Quasi-Monte Carlo methods for PDE uncertainty quantification
Autumn School – Uncertainty Quantification for High-Dimensional Problems

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 $\boldsymbol{\gamma} := (\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1,\ldots,s\}}$ 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

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

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

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

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

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

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

where $\varphi(n) = |\{k \in \mathbb{N} : 1 \leq k \leq n-1,\ \gcd(k,n) = 1\}|$ 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

$$\text{R.M.S. error} \\ \leq \frac{\|f\|_{L^2(D)}}{a_{\min}} \bigg(\frac{1}{\varphi(n)} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}}^{\lambda} \Big(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}}\Big)^{|\mathfrak{u}|}\bigg)^{\frac{1}{2\lambda}} \bigg(\sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \frac{(|\mathfrak{u}|!)^2 \prod_{j\in\mathfrak{u}} b_j^2}{\gamma_{\mathfrak{u}}}\bigg)^{\frac{1}{2}}. \tag{3}$$

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

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

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

Under which conditions can the R.M.S. error be bounded independently of the dimension s?

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

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

This leads to the discretized solution

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

where $G \in \mathbb{R}^{100\times 101}$, $\boldsymbol{u}(\boldsymbol{y}) = [u(x_1,\boldsymbol{y}),\ldots,u(x_{100},\boldsymbol{y})]^{\mathrm{T}}$, $\boldsymbol{a}(\boldsymbol{y}) = [a(x_0,\boldsymbol{y}),\ldots,a(x_{100},\boldsymbol{y})]^{\mathrm{T}}$, 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 $F(\boldsymbol{y}) = u(0.5, \boldsymbol{y} - \frac{\mathbf{1}}{\mathbf{2}})$, $\boldsymbol{y} \in [0,1]^s$. We can apply a randomly shifted rank-1 lattice rule by drawing R shifts $\boldsymbol{\Delta}_1,\ldots,\boldsymbol{\Delta}_R$ from $\mathcal{U}([0,1]^s)$ and computing the cubatures

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

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.,

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

What convergence rate do you observe?

For $s = 10$ and $n \in \{2^{10}, 2^{11}, \ldots, 2^{20}\}$, you can use the following precomputed ("off-the-shelf") generating vector:

$$\boldsymbol{z} = [1, 182667, 279195, 223491, 205755, 359329, 198937, 246491, 466233, 379083]^{\mathrm{T}}.$$

Tailored lattices with arbitrary s and n for this integration problem can be obtained by using a CBC algorithm with the weights (4) as inputs. Some implementations and "off-the-shelf" lattice rules are available at [1, 2, 3].

Note: "Off-the-shelf" lattice rules tend to work pretty well in practice and it is quite common to simply use some of the precomputed ones available at [1, 3]. However, strictly speaking, one loses the convergence guarantee when the generating vector is not obtained using a CBC algorithm with weights appropriately tailored for the integration problem.

References

[1] F. Y. Kuo. Lattice rule generating vectors. `https://web.maths.unsw.edu.au/~fkuo/lattice/`

[2] F. Y. Kuo and D. Nuyens. *QMC4PDE*. `https://people.cs.kuleuven.be/~dirk.nuyens/qmc4pde/`

[3] D. Nuyens. *Magic Point Shop*. `https://people.cs.kuleuven.be/~dirk.nuyens/qmc-generators/`