Solving the steady state diffusion equation with uncertainty
Final Presentation

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Problem

The equation to be solved is

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

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

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

$$u(x,\omega) = g(x) \text{ on } \partial D_D$$
$$\frac{\partial u}{\partial n} = 0 \text{ on } \partial D_n \ .$$

- Models groundwater flow through a porous medium [15].

Outline

1. Approximate the random field using the Karhunen-Loéve expansion.
2. Solve the PDE using stochastic Galerkin method.
3. Compare mean and variance of the solution to those obtained using the Monte-Carlo method.

Karhunen-Loéve expansion

The expansion is

$$a(x,\vec{\xi}) = a_0(x) + \sum_{s=1}^{\infty} \sqrt{\lambda_s} a_s(x) \xi_s \ . \tag{2}$$

- $a_0(x)$ is the mean of the random field.
- The random variables ξ_s are uncorrelated with $E[\xi_s] = 0$, $Var[\xi_s] = 1$.
- The λ_s and $a_s(x)$ are eigenpairs which satisfy

$$(\mathcal{C} a_s)(x_1) = \int_D C(x_1, x_2) a_s(x_2) dx_2 = \lambda_s a_s(x_1) \ , \tag{3}$$

where $C(x_1, x_2)$ is the covariance function of the random field.

Discretization of the eigenvalue problem

- The square domain D is discretized intervals of equal size h in each direction.
- The eigenvalues of the covariance operator satisfy

$$h^2 CV = \Lambda V \ . \tag{4}$$

where $C_{ij} = C(x_i, x_j)$.
- The approximation of the eigenfunctions are

$$a_s(x_i) = \frac{1}{h} V_{is} \tag{5}$$

Discretization of the eigenvalue problem

- Alternatively, q samples of the random field can be used to form the sample covariance matrix:

$$\widehat{C}_{ij} = \frac{1}{q}\sum_{k=1}^{q}(a(x_i,\omega_k) - \hat{a}_i)(a(x_j,\omega_k) - \hat{a}_j) \tag{6}$$

where $\widehat{a}_i$ is the sample mean.

Covariance function

- The covariance function for the Gaussian random field with mean μ and variance σ^2 is

$$C_g((x_1, y_1), (x_2, y_2)) = \sigma^2 \exp\left(\frac{-|x_1 - x_2|}{b_x} + \frac{-|y_1 - y_2|}{b_y}\right) \tag{7}$$

  where b_x, b_y are the correlation lengths.
- The eigenvalues and eigenfunctions have analytic expressions for this covariance function.

Validation of eigenpairs

- Two methods for finding eigenpairs verified by comparing with analytic expressions for the Gaussian random field.

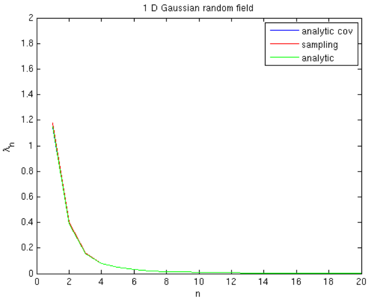


Figure: Eigenvalues of Gaussian random field with parameters $b = 1$, $q = 10000$ computed using analytic expression and the two covariance matrices.

Covariance function

- The covariance function for the lognormal random field can be written as a function of the Gaussian covariance function.

$$C_l((x_1, y_1), (x_2, y_2)) = e^{2\mu+\sigma^2}(e^{C_g((x_1,y_1),(x_2,y_2))} - 1) \quad [9]. \quad (8)$$

- This expression is used to build the covariance matrix and find the eigenpairs.
- The sampling method would allow this model to be used when structure of the random field is unknown but can be sampled at various points in space.

Karhunen-Loéve expansion

The lognormal random field can be approximated two ways:

$$k(x,\xi) = \exp[a_0(x) + \sum_{i=1}^{m_g} \sqrt{\lambda_i} a_i(x)\xi_i] \tag{9}$$

$$\widehat{k}(x,\eta) = k_0(x) + \sum_{i=1}^{m_l} \sqrt{\mu_i} k_i(x)\eta_i \; . \tag{10}$$

- $\{\xi_i\}$ are independent Gaussian random variables, so the joint probability density function, $\rho(\xi)$, is known.
- The joint density function of the random variables, η_i, is needed.
- Let $m = \max(m_g, m_l)$ and the joint density function, $\widehat{\rho}(\eta)$, is found using a change of variables.

Probability density function

- Define matrices $A = [a_1|a_2|...|a_m]$ and $K = [k_1|k_2|...|k_m]$ where the columns are the eigenfunctions evaluated at the points in the spatial discretization.
- Define the mass matrix $B_{ij} = \int_D \phi_i(x)\phi_j(x)dx$.
- A was normalized so that $A^T BA = I$.
- Define the diagonal matrices $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_m)$ and $M = \mathrm{diag}(\mu_1, \mu_2, ..., \mu_m)$.
- Define vectors $\xi = [\xi_1, \xi_2, ..., \xi_m]^T$ to be the standard normal random variables in the Gaussian random field and $\eta = [\eta_1, \eta_2, ..., \eta_m]^T$ to be the unknown random variables in the lognormal expansion.

Probability density function

$$\Lambda A^T B(k(x,\xi) - a_0(x)) = \Lambda A^T B(\widehat{k}(x,\eta) - a_0(x)) \,. \tag{11}$$

$$\xi = g(\eta) = \Lambda A^T B(\ln(k_0 + KM\eta) - a_0) \,. \tag{12}$$

- $\widehat{\rho}(\eta) = \rho(g(\eta))|J(\eta)|$ describes the density for η such that $k_0 + KM\eta > 0$.
- $|J(\eta)|$ is the absolute value of the determinant of the Jacobian, which we can find since $g(\eta)$ is differentiable.

Probability density function

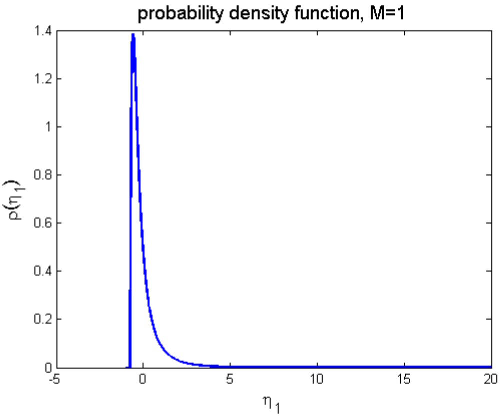


Figure: Probability density function for 1d field $m = 1$, $b = 10$.

Probability density function

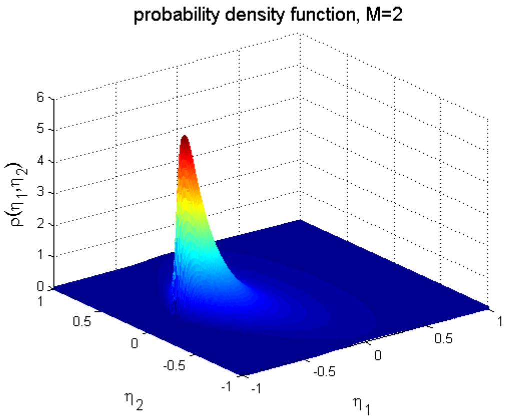


Figure: Probability density function for $m = 2$, $b = 10$.

Probability density function

- The joint density function can be used to find the marginal density functions which have mean 0 and variance 1 as expected.
- Samples of $k(x, \xi)$ were generated with m $N(0, 1)$ samples for each instance.
- To find samples of $\widehat{k}(x, \eta)$, accept/reject sampling is used.
- Uniform samples over the support of density function are generated and the probability density function evaluated at those values.
- In addition another uniform sample on (0,1) is generated, if this value is above the value of the pdf it is kept as a sample of the distribution.
- The sample mean of $k(x, \xi)$ and $\widehat{k}(x, \eta)$ can now be compared.

Probability density function

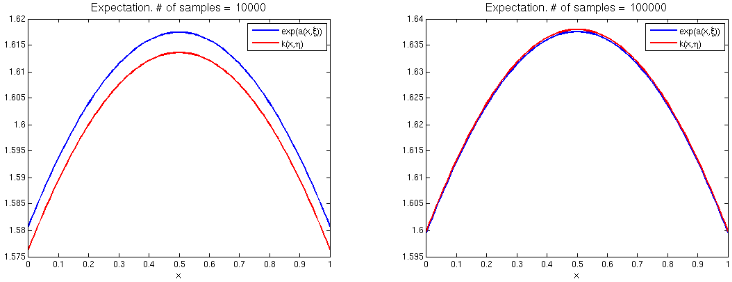


Figure: Compare $E[\widehat{k}(x,\eta)]$ and $E[k(x,\xi)]$ using Monte-Carlo method. Lognormal samples found using accept/reject technique.

Deterministic diffusion equation

- For the Monte-Carlo method the deterministic diffusion equation needs to be solved.

$$-\nabla \cdot (k(x)\nabla u(x)) = f(x)\ . \qquad (13)$$

- Let D be square and discretize with bilinear elements on quadrilaterals of size h by h.
- Let $\phi_j(x)$ denote the basis functions.

Deterministic diffusion equation

Find $u(x) \in H^1_E(D) = \{u \in H^1(D) : u = g(x) \text{ on } \partial D_d\}$ such that

$$\int_D k(x)\nabla u(x) \cdot \nabla v(x) dx = \int_D f(x)v(x)dx \tag{14}$$

is satisfied for all $v(x) \in H^1_0(D)$.

Deterministic diffusion equation

- The finite element solution is

$$u_h(x) = \sum_{j=1}^{n} u_j \phi_j(x) + \sum_{j=n+1}^{n+n_d} u_j \phi_j(x) \; . \tag{15}$$

  where n is the number of elements on the interior and n_d is the number of elements on the boundary.

- To find the coefficients u_j, solve $Au = b$ where

$$A_{ij} = \int_D k(x) \nabla \phi_j(x) \cdot \nabla \phi_i(x) \, dx \tag{16}$$

$$b_i = \int_D \phi_i(x) f(x) \, dx - \sum_{j=n+1}^{n+n_d} u_j \int_D k(x) \nabla \phi_j(x) \cdot \nabla \phi_i(x) \, dx \tag{17}$$

Deterministic diffusion equation

- Implemented with Matlab package Incompressible Flow & Iterative Solver Software(IFISS) [10].
- $D = [0,1] \times [0,1]$.
- $f(x) = 1,\ g(x) = 0,\ k(x) = 1,\ h = 0.0625,\ n_d = 64,\ n = 225$
- Analytic solution [1]:

$$u(x,y) = \frac{16}{\pi^4} \sum_{l=0}^{\infty} \sum_{k=0}^{\infty} \frac{\sin((2k+1)\pi x)\sin((2l+1)\pi y)}{(2k+1)(2l+1)((2k+1)^2 + (2l+1)^2)} \tag{18}$$

$$\frac{||u_h(x) - u(x)||_2}{||u(x)||_2} = 3.31 \times 10^{-3} \tag{19}$$

Deterministic diffusion equation

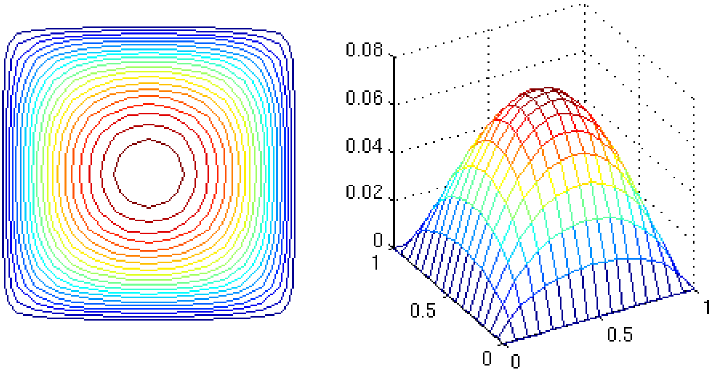


Figure: Deterministic solution, $k(x) = 1$

Monte Carlo Method

- Use the deterministic solver for each of q finite element problems, denoting the solution $u_h^i(x)$ for $i = 1, \ldots, q$.
- The sample mean of the solution is

$$\mathrm{E}_q[u_h] = \frac{1}{q}\sum_{i=1}^{q} u_h^i(x) \ . \tag{20}$$

$$\mathrm{Var}_q[u_h] = \frac{1}{q-1}\sum_{i=1}^{q}(u_h^i(x)^2 - E_q[u_h]^2) \tag{21}$$

- The error in the mean is
$E[u] - E_q[u_h] = E[u] - E[u_h] + E[u_h] - E_q[u_h]$.

Monte Carlo Method

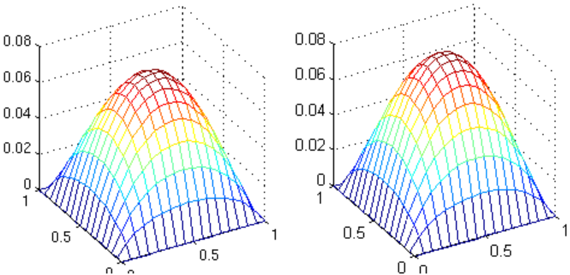
- Using the KL expansion from the Gaussian random field

$$k(x, \vec{\xi}) = \exp[a_0(x) + \sum_{s=1}^{m_g} \sqrt{\lambda_s} a_s(x) \xi_s] \tag{22}$$

  where ξ_s are independent and $N(0,1)$ [13].
- Sample the m_g standard normal random variables q times to produce samples $k_i(x)$ for $i = 1, ..., q$.
- Running method with $\sigma = 0$ differs from the deterministic solution $\sim 10^{-15}$.

Monte Carlo Method

Figure: Monte Carlo solution: $E[k(x,\xi)] = 1$, $f(x) = 1$, $m = 5$, $g(x) = 0$.



(a) $\sigma = 0.001, q = 100$ (b) $\sigma = 0.5, q = 100000$

Stochastic weak formulation

- Write the solution as combination of basis functions which can be used to estimate statistical properties of the solution.
- The stochastic basis functions are analagous to the spatial basis functions used in the deterministic method.
- Using the KL expansion, the probability space, Ω, is approximated by Γ, where Γ is the support of the joint density function of the random variables in the expansion.
- The weak formulation of the problem is to find $u \in H^1(D) \otimes L^2(\Gamma)$ such that the following holds for all $v \in H^1_0(D) \otimes L^2(\Gamma)$

$$\int_\Gamma \int_D \widehat{k}(x,\eta) \nabla u \cdot \nabla v \widehat{\rho}(\eta)\, dx\, d\eta = \int_\Gamma \int_D f v \widehat{\rho}\,(\eta) dx\, d\eta \quad (23)$$

Chaos polynomials

- The spatial discretization uses the same bilinear elements as the deterministic problem ($\phi_i(x)$).
- The stochastic discretization uses chaos polynomials

$$\psi_{\mathbf{j}}(\eta) = \psi_{j_1}(\eta_1)\psi_{j_2}(\eta_2)...\psi_{j_m}(\eta_m) \; . \qquad (24)$$

- The chaos polynomials are chosen to be orthonormal so that $E[\psi_{\mathbf{i}}(\eta)\psi_{\mathbf{j}}(\eta)] = \delta_{\mathbf{ij}}$.

Chaos polynomials

- The number of basis polynomials is chosen by setting an upper bound (N) on the degree of the polynomials.

$$\deg(\psi_{\mathbf{j}}) = \deg(\psi_{j_1}) + ... + \deg(\psi_{j_m}) \leq N \ \ \forall \mathbf{j} \tag{25}$$

- The polynomials can be reindexed $j = 1, ..., n_\eta$ where

$$n_\eta = \binom{N+m}{m} . \tag{26}$$

Stochastic Galerkin method

- The solution is written as a combination of products of the two basis functions.

$$u_h(x,\eta) = \sum_{i=1}^{n_x} \sum_{j=1}^{n_\eta} u_{ij}\phi_i(x)\psi_j(\eta) \qquad (27)$$

$$v(x,\eta) = \phi(x)\psi(\eta) \qquad (28)$$

- The problem is to find the coefficients u_{ij} which satisfy

$$\sum_{i=1}^{n_x} \sum_{j=1}^{n_\eta} \int_\Gamma \int_D u_{ij}\widehat{k}(x,\eta)\nabla\phi_i(x)\cdot\nabla\phi_k(x)\psi_j(\eta)\psi_l(\eta)\widehat{\rho}(\eta)dxd\eta$$

$$= \int_\Gamma \int_D f(x)\phi_k(x)\psi_l(\eta)\widehat{\rho}(\eta)dxd\eta \quad (29)$$

for each $k = 1, ..., n_x$ and $l = 1, ..., n_\eta$.

Stochastic Galerkin method

- Define $\mu_0 = 1$ and $\eta_0 = 1$, so the KL expansion can be written

$$\widehat{k}(x,\eta) = \sum_{s=0}^{m} \sqrt{\mu_s} k_s(x) \eta_s \ . \tag{30}$$

- The solution u can be found by solving $\widehat{A}u = b$ where

$$\widehat{A} = \sum_{p=0}^{m} G_p \otimes A_p \tag{31}$$

$$[A_p]_{ik} = \int_D \sqrt{\mu_p} k_p(x) \nabla \phi_i(x) \cdot \nabla \phi_k(x) dx \tag{32}$$

$$[G_p]_{jl} = \int_\Gamma \eta_p \psi_j(\eta) \psi_l(\eta) \widehat{\rho}(\eta) d\eta \tag{33}$$

$$b = \int_D f(x) \phi_k(x) dx \int_\Gamma \psi_l(\eta) \widehat{\rho}(\eta) d\eta \tag{34}$$

Stochastic Galerkin method

- The mean and the variance of the solution are

$$\mathrm{E}\left[u(x,\eta)\right] = \sum_{i=1}^{n_x} u_{i1}\phi_i(x) \tag{35}$$

$$\mathrm{Var}\left[u(x,\eta)\right] = \sum_{i=1}^{n_x}\sum_{k=1}^{n_x}\sum_{j=2}^{n_\eta} u_{ij}u_{kj}\phi_i(x)\phi_k(x) \tag{36}$$

Orthogonal polynomials

- Introduce the assumption $\widehat{\rho}(\eta) = \widehat{\rho}_1(\eta_1)\widehat{\rho}_2(\eta_2)...\widehat{\rho}_m(\eta_m)$.
- The integral for $[G_p]_{jl}$ becomes

$$[G_p]_{jl} = \int_{\Gamma_1} \psi_j(\eta_1)\psi_j(\eta_1)\psi_l(\eta_1)\widehat{\rho}_1(\eta_1)d\eta_1 ... \int_{\Gamma_p} \eta_p\psi_j(\eta_p)\psi_l(\eta_p)\widehat{\rho}_p(\eta_p)d\eta_p ... \int_{\Gamma_m} \psi_j(\eta_m)\psi_l(\eta_m)\widehat{\rho}_m(\eta_m)d\eta_m \quad (37)$$

- For each of the random variables the ith component of the orthogonal polynomials $\psi_j(\eta_i)$ is constructed using the three-term recurrence relation, where the coefficients are found using the Stieljtes procedure.

Orthogonal polynomials

- The $k+1$ degree polynomial is:

$$\psi_{k+1}(\eta_i) = (\eta_i - \alpha_k)\psi_k(\eta_i) - \beta_k\psi_{k-1}(\eta_i) \tag{38}$$

for $k = 0, 1, ...,$ where $\psi_{-1}(\eta_i) = 0$ and $\psi_0(\eta_i) = 1$.

- The recurrence coefficients are

$$\alpha_k = \frac{\int \eta_i\psi_k(\eta_i)\psi_k(\eta_i)\rho_i(\eta_i)d\eta_i}{\int \psi_k(\eta_i)\psi_k(\eta_i)\rho_i(\eta_i)d\eta_i} \tag{39}$$

for $k = 0, 1, 2, ...$ and

$$\beta_k = \frac{\int \psi_k(\eta_i)\psi_k(\eta_i)\rho_i(\eta_i)d\eta_i}{\int \psi_{k-1}(\eta_i)\psi_{k-1}(\eta_i)\rho_i(\eta_i)d\eta_i} \tag{40}$$

for $k = 1, 2, ...$

Stieljtes procedure

- Let $[a, b]$ be the support of $\rho_i(\eta_i)$ and discretize with R points.
- The coefficients are:

$$\alpha_{k,R} = \frac{\sum_{t=1}^{R} \eta_{i_t} w_t \psi_{k,R}(\eta_{i_t})\psi_{k,R}(\eta_{i_t})\rho_i(\eta_{i_t})}{\sum_{t=1}^{R} w_t \psi_{k,R}(\eta_{i_t})\psi_{k,R}(\eta_{i_t})\rho(\eta_{i_t})} \tag{41}$$

$$\beta_{k,R} = \frac{\sum_{t=1}^{R} w_t \psi_{k,R}(\eta_{i_t})\psi_{k,R}(\eta_{i_t})\rho_i(\eta_{i_t})}{\sum_{t=1}^{R} w_t \psi_{k-1,R}(\eta_{i_t})\psi_{k-1,R}(\eta_{i_t})\rho(\eta_{i_t})} \tag{42}$$

Stieljtes procedure

- The weights and nodes are found using a Fejer quadrature where the nodes are related to the roots of the Chebyshev polynomials.

$$\eta_v = \frac{1}{2}(b-a)\cos\left(\frac{2v-1}{2M}\right) + \frac{1}{2}(a+b) \tag{43}$$

$$w_v = \frac{1}{M}\left(1 - 2\sum_{n=1}^{\lfloor M/2 \rfloor} \frac{\cos(2n(\frac{2v-1}{2M}))}{4n^2-1}\right) \tag{44}$$

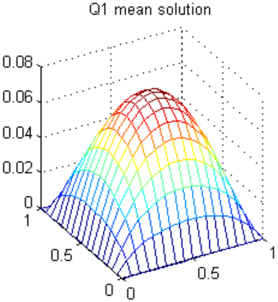
for $v = 1, ..., M$.

Stieljtes procedure

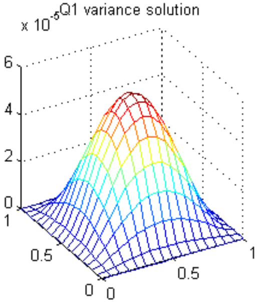
- The procedure was implemented for Matlab by Gautschi [4] where the interval is broken up into component intervals.
- This procedure was called to construct the polynomials for each of the m marginal density functions.

Results, $m = 1$

Figure: Stochastic Galerkin solution: $E[k(x,\eta)] = 1$, $f(x) = 1$, $m = 1$, $\sigma = 0.1$, $b_x = b_y = 10$.



(a) Mean



(b) Variance

Results, $m = 1$

- Validation of the stochastic Galerkin method is acheived by comparing with the Monte-Carlo solution.
- With standard deviation, $\sigma = 0.1$, and correlation lengths, $b_x = b_y = 10$ the first eigenvalue includes 93.22% of the variance.

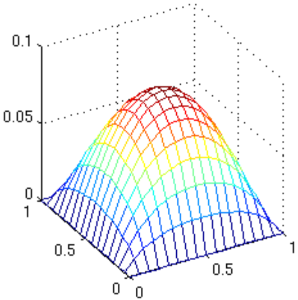
$$\frac{||E[u]_{MC} - E[u]_{SG}||_2}{||E[u]_{MC}||_2} = 4.61 \times 10^{-4}$$

$$\frac{||sd_{MC} - sd_{SG}||_2}{||sd_{MC}||_2} = 9.00 \times 10^{-3}$$

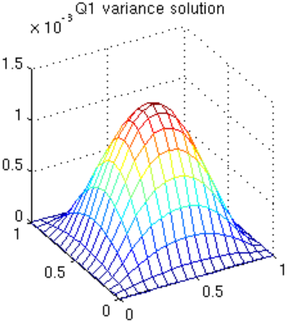
- Given the small standard deviation, the solution is not so different from the deterministic result.

Results, $m = 2$

Figure: Stochastic Galerkin solution: $E[k(x,\eta)] = 1$, $f(x) = 1$, $m = 2$, $\sigma = 0.5$, $b_x = b_y = 10$.



(a) Mean



(b) Variance

Results, $m = 2$

- Assume $\widehat{\rho}(\eta) = \rho_1(\eta_1)\rho_2(\eta_2)$.
- $\sigma = 0.5$ and $b_x = b_y = 10$, which incorporates 94.67% of the variance in the first two eigenvalues.

$$\frac{||E[u]_{MC} - E[u]_{SG}||_2}{||E[u]_{MC}||_2} = 3.95 \times 10^{-3}$$

$$\frac{||sd_{MC} - sd_{SG}||_2}{||sd_{MC}||_2} = 1.32 \times 10^{-1}$$

Results, $m = 2$

- The Monte-Carlo method with $q = 100,000$ takes approximately 3.5 hours.
- The stochastic Galerkin method took approximately 0.5 hours.
- Unlike the Monte-Carlo method, the SG method scales as a function of the number of random variables.
- The majority of the time spent on the stochastic Galerkin method is in computing the two marginal density functions needed.

Deliverables

- Code to compute the moments of the solution using the Monte-Carlo method
  - Verified using $\sigma = 0$ and comparing with deterministic solution.
- Code to compute the moments of the solution using a KL expansion and stochastic Galerkin method.
  - Implemented for expansions of up to two random variables and standard deviation up to $\sigma = 0.5$ and verified using the Monte-Carlo results.
- Comparison of the results for varying number of terms in the KL expansion.
- Comparison of computational cost for the two methods

Conclusion

- The stochastic Galerkin method for performs faster than Monte-Carlo methods for $m = 1$ and $m = 2$.
- A different quadrature routine to compute the marginal density functions could improve computation time.
- The assumption about separability of the density function does not hold for standard deviations much higher than $\sigma = 0.5$.
- Having the joint density function illustrates using the direct expansion of the lognormal random field can be used to solve this problem.
- The stochastic collocation method does not require orthogonal polynomials, so no assumption of separability would be needed.

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