loéve expansion

The expansion is

\[ a(x, \xi) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \xi_s. \]  (2)
Karhunen-Loéve expansion

The expansion is

\[ a(x, \xi) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \xi_s. \]  

(2)

- \( \mu(x) \) is the mean of the random field.
Karhunen-Loéve expansion

The expansion is

\[ a(x, \xi) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \xi_s. \]  

(2)

- \( \mu(x) \) is the mean of the random field.
- The random variables \( \xi_s \) are uncorrelated.
The expansion is

\[ a(x, \xi) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \xi_s . \] (2)

- \( \mu(x) \) is the mean of the random field.
- The random variables \( \xi_s \) are uncorrelated.
- The \( \lambda_s \) and \( f_s(x) \) are eigenpairs which satisfy

\[
(Cf)(x) = \int_D C(x, y) f(y) dy = \lambda f(x) ,
\] (3)

where \( C(x, y) \) is the covariance function of the random field.
Covariance matrix

The covariance matrix for a finite set of points $x_i$ in the spatial domain is

$$C(x_i, x_j) = \int_{\Omega} (a(x_i, \omega) - \mu(x_i))(a(x_j, \omega) - \mu(x_j))dP(\omega) , \quad (4)$$

where

$$\mu(x) = \int_{\Omega} a(x, \omega)dP(\omega) . \quad (5)$$
Covariance matrix

The covariance matrix for a finite set of points $x_i$ in the spatial domain is

$$C(x_i, x_j) = \int_{\Omega} (a(x_i, \omega) - \mu(x_i))(a(x_j, \omega) - \mu(x_j))dP(\omega) ,$$  \hspace{1cm} (4)

where

$$\mu(x) = \int_{\Omega} a(x, \omega)dP(\omega) .$$  \hspace{1cm} (5)

Denote the approximation to this matrix

$$C_{ij} = C(x_i, x_j) .$$  \hspace{1cm} (6)
Covariance matrix

- The eigenpairs of the covariance matrix are related to the eigenpairs of the random field.
Covariance matrix

- The eigenpairs of the covariance matrix are related to the eigenpairs of the random field.
- This is found by taking a discrete approximation to the continuous eigenvalue problem in Equation 3.
Covariance matrix

- The eigenpairs of the covariance matrix are related to the eigenpairs of the random field.
- This is found by taking a discrete approximation to the continuous eigenvalue problem in Equation 3.
- For a one-dimensional domain with uniform interval size $h$, the discretization of this problem is

$$hCV = \Lambda V .$$  

(7)
Covariance matrix

- The eigenpairs of the covariance matrix are related to the eigenpairs of the random field.
- This is found by taking a discrete approximation to the continuous eigenvalue problem in Equation 3.
- For a one-dimensional domain with uniform interval size $h$, the discretization of this problem is
  \[ hCV = \Lambda V. \] (7)

- For a uniform two-dimensional domain with interval sizes $h_x$ and $h_y$, the problem to solve is
  \[ h_x h_y CV = \Lambda V. \] (8)
Covariance matrix

- When the covariance function for a random field is known, the covariance matrix is constructed by evaluating the function at each pair of points.
Covariance matrix

- When the covariance function for a random field is known, the covariance matrix is constructed by evaluating the function at each pair of points.

- Otherwise, $n$ samples can be taken at each spatial point to form the sample covariance matrix, $\hat{C}$.

\[ \hat{C}_{ij} = \frac{1}{n} \sum_{k=1}^{n} (a(x_i, \xi_k) - \hat{\mu}_i)(a(x_j, \xi_k) - \hat{\mu}_j) \]  \hspace{1cm} (9)

\[ \hat{\mu}_i = \frac{1}{n} \sum_{k=1}^{n} a(x_i, \xi_k) . \] \hspace{1cm} (10)
Sample covariance matrix

- We are interested in the eigenpairs of $\hat{C}$, but do not need to construct the entire matrix.
Sample covariance matrix

- We are interested in the eigenpairs of $\hat{C}$, but do not need to construct the entire matrix.
- Define a matrix:

$$B_{ik} = a(x_i, \omega_k) - \hat{\mu}_i$$  \hspace{1cm} (11)
Sample covariance matrix

- We are interested in the eigenpairs of $\hat{\mathbf{C}}$, but do not need to construct the entire matrix.
- Define a matrix:
  
  $$B_{ik} = a(x_i, \omega_k) - \hat{\mu}_i$$  

  (11)

- Then the sample covariance matrix can be written as
  
  $$\hat{\mathbf{C}} = \frac{1}{n} \mathbf{B} \mathbf{B}^T.$$  

  (12)
Sample covariance matrix

- Consider the singular value decomposition of \( B = U \Sigma V^T \).
Sample covariance matrix

- Consider the singular value decomposition of \( B = U\Sigma V^T \).
- The eigenvalues of \( \hat{C} \) will be \( \frac{1}{n}\Sigma^2 \).
- The eigenvectors of \( \hat{C} \) will be the columns of \( U \).
Consider the singular value decomposition of $B = U\Sigma V^T$.

The eigenvalues of $\hat{C}$ will be $\frac{1}{n} \Sigma^2$.

The eigenvectors of $\hat{C}$ will be the columns of $U$.

Using this approach ensures that small numerical errors will not produce imaginary eigenvalues.
A Gaussian random field in one dimension has covariance function

\[ C(x_1, x_2) = \sigma^2 \exp(-|x_1 - x_2|/b) \]  

(13)
A Gaussian random field in one dimension has covariance function

\[ C(x_1, x_2) = \sigma^2 \exp\left(-|x_1 - x_2|/b\right) \]  

(13)

\( \sigma^2 \) is the (constant) variance of the stationary random field and \( b \) is the correlation length.
A Gaussian random field in one dimension has covariance function

\[ C(x_1, x_2) = \sigma^2 \exp(-|x_1 - x_2|/b) \]  

(13)

- \( \sigma^2 \) is the (constant) variance of the stationary random field and \( b \) is the correlation length.

- Large values of \( b \): random variables at points that are near each other are highly correlated.
Gaussian random field

- Exact solutions for the eigenvalues and eigenfunctions are known [9].

\[
\begin{align*}
\lambda_n &= \sigma^2 \frac{2b}{\omega_n^2 + b^2} \\
\lambda_n^* &= \sigma^2 \frac{2b}{\omega_n^{*2} + b^2}
\end{align*}
\]
Gaussian random field

- Exact solutions for the eigenvalues and eigenfunctions are known [9].

\[
\lambda_n = \sigma^2 \frac{2b}{\omega_n^2 + b^2} \quad (14)
\]

\[
\lambda_n^* = \sigma^2 \frac{2b}{\omega_n^*2 + b^2} \quad (15)
\]

where \( \omega_n \) and \( \omega_n^* \) solve the following:

\[
b - \omega \tan(\omega a) = 0 \quad (16)
\]

\[
\omega^* + b \tan(\omega^* a) = 0 . \quad (17)
\]
Gaussian random field

- The random variables in the expansion are $\xi_s \sim N(0, 1)$.

$$a(x, \xi) = \mu(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} f_n(x) \xi_n$$  \hspace{1cm} (18)
Gaussian random field

- The random variables in the expansion are $\xi_s \sim N(0, 1)$.

$$a(x, \vec{\xi}) = \mu(x) + \sum_{n=1}^{\infty} \sqrt{\lambda_n} f_n(x) \xi_n$$  \hspace{1cm} (18)

- For a two-dimensional Gaussian field

$$C((x_1, y_1), (x_2, y_2)) = \sigma^2 \exp \left( \frac{-|x_1 - x_2|}{b_1} - \frac{-|y_1 - y_2|}{b_2} \right)$$  \hspace{1cm} (19)
Verification for 1D Gaussian random field

Three methods were used to find the eigenvalues of a one-dimensional $N(0, 1)$ Gaussian random field on $D = [-1, 1]$ with step size $h = .02$. 

1. Solve for the eigenfrequencies using Newton's method.
2. Build the analytic covariance matrix.
3. Build the sample covariance matrix.

Implemented using Matlab and made use of functions written by E. Ullman 2007-10.
Verification for 1D Gaussian random field

Three methods were used to find the eigenvalues of a one-dimensional $N(0, 1)$ Gaussian random field on $D = [-1, 1]$ with step size $h = .02$.

1. Solve for the eigenfrequencies using Newton’s method.
Verification for 1D Gaussian random field

Three methods were used to find the eigenvalues of a one-dimensional $N(0, 1)$ Gaussian random field on $D = [-1, 1]$ with step size $h = .02$.

1. Solve for the eigenfrequencies using Newton’s method.
2. Build the analytic covariance matrix.
Verification for 1D Gaussian random field

Three methods were used to find the eigenvalues of a one-dimensional $N(0, 1)$ Gaussian random field on $D = [-1, 1]$ with step size $h = .02$.

1. Solve for the eigenfrequencies using Newton’s method.
2. Build the analytic covariance matrix.
3. Build the sample covariance matrix.
Verification for 1D Gaussian random field

Three methods were used to find the eigenvalues of a one-dimensional $N(0, 1)$ Gaussian random field on $D = [-1, 1]$ with step size $h = .02$.

1. Solve for the eigenfrequencies using Newton’s method.
2. Build the analytic covariance matrix.
3. Build the sample covariance matrix.

Implemented using Matlab and made use of functions written by E. Ullman 2007-10.
Figure: Eigenvalues of Gaussian random field with parameters $b = 1$, $n = 10000$ for the three methods. Methods 1 and 2 produce nearly identical results.
Gaussian random field 1D

(a) n=100  
(b) n=1000  
(c) n=10000

Figure: The eigenvalues of the sampling method converge as the number of samples, $n$ is increased.
Gaussian random field 1D

Figure: The effect of correlation length, $b$, on the eigenvalues

(a) $b = 0.01$, $n=100000$    (b) $b = 0.1$, $n=1000$    (c) $b = 3$, $n=10000$
Gaussian random field

- Verified three methods using a two-dimensional domain $D = [0, 1] \times [0, 1]$ as well.

- Eigenvectors also agree.
Lognormal random field

- If $a(x, \xi)$ is a Gaussian random variable, $k(x, \xi) = \exp(a(x, \xi))$ is lognormal at every point in the spatial domain.
Lognormal random field

- If $a(x, \xi)$ is a Gaussian random variable, $k(x, \xi) = \exp(a(x, \xi))$ is lognormal at every point in the spatial domain.
- If $X \sim N(\mu, \sigma)$ and $X = \ln(Y)$, the lognormal random variable $Y$ has the following results [10]:

$$E[Y] = e^{\sigma^2/2}$$

$$\text{Var}[Y] = e^{2\mu+\sigma^2} (e^{\sigma^2} - 1)$$

$$LC(x_1, x_2) = e^{2\mu+\sigma^2} (e^{C(x_1, x_2)} - 1).$$
Figure: The eigenvalues obtained using the sample covariance matrix, converge to the analytic covariance matrix results as the number of samples is increased. Tests use correlation length $b = 1$. 
Summary

- Confirmed sampling procedure for determining eigenpairs of a lognormal field.
Confirmed sampling procedure for determining eigenpairs of a lognormal field.

Ultimately analytic covariance function will be used to compute the eigenpairs used in the KL expansion of $k$:

$$k(x, \vec{\eta}) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \eta_s .$$  \hspace{1cm} (23)
Summary

- Confirmed sampling procedure for determining eigenpairs of a lognormal field.
- Ultimately analytic covariance function will be used to compute the eigenpairs used in the KL expansion of $k$:

$$k(x, \eta) = \mu(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} f_s(x) \eta_s .$$

(23)

- What is the distribution of the $\eta_s$?
Schedule

Stage 2: December
- Finish construction of the principal components analysis
- Write code which generates Monte-Carlo solutions

Stage 3: January- February
- Run the Monte-Carlo simulations
- Write solution method

Stage 4: March - April
- Run numerical method
- Analyze accuracy and validity of the method
References


References


