List of Exercises
Numerical methods for random partial differential equations: hierarchical approximation and machine learning approaches

MATH4UQ — RWTH Aachen University

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1 MLMC under approximate sampling

1.1 Objective

This exercise gives hands-on experience on multilevel Monte Carlo sampling methods for approximate (discretized) sampling. It also makes the student work on sampling Gaussian random fields and thus experimenting with Karhunen-Loève and Fourier expansions.

1.2 Problem

Next we look at the solution of a one dimensional boundary value problem

$$-(a(x,\omega)u'(x,\omega))' = \underbrace{4\pi^2\cos(2\pi x)}_{=:f(x)}, \text{ for } x \in (0,1)$$

with $u(0,\cdot) = u(1,\cdot) = 0$. In this case, we are interested in computing the expected value of the following QoI

$$Q(u(\omega)) = \int_0^1 u(x,\omega)dx.$$

We use an $I+1$ uniform grid $0 = x_0 < x_1 < \ldots < x_I = 1$ on $[0,1]$ with uniform spacing $h = x_i - x_{i-1} = 1/I$, $i = 1,\ldots,I$. Using this grid we can build a piecewise linear FEM approximation,

$$u_h(x,\omega) = \sum_{i=1}^{I-1} \mathbf{u}_{h,i}(\omega)\varphi_i(x),$$

yielding a tridiagonal linear system for the nodal values, $A(\omega)\mathbf{u}_h(\omega) = F$, with

$$\begin{aligned}
A_{i,i-1}(\omega) =& -\frac{a(x_{i-1/2},\omega)}{h^2} \\
A_{i,i}(\omega) =& \frac{a(x_{i-1/2},\omega) + a(x_{i+1/2},\omega)}{h^2} \\
A_{i,i+1}(\omega) =& -\frac{a(x_{i+1/2},\omega)}{h^2}
\end{aligned}$$

and

$$F_i = f(x_i).$$

Here we used the notation $x_{i+1/2} = \frac{x_i + x_{i+1}}{2}$ and $x_{i-1/2} = \frac{x_i + x_{i-1}}{2}$.

The integral in $Q(u_h)$ can be then computed exactly by a trapezoidal method, yielding

$$Q(u_h) = h\sum_{i=1}^{I-1} \mathbf{u}_{h,i}.$$

1.3 Models for the random coefficient a.

We look at two different models for $a(x,\omega)$, namely

1.3.1 Model 1: Piecewise constant coefficient

$$a(x,\omega) = 1 + \sigma \sum_{n=1}^{N} Y_n(\omega)\mathbb{I}_{[\hat{x}_{n-1},\hat{x}_n]}(x),$$

with equispaced nodes $\hat{x}_n = \frac{n}{N}$ for $0 \le n \le N$ and i.i.d. uniform random variables $Y_n \sim U([-\sqrt{3},\sqrt{3}])$. Consider different uniform mesh refinements, i.e. values of $I = N\,2^\ell$, $\ell \ge 0$, and different number of input random variables $N = 10$, $N = 20$ and $N = 40$. Remember to choose σ ensuring coercivity, namely $1 - \sigma\sqrt{3} > 0$.

1.3.2 Model 2: Log-Normal

$$a(x,\omega) = \exp(\kappa(x,\omega)),$$

where $\kappa(x,\omega)$ is a stationary Gaussian random field with mean zero and the Matérn covariance function

$$C(x,y) = \sigma^2 \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(\sqrt{2\nu}\frac{|x-y|}{\rho}\right)^\nu K_\nu\left(\sqrt{2\nu}\frac{|x-y|}{\rho}\right),$$

where Γ is the gamma function and K_ν is the modified Bessel function of the second kind. We look at the following special cases of C

$$\begin{aligned}
\nu = 0.5, \quad C(x,y) &= \sigma^2 \exp\left(-\tfrac{|x-y|}{\rho}\right)\\
\nu = 1.5, \quad C(x,y) &= \sigma^2 \left(1+\tfrac{\sqrt{3}|x-y|}{\rho}\right)\exp\left(-\tfrac{\sqrt{3}|x-y|}{\rho}\right)\\
\nu = 2.5, \quad C(x,y) &= \sigma^2 \left(1+\tfrac{\sqrt{5}|x-y|}{\rho}+\tfrac{\sqrt{3}|x-y|^2}{\rho^2}\right)\exp\left(-\tfrac{\sqrt{5}|x-y|}{\rho}\right)\\
\nu \to \infty, \quad C(x,y) &= \sigma^2 \exp\left(-\tfrac{|x-y|^2}{2\rho^2}\right).
\end{aligned}$$

Moreover we choose $\rho = 0.1$ and $\sigma^2 = 2$.

1.4 Possible numerical approximations of Log-Normal random fields

1. Given a grid, consider multivariate Gaussian random vector X_h with mean μ_h covariance matrix Σ_h consisting of the Gaussian random field's covariance function evaluated on the grid. Let A such that $\Sigma_h = AA^T$ (e.g., via Cholesky or spectral decomposition). Sampling of X_h then via the representation $X_h = \mu_h + A\,Z$, where $Z \sim \mathcal{N}(0, I)$.

2. We expand $\kappa(x,\omega)$ using truncated Karhunen-Loève expansion with N terms

$$\kappa(x,\omega) \approx \sum_{n=1}^{N} \sqrt{\lambda_n} Y_n(\omega) e_n(x)$$

   Where $\{Y_k\}$ is a set of i.i.d. standard Gaussian. To find the eigenfunctions and eigenvalues of C we solve the eigenvalue problem

$$\int_0^1 C(x,y) e_n(y)\, \mathrm{d}y = \lambda_n e_n(x) \tag{1}$$

   We do this by discretizing C as a matrix by evaluating the function $C(x_{i+\frac{1}{2}}, x_{j+\frac{1}{2}})$ over the grid $\{x_{i+\frac{1}{2}}\}_{i=0}^{I-1} \times \{x_{i+\frac{1}{2}}\}_{i=0}^{I-1}$ with $N \le I$. Then use `MATLAB`'s function `eig()`. This discretization corresponds to a piecewise constant FEM approximation to the eigenvalue problem (1). Make sure that the computed eigenfunctions have norm 1 with respect to the continuous $L^2([0,1])$ norm.

3. Now, with the same covariance field as before, use a Fourier expansion of a periodic extension of it, namely

$$Cov_\kappa^{\#}(x-y) = \sum_{n=0}^{\infty} \kappa_n^2 \cos\left(\frac{n\pi(x-y)}{L_p}\right).$$

   Take $L_p = 2$ for instance. As a result, the stationary random field κ admits the exact representation in $[0, L_p]$

$$\kappa(\omega, x) = \sum_{n=0}^{\infty} \kappa_n \left(y_n(\omega)\cos\left(\frac{n\pi x}{L_p}\right) + z_n(\omega)\sin\left(\frac{n\pi x}{L_p}\right)\right)$$

and

- $\mathbb{E}[y_n] = \mathbb{E}[z_n] = 0$
- $Var[y_n] = Var[z_n] = 1$
- $\{y_n, z_n\}_n$ uncorrelated.

Here take iid y_n, z_n with standard Normal distribution.

1.5 Numerical approximation of $\mathbb{E}[Q(u)]$.

When working with Model 2 for $a(x, \omega)$, use the last task of 1.4 in homework 1 to deduce a relevant choice of N. Moreover, pick two different values of the parameter ν.

1. Compute, using multilevel Monte Carlo, the approximation of $\mathbb{E}[Q(u)]$ and **Model 2** only. Implement your MLMC sampling algorithm, keep in mind to use an optimal number of samples. Choose the number of samples and the number of levels such that the *total* relative error is less than 10%, 5% and 1%, respectively. Report your computational work. Does it match the predictions from MLMC theory?

   You may compare with the function `mlmc()` provided by Mike Giles and write `sums = mlmc_l(M,l,N)` to evaluate N samples at level l with level separation M. Look in `mlmc_test.m` for an example implementation.

2. Approximate the probability $P(Q(u) < K)$ using importance sampling and MLMC. Use for all levels the same importance sampling that you did in homework 1. Compute with different values of K, namely $K = -5$, $K = -10$, and $K = -20$. Choose the number of samples and the number of levels so that the relative error is less than 5%.

3. Redo at least one of either part **1** or part **2** using ML-QMC.

4. Redo question 5 ii) of homework 2 by using MLMC to estimate the exponential moments of $Q(u)$

$$\mathbb{E}[\exp(-\theta Q(u))] \approx \sum_{\ell=0}^{L} \mathbb{E}[\exp(-\theta Q(u_{h_\ell}))] - \mathbb{E}[\exp(-\theta Q(u_{h_{\ell-1}}))]$$