Uncertainty Quantification and Quasi-Monte Carlo — Exercise 4
Sommersemester 2025
Return your written solutions either in person or by email
to vesa.kaarnioja@fu-berlin.de by Tuesday 27 May 2025, 10:15 am
Please make sure to return your source code for all programming tasks

1. Repeat task 3 from Exercise 3, but instead of using a Monte Carlo sample average to compute the expected value, use instead an *off-the-shelf lattice rule*. Download the file `offtheshelf.txt` from the course webpage. The file contains an *extensible*, 100-dimensional generating vector $\boldsymbol{z} \in \mathbb{N}^{100}$. For $n = 2^k$, $k \in \{10, 11, \ldots, 20\}$, you can compute the n-point QMC point set using the formula
$$\boldsymbol{y}_i = \mathrm{mod}\bigg(\frac{i\boldsymbol{z}}{n}, 1\bigg) - 0.5, \quad i = 0, 1, \ldots, n-1.$$
The QMC estimator using this *deterministic* point set is
$$\mathbb{E}[u(\boldsymbol{x}, \cdot)] \approx \frac{1}{n}\sum_{i=0}^{n-1} u(\boldsymbol{x}, \boldsymbol{y}_i).$$
To solve the PDE numerically for each $\boldsymbol{y}_i$, you can modify the script `fem.py` available on the course webpage. Fix $s = 100$ and estimate the $L^2(D)$ error of the QMC approximation by using a QMC estimate corresponding to $n' \gg n$ as a reference solution. What convergence rate do you obtain?

2. Repeat task 4 from Exercise 3, but instead of using a Monte Carlo sample average to compute the expected value, use instead an *off-the-shelf lattice rule*. Download the file `offtheshelf.txt` from the course webpage. The file contains an *extensible*, 100-dimensional generating vector $\boldsymbol{z} \in \mathbb{N}^{100}$. For $n = 2^k$, $k \in \{10, 11, \ldots, 20\}$, you can compute the n-point QMC point set using the formula
$$\boldsymbol{y}_i = \mathrm{mod}\bigg(\frac{i\boldsymbol{z}}{n}, 1\bigg) - 0.5, \quad i = 0, 1, \ldots, n-1.$$
The QMC estimators using this *deterministic* point set are
$$\mathbb{E}[\lambda(\cdot)] \approx \frac{1}{n}\sum_{i=0}^{n-1} \lambda(\boldsymbol{y}_i) \quad \text{and} \quad \mathbb{E}[u(\boldsymbol{x}, \cdot)] \approx \frac{1}{n}\sum_{i=0}^{n-1} u(\boldsymbol{x}, \boldsymbol{y}_i).$$
To solve the PDE numerically for each $\boldsymbol{y}_i$, you can modify the script `fem.py` available on the course webpage. Fix $s = 100$ and estimate the Euclidean error of $\mathbb{E}[\lambda(\cdot)]$ and the $L^2(D)$ error of the QMC approximations by using a QMC estimate corresponding to $n' \gg n$ as a reference solution. What convergence rate(s) do you obtain?

   Tasks 1 and 2: If computing the reference solution using $n = 2^{20}$ takes too long, you can of course use a smaller value like $n = 2^{16}$ instead.

The exercises continue on the next page.

3. Let $s, n \in \mathbb{N}$, $z_1, \ldots, z_s \in \mathbb{U}_n := \{k \in \mathbb{N} \mid 1 \leq k \leq n,\ \gcd(k,n) = 1\}$, and $\gamma_{\mathfrak{u}} \in \mathbb{R}_+$ for all $\varnothing \neq \mathfrak{u} \subseteq \{1, \ldots, s\}$. During the lectures, we derived the following formula for the *shift-averaged worst-case error* for integrands belonging to unanchored, weighted Sobolev spaces:

$$[e^{\mathrm{sh}}_{n,s}(z_1, \ldots, z_s)]^2 = \frac{1}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} B_2\bigg(\bigg\{\frac{kz_j}{n}\bigg\}\bigg),$$

where the braces $\{x\} := x - \lfloor x \rfloor$ denote the *fractional part* of a non-negative real number $x \geq 0$, $\lfloor x \rfloor := \max\{k \in \mathbb{Z} : k \leq x\}$ for $x \in \mathbb{R}$, and $B_2(x) := x^2 - x + \frac{1}{6}$ is the Bernoulli polynomial of degree 2.

(a) When $s = 1$, show that

$$[e^{\mathrm{sh}}_{n,1}(z_1)]^2 = \frac{\gamma_{\{1\}}}{6n^2}.$$

(b) Use part (a) to conclude that

$$[e^{\mathrm{sh}}_{n,1}(z_1)]^2 \leq \bigg(\frac{1}{\varphi(n)} \gamma_{\{1\}}^{\lambda} \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\bigg)^{1/\lambda} \quad \text{for all } \lambda \in \big(\tfrac{1}{2}, 1\big],$$

where $\varphi(n) := |\mathbb{U}_n|$ is the *Euler totient function* for $n \in \mathbb{N}$, where the bars $|\cdot|$ denote the cardinality of a set, and $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$ is the *Riemann zeta function* for $x > 1$.

4. Let $B_2(x) := x^2 - x + \frac{1}{6}$ be the Bernoulli polynomial of degree 2 and let $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\ldots,s\}}$ be a sequence of positive weights. Recall that the weighted, unanchored Sobolev space $H_{s,\boldsymbol{\gamma}}$ is characterized by the reproducing kernel

$$K_{s,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) := \sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \eta(x_j, y_j), \quad \boldsymbol{x}, \boldsymbol{y} \in [0,1]^s,$$

where

$$\eta(x, y) := \tfrac{1}{2} B_2(|x - y|) + (x - \tfrac{1}{2})(y - \tfrac{1}{2}), \quad x, y \in [0,1].$$

Show that

$$\int_{[0,1]^s} K_{s,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{y} = 1,$$

$$\int_{[0,1]^s} \int_{[0,1]^s} K_{s,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \,\mathrm{d}\boldsymbol{y} = 1,$$

$$\int_{[0,1]^s} K_{s,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} = \sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}} (\tfrac{1}{6})^{|\mathfrak{u}|}.$$