HW 1 Hints pt. 1

Montag, 24. April 2023 13:09

24.04.2021

Homework 1: Feedback

1) MC under exact sampling:

Estimate by Monte Carlo (MC)

$$g = \int_{[0,1]^N} f(x)\, dx$$

where f is known.

- You are given 6 choices of f.

In examples 1, 2, 4, 5 and 6 g is known in closed form.

To get a reference value of example 3 one possibility is to run MC with a sufficiently large number of samples.

Homework 1
Numerical methods for random partial differential equations: hierarchical approximation and machine learning approaches

April 14, 2023

IMPORTANT: Please refer to the course syllabus and the course outline for what an acceptable level on a handed in homework is.

1 MC under exact sampling

1.1 Objective

Hands-on experience on Monte Carlo sampling methods under the idealised assumptions of exact sampling. Tasks include the numerical versification and computable confidence regions. The idea is to connect theory and practical aspects and experiment with the methods.

1.2 Problem

We are interested in calculating the following quantity

$$g = \int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x}$$

for some given function f. We try different cases, which mainly differ by the degree of regularity of the function f. In this exercise f is known and the problem is simply integrating the function in a high dimension N.

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1.3 Model problems

We look at different examples of f for some real constants $\{c_n, w_n\}_{n=1}^N$ taken from

1. Oscillatory: $f(\mathbf{x}) = \cos\left(2\pi w_1 + \sum_{n=1}^N c_n x_n\right)$, with $c_n = 9/N$, $w_1 = \frac{1}{2}$.
   Exact solution:
   $$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \Re\left(e^{i2\pi w_1} \prod_{n=1}^N \frac{1}{ic_n}(e^{ic_n} - 1)\right)$$
   (here i denote the imaginary unit and $\Re(z)$ the real part of $z \in \mathbb{C}$)
2. Product peak: $f(\mathbf{x}) = \prod_{n=1}^N \left(c_n^{-2} + (x_n - w_n)^2\right)^{-1}$, with $c_n = 7.25/N$ and $w_n = \frac{1}{2}$.
   Exact solution:
   $$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N c_n \left(\arctan(c_n(1-w_n)) + \arctan(c_n w_n)\right)$$
3. Corner peak: $f(\mathbf{x}) = \left(1 + \sum_{n=1}^N c_n x_n\right)^{(-N+1)}$
   with $c_n = 1.85/N$.
4. Gaussian: $f(\mathbf{x}) = \exp\left(-\sum_{n=1}^N c_n^2 (x_n - w_n)^2\right)$, with $c_n = 7.03/N$ and $w_n = \frac{1}{2}$.
   Exact solution:
   $$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N \frac{\sqrt{\pi}}{2c_n} \left(\mathrm{erf}(c_n(1-w_n)) + \mathrm{erf}(c_n w_n)\right)$$
5. Continuous: $f(\mathbf{x}) = \exp\left(-\sum_{n=1}^N c_n |x_n - w_n|\right)$,with $c_n = 2.04/N$ and $w_i = \frac{1}{2}$.
   Exact solution:
   $$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \prod_{n=1}^N \frac{1}{c_n}\left(2 - e^{-c_n w_n} - e^{-c_n(1-w_n)}\right)$$
6. Discontinuous: $f(\mathbf{x}) = \begin{cases} 0 & \text{if } x_1 > w_1 \text{ or } x_2 > w_2 \\ \exp\left(\sum_{n=1}^N c_n x_n\right) & \text{otherwise} \end{cases}$, with $c_i = 4.3/N$, $w_1 = \frac{\pi}{4}$ and $w_2 = \frac{\pi}{5}$.
   Exact solution:
   $$\int_{[0,1]^N} f(\mathbf{x})\, d\mathbf{x} = \frac{1}{\prod_{n=1}^N c_n}(e^{c_1 w_1} - 1)(e^{c_2 w_2} - 1) \prod_{n=3}^N (e^{c_n} - 1)$$

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Tasks:

1) Recall the MC estimator first and write a code to estimate g for different choices of f.

2) Discuss how to estimate the MC error using the Central Limit Theorem. Compare the exact error and the error estimate. For this plot both errors as a function of the number of samples. Estimate the convergence rate. Consider different values of N.

4) First, observe that

$$\frac{1}{2\pi}\int_{\mathbb{R}^2} \max\left(e^{x_1} + e^{x_2} - K, 0\right) e^{-\frac{(x_1^2+x_2^2)}{2}}\, dx_1 dx_2 = E\left[\max\left(e^{X_1} + e^{X_2} - K, 0\right)\right]$$

where X_1 and X_2 are indep standard Gaussians.

- Use MC to estimate it for different values of K. What happens

1.4 Numerical tasks

1. Write a Monte Carlo estimator to numerically estimate (some of) these integrals. Use `MATLAB`'s function `rand(N,M)` to generate M random points in the hypercube $[0,1]^N$.
2. Estimate the error using the Central Limit Theorem. Plot the exact error and error estimates versus the number of samples used. Estimate the convergence rate. Report the square of the coefficient of variation for all cases.
   Do your computations at least for $N = 2$ and $N = 20$.
3. Repeat the previous problem using Berry-Esseen theorem.
4. Consider the approximation of the following integral, for values of $K = 3$ and $K = 6$
   $$\frac{1}{2\pi}\int_{\mathbb{R}^2} \max\left(e^{x_1} + e^{x_2} - K, 0\right) e^{\frac{-(x_1^2+x_2^2)}{2}}\, dx_1 dx_2$$
   Use importance sampling based on the shift-dilation technique, and compare it to the standard Monte Carlo estimator. Use Central Limit Theorem to control the error.

2 MC for PDEs using approximate sampling

2.1 Objective

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

2.2 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,

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

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Var = sigma^2

coeff. of variation: sigma / E[X]

3) Berry-Esseen states: Let $X_1, X_2, \ldots$ be iid real-valued random variables with

$$E[X_i] = 0,$$
$$E[X_i^2] = \sigma^2 > 0 \quad \text{and}$$
$$E[|X_i|^3] < \infty.$$

Define $Y_M = \frac{1}{M}\sum_{i=1}^{M} X_i$ and

$$\lambda := \sigma^{-1}\left(E[|Y - E[Y]|^3\right)^{\frac{1}{3}}.$$

Then

$$\Big|\underbrace{F_{Y_M}(x)}_{P(Y_M \le x)} - \underbrace{\phi(x)}_{\text{CDF of a standard normal random variable}}\Big| \le \frac{C_{BE}\lambda^3}{(1+|x|)^3\sqrt{M}} \quad \forall x \in \mathbb{R}$$

$C_{BE} \approx 30.5118$ constant

Use this to derive: $$P\left(|g - \hat{g}| \le \frac{c_0 \sigma}{\sqrt{M}}\right) \ge 2\phi(c_0) - 1 - 2\frac{C_{BE}\lambda^3}{(1+c_0)^3\sqrt{M}} \quad \forall c_0 > 0$$

• Use MC to estimate it for different values of K. What happens when K increases.

• Consider the use of Importance Sampling.

Idea: Consider shifting the distribution of X_1 and X_2 by μ_1 and μ_2 respectively

Use this to derive: $P\left(|g-\hat{g}| \le \frac{c_0 \sigma}{\sqrt{M}} \right) \ge 2\phi(c_0) - 1 - 2\frac{C_{BE}\,\lambda^3}{(1+c_0)^3\sqrt{M}} \quad \forall c_0 > 0$

MC estimator of g

(What is the advantage of this compared to the CLT?)

Remember: The goal in importance sampling is to minimize $\int_{\mathbb{R}^2} \frac{(g_K\, p)^2}{\hat{p}}(x)\, dx$

$g_K = \max(e^{x_1} + e^{x_2} - K, 0)$

A possibility to choose μ_1 and μ_2:

$$(\mu_1^*, \mu_2^*) = \underset{x_1, x_2}{\operatorname{argmax}}\ \underbrace{\max(e^{x_1} + e^{x_2} - K, 0) \cdot p_{X_1}(x_1) \cdot p_{X_2}(x_2)}$$

where

strongly suggest to look at plots of this function!

$$p_{X_1}(x) = p_{X_2}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

provide a 3D plot of the optimal density

$$p^* \propto p_{X_1}(x_1) \cdot p_{X_2}(x_2) \cdot \max(e^{x_1} + e^{x_2} - K, 0)$$

plot also the IS density using mean shifting with μ_1^* and μ_2^*

Remark: Assume we want to estimate:

$$E\left[F(\underline{X})\right]$$ by Importance Sampling.

- In the case where $F \geq 0$

$$\rho^* \propto \rho \cdot F$$

is multimodal, then the idea of shifting the mean is not efficient and can lead to a result that is worse than the standard MC.