Uncertainty Quantification and Quasi-Monte Carlo Exercise 6
Sommersemester 2025
Return your written solutions either in person or by email
to vesa.kaarnioja@fu-berlin.de by Tuesday 10 June 2025, 10:15 am
Please make sure to return your source code for all programming tasks

Let $U_s := [-1/2, 1/2]^s$ and $D = (0, 1)$. Consider the Dirichlet–Neumann problem

$$\begin{cases} -\dfrac{\partial}{\partial x}\left(a(x, \boldsymbol{y})\dfrac{\partial}{\partial x}u(x, \boldsymbol{y})\right) = f(x), & x \in D,\ \boldsymbol{y} \in U_s, \\ u(0, \boldsymbol{y}) = 0 = \dfrac{\partial}{\partial x}u(1, \boldsymbol{y}), & \boldsymbol{y} \in U_s, \end{cases}$$

endowed with the parametric coefficient

$$a(x, \boldsymbol{y}) := a_0(x) + \sum_{j=1}^{s} y_j \psi_j(x), \quad x \in D,\ \boldsymbol{y} = (y_j)_{j=1}^s \in U_s,$$

where $a_0 \in L^\infty(D)$ and $\psi_j \in L^\infty(D)$ for all $j \geq 1$. Furthermore, we assume that $f \in L^2(D)$ is given and there exist constants $a_{\min}, a_{\max} > 0$ such that $0 < a_{\min} \leq a(x, \boldsymbol{y}) \leq a_{\max} < \infty$ for all $x \in D$ and $\boldsymbol{y} \in U_s$.

The solution is given by

$$u(x, \boldsymbol{y}) = \int_0^x \left(\int_w^1 f(z)\,\mathrm{d}z \right) \frac{1}{a(w, \boldsymbol{y})}\,\mathrm{d}w, \quad x \in D,\ \boldsymbol{y} \in U_s. \tag{1}$$

1. Show that

$$|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} u(x, \boldsymbol{y})| \leq \frac{\|f\|_{L^2(D)}}{a_{\min}} |\boldsymbol{\nu}|! \boldsymbol{b}^{\boldsymbol{\nu}} \quad \text{for all } x \in D,\ \boldsymbol{y} \in U_s,\ \boldsymbol{\nu} \in \mathbb{N}_0^s,$$

   where $\boldsymbol{b} = (b_j)_{j=1}^s$ with $b_j = \frac{\|\psi_j\|_{L^\infty(D)}}{a_{\min}}$, $\boldsymbol{b}^{\boldsymbol{\nu}} = \prod_{j=1}^s b_j^{\nu_j}$, and $|\boldsymbol{\nu}| := \sum_{j=1}^s \nu_j$.

2. Let $\boldsymbol{\gamma} := (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\dots,s\}}$ be a sequence of positive real numbers. During the lectures we considered an unanchored, weighted Sobolev space $H_{s,\boldsymbol{\gamma}}$ equipped with the norm

$$\|f\|_{s,\boldsymbol{\gamma}}^2 = \sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \frac{1}{\gamma_{\mathfrak{u}}} \int_{[0,1]^{|\mathfrak{u}|}} \left(\int_{[0,1]^{s-|\mathfrak{u}|}} \frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{y}_{\mathfrak{u}}} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right)^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}}, \quad f \in H_{s,\boldsymbol{\gamma}},$$

   where $\mathrm{d}\boldsymbol{y}_{\mathfrak{u}} := \prod_{j \in \mathfrak{u}} \mathrm{d}y_j$ and $\mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} := \prod_{j \in \{1,\dots,s\} \setminus \mathfrak{u}} \mathrm{d}y_j$ for $\mathfrak{u} \subseteq \{1, \dots, s\}$.

   Fix $x \in D$ and define $F(\boldsymbol{y}) = u(x, \boldsymbol{y} - \frac{\mathbf{1}}{\mathbf{2}})$ for $\boldsymbol{y} \in [0, 1]^s$. Show that

$$\|F\|_{s,\boldsymbol{\gamma}}^2 \leq \frac{\|f\|_{L^2(D)}^2}{a_{\min}^2} \sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j \in \mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}}. \tag{2}$$

3. Let us consider the QMC approximation of the integral $\int_{[0,1]^s} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$. Using s, n, and $\boldsymbol{\gamma}$ as inputs in a component-by-component (CBC) algorithm, it is possible to construct a QMC rule satisfying the error bound

$$\text{R.M.S. error} \le \left(\frac{1}{\varphi(n)} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1,\dots,s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{\frac{1}{2\lambda}} \|F\|_{s,\boldsymbol{\gamma}} \quad \text{for all } \lambda \in (\tfrac{1}{2}, 1],$$

where $\varphi(n) = |\{k \in \mathbb{N} : 1 \le k \le n,\ \gcd(k,n) = 1\}|$ is the Euler totient function and $\zeta(x) = \sum_{k=1}^{\infty} k^{-x}$ is the Riemann zeta function for $x > 1$.

By plugging in (2), we obtain the error bound

$$\begin{aligned}&\text{R.M.S. error}\\ &\le \frac{\|f\|_{L^2(D)}}{a_{\min}} \left(\frac{1}{\varphi(n)} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1,\dots,s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\right)^{|\mathfrak{u}|}\right)^{\frac{1}{2\lambda}} \left(\sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j \in \mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}}\right)^{\frac{1}{2}}.\end{aligned} \tag{3}$$

Show that the upper bound (3) is minimized by choosing the weights

$$\gamma_{\mathfrak{u}} = \left(|\mathfrak{u}|! \prod_{j \in \mathfrak{u}} \frac{b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^{\lambda}}}\right)^{\frac{2}{1+\lambda}}, \quad \mathfrak{u} \subseteq \{1,\dots,s\}, \tag{4}$$

where we use the convention that an empty product is equal to 1.

4. Let us consider a simple numerical discretization of (1). Let $x_k = hk$, $h = \frac{1}{100}$, $k \in \{0,\dots,100\}$. For simplicity, let $f(x) = 1$. The integral in (1) can be discretized, e.g., using the trapezoidal rule as

$$\int_0^{x_k} g(w,\boldsymbol{y})\,\mathrm{d}w \approx h \sum_{i=1}^{k} \frac{g(x_i,\boldsymbol{y}) + g(x_{i-1},\boldsymbol{y})}{2} \text{ for } k \in \{1,\dots,100\} \text{ with } g(w,\boldsymbol{y}) := \frac{1-w}{a(w,\boldsymbol{y})}.$$

This leads to the discretized solution

$$\boldsymbol{u}(\boldsymbol{y}) = G\frac{1}{\boldsymbol{a}(\boldsymbol{y})}, \tag{5}$$

where $G \in \mathbb{R}^{100\times 101}$, $\boldsymbol{u}(\boldsymbol{y}) = [u(x_1,\boldsymbol{y}),\dots,u(x_{100},\boldsymbol{y})]^{\mathrm{T}}$, $\boldsymbol{a}(\boldsymbol{y}) = [a(x_0,\boldsymbol{y}),\dots,a(x_{100},\boldsymbol{y})]^{\mathrm{T}}$, and $\frac{1}{\boldsymbol{a}(\boldsymbol{y})} = \big(\frac{1}{a(x_{i-1},\boldsymbol{y})}\big)_{i=1}^{101}$ denotes the elementwise reciprocal vector of $\boldsymbol{a}$.

   (a) In tasks 1–3, we analyzed the use of QMC for the *non-discretized problem*. Are the conclusions still valid for the numerically discretized solution (5)?

   (b) Fix $x = 0.5$ ($= x_{50}$ in our discretization) and consider the function $F(\boldsymbol{y}) = u(0.5, \boldsymbol{y} - \mathbf{1/2})$, $\boldsymbol{y} \in [0,1]^s$. We can apply a randomly shifted rank-1 lattice rule by drawing R shifts $\boldsymbol{\Delta}_1,\dots,\boldsymbol{\Delta}_R$ from $\mathcal{U}([0,1]^s)$ and computing the cubatures

$$Q_n^{(r)} F = \frac{1}{n} \sum_{k=1}^{n} F(\operatorname{mod}(\boldsymbol{t}_k + \boldsymbol{\Delta}_r, 1)) \quad \text{for } r \in \{1,\dots,R\},$$

where $\boldsymbol{t}_k = \mathrm{mod}(\frac{k\boldsymbol{z}}{n}, 1)$. As our approximation of $\int_{[0,1]^s} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}$, we take the average

$$\overline{Q}_{n,R}F = \frac{1}{R}\sum_{r=1}^{R} Q_n^{(r)}F.$$

We can estimate the root-mean-square error by computing

$$E_{n,R} = \sqrt{\frac{1}{R(R-1)}\sum_{r=1}^{R}(\overline{Q}_{n,R}F - Q_n^{(r)}F)^2}.$$

Fix a "reasonable" number of random shifts (e.g., you may choose $R = 4$ or $R = 8$ or $R = 16$ ...) and compute $E_{n,R}$ for increasing n. As the parameterization of the diffusion coefficient, you can consider, e.g.,

$$a(x, \boldsymbol{y}) = 1 + \sum_{j=1}^{s} y_j j^{-2}\sin(\pi j x), \quad x \in D,\ \boldsymbol{y} \in [-1/2, 1/2]^s.$$

Fix $s = 100$ and, for increasing n, use two different generating vectors:

(i) a generating vector obtained using the fast CBC algorithm with weights (4);

(ii) an "off-the-shelf" generating vector `offtheshelf.txt` available on the course webpage.

Compute the root-mean-square errors for both point sets and compare the results.