Uncertainty Quantification and Quasi-Monte Carlo — Bonus exercises
Wintersemester 2022/23
*These exercises will not be graded and do not need to be returned.*

1. Consider the elliptic PDE problem

$$\begin{cases} -\nabla\cdot(a(\boldsymbol{x})\nabla u(\boldsymbol{x})) = f(\boldsymbol{x}), & \boldsymbol{x}\in D,\\ u(\boldsymbol{x}) = 0, & \boldsymbol{x}\in\partial D.\end{cases}$$

   Implement a finite element solver for this PDE in Python. You may consider the domain $D=(0,1)^2$ and model your code according to the MATLAB solver available on the course webpage (you are also welcome to do something more sophisticated).

   Test the program you wrote using the following parameters: $a(x_1,x_2)=1$, $f(x_1,x_2)=x_1+x_2$, and $D=(0,1)^2$. Does your FE solution resemble the function illustrated on slide 25 of `https://vesak90.userpage.fu-berlin.de/week5.pdf`?

2. 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

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

   where

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

   Show that

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

3. Let $K_{s,\boldsymbol{\gamma}}$ and $\eta$ be defined as in (1) and (2), respectively. Show that

$$\int_0^1 \eta(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta = B_2(|x-y|) \quad \text{for } x,y\in[0,1],$$

   where $\{x\} := x - \lfloor x\rfloor$ is the fractional part of $x\geq 0$ and $\lfloor x\rfloor := \max\{k\in\mathbb{Z}\mid k\leq x\}$ is the floor function. Use the above to deduce that the shift-invariant kernel associated with $K_{s,\boldsymbol{\gamma}}$, i.e.,

$$K^{\mathrm{sh}}_{s,\boldsymbol{\gamma}}(\boldsymbol{x},\boldsymbol{y}) := \int_{[0,1]^s} K_{s,\boldsymbol{\gamma}}(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}$$

can be written as

$$K_{s,\boldsymbol{\gamma}}^{\rm sh}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1,\ldots,s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} B_2(|x_j-y_j|).$$

Moreover, if the weights are *product weights*, i.e., they can be written as

$$\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j \quad \text{for } \mathfrak{u}\subseteq\{1,\ldots,s\},$$

where $\gamma_1,\ldots,\gamma_s > 0$ and we interpret an empty product as 1, show that the above expression simplifies to

$$K_{s,\boldsymbol{\gamma}}^{\rm sh}(\boldsymbol{x},\boldsymbol{y}) = \prod_{j=1}^{s}(1+\gamma_j B_2(|x_j-y_j|)).$$

4. Let $f \in C([0,1)^s)$ be a 1-periodic function with respect to each of its variables and define

$$r_\alpha(\boldsymbol{\gamma},\boldsymbol{h}) := \gamma_{\mathrm{supp}(\boldsymbol{h})}^{-1} \prod_{j\in\mathrm{supp}(\boldsymbol{h})} |h_j|^\alpha \quad \text{for } \alpha>1 \text{ and } \boldsymbol{h}\in\mathbb{Z}^s,$$

where $\mathrm{supp}(\boldsymbol{h}) := \{j\in\{1,\ldots,s\} : h_j \neq 0\}$ and $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1,\ldots,s\}}$ denotes a collection of positive weights.

Recall from the lectures that

$$\frac{1}{n}\sum_{k=1}^{n} f\left(\left\{\frac{k\boldsymbol{z}}{n}\right\}\right) - \int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \sum_{\boldsymbol{h}\in\Lambda^\perp\setminus\{\boldsymbol{0}\}} \widehat{f}(\boldsymbol{h}),$$

where $\widehat{f}(\boldsymbol{h}) := \int_{[0,1]^s} f(\boldsymbol{x})\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{h}\cdot\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x}$ and the dual lattice $\Lambda^\perp := \{\boldsymbol{h}\in\mathbb{Z}^s \mid \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod{n}\}$ is determined entirely by the generating vector $\boldsymbol{z}\in\mathbb{Z}^s$ and $n\in\mathbb{N}$.

Show that

$$\left|\frac{1}{n}\sum_{k=1}^{n} f\left(\left\{\frac{k\boldsymbol{z}}{n}\right\}\right) - \int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\right| \le P_\alpha(\boldsymbol{\gamma},\boldsymbol{z})\|f\|_\alpha,$$

where

$$P_\alpha(\boldsymbol{\gamma},\boldsymbol{z}) := \sum_{\boldsymbol{h}\in\Lambda^\perp\setminus\{\boldsymbol{0}\}} \frac{1}{r_\alpha(\boldsymbol{\gamma},\boldsymbol{h})} \quad \text{for } \alpha>1 \tag{3}$$

and

$$\|f\|_\alpha := \sup_{\boldsymbol{h}\in\mathbb{Z}^s} |\widehat{f}(\boldsymbol{h})| r_\alpha(\boldsymbol{\gamma},\boldsymbol{h}) \quad \text{for } \alpha>1. \tag{4}$$

5. Let $\alpha \geq 2$ be an even integer. Show that (3) can be written as

$$P_\alpha(\boldsymbol{\gamma}, \boldsymbol{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \omega\Big(\Big\{\frac{k z_j}{n}\Big\}\Big),$$

where

$$\omega(x) := (2\pi)^\alpha \frac{B_\alpha(x)}{(-1)^{\alpha/2+1}\alpha!}, \ x \in [0,1],$$

and $B_\alpha(x) := \frac{(-1)^{\alpha/2+1}\alpha!}{(2\pi)^\alpha} \sum_{h \in \mathbb{Z}\setminus\{0\}} \frac{\mathrm{e}^{2\pi \mathrm{i} h x}}{h^\alpha}$, $x \in [0,1]$, is the (Fourier series representation of the) *Bernoulli polynomial of degree $\alpha$*.

*Hint:* This is actually pretty difficult, so you can either assume product weights $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ or an unweighted setting with $\gamma_{\mathfrak{u}} \equiv 1$. The character property on slide 7 of `https://vesak90.userpage.fu-berlin.de/week7.pdf` may also be helpful.

*Significance:* If one wanted to develop a CBC algorithm for certain classes of smooth, periodic functions, one could use the expression derived for $P_\alpha(\boldsymbol{\gamma}, \boldsymbol{z})$ in task 5 as the search criterion! (Compare with the shift-averaged worst-case error from the lectures.) For further details, see, e.g., "Good lattice rules in weighted Korobov spaces with general weights" by Dick, Sloan, Wang, and Woźniakowski (2006).

6. Let $\alpha \geq 2$ be an even integer. Show that the norm (4) can be bounded by

$$\|f\|_\alpha \leq \max_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \frac{1}{(2\pi)^{\alpha|\mathfrak{u}|}\gamma_{\mathfrak{u}}} \int_{[0,1]^{|\mathfrak{u}|}} \bigg| \int_{[0,1]^{s-|\mathfrak{u}|}} \bigg( \prod_{j \in \mathfrak{u}} \frac{\partial^\alpha}{\partial y_j^\alpha} \bigg) f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \bigg| \, \mathrm{d}\boldsymbol{y}_{\mathfrak{u}},$$

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

*Hint:* Like the previous task, you can also assume either product weights or $\gamma_{\mathfrak{u}} \equiv 1$ if this seems challenging.

7. Let $\mathscr{F} := \{\boldsymbol{m} \in \mathbb{N}_0^{\mathbb{N}} \mid |\boldsymbol{m}| := \sum_{j=1}^\infty m_j < \infty\}$ denote the set of finitely supported multi-indices. Let $\boldsymbol{b} = (b_j)_{j \geq 1}$ be a sequence of non-negative numbers and let $(\mathbb{A}_{\boldsymbol{\nu}})_{\boldsymbol{\nu} \in \mathscr{F}}$ and $(\mathbb{B}_{\boldsymbol{\nu}})_{\boldsymbol{\nu} \in \mathscr{F}}$ be non-negative numbers satisfying the inequality

$$\mathbb{A}_{\boldsymbol{\nu}} \leq \sum_{j \in \mathrm{supp}(\boldsymbol{\nu})} \nu_j b_j \mathbb{A}_{\boldsymbol{\nu}-\boldsymbol{e}_j} + \mathbb{B}_{\boldsymbol{\nu}} \quad \text{for all } \boldsymbol{\nu} \in \mathscr{F} \text{ (including } \boldsymbol{\nu} = \boldsymbol{0}),$$

where $\mathrm{supp}(\boldsymbol{\nu}) := \{j \in \mathbb{N} \mid \nu_j \neq 0\}$. Prove that

$$\mathbb{A}_{\boldsymbol{\nu}} \leq \sum_{\boldsymbol{m} \leq \boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} |\boldsymbol{m}|! \boldsymbol{b}^{\boldsymbol{m}} \mathbb{B}_{\boldsymbol{\nu}-\boldsymbol{m}} \quad \text{for all } \boldsymbol{\nu} \in \mathscr{F}.$$

8. Let $D \subset \mathbb{R}^d$, $d \in \{2,3\}$, be a bounded Lipschitz domain and let $U := [-1/2, 1/2]^{\mathbb{N}}$ be a set of parameters. Define

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

which is assumed to satisfy the following:

(A1) there exist $a_{\min}, a_{\max} > 0$ such that $0 < a_{\min} \le a(\boldsymbol{x},\boldsymbol{y}) \le a_{\max} < \infty$ for all $\boldsymbol{x} \in D$ and $\boldsymbol{y} \in D$.

(A2) $a_0 \in L^\infty(D)$ and $\psi_j \in L^\infty(D)$ for all $j \ge 1$.

(A3) $\sum_{j=1}^\infty \|\psi_j\|_{L^\infty(D)}^p < \infty$ for some $p \in (0,1)$.

Consider the *coupled PDE system*

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla u(\boldsymbol{x},\boldsymbol{y})) = f(\boldsymbol{x}), & \boldsymbol{x} \in D,\ \boldsymbol{y} \in U, \\ u(\boldsymbol{x},\boldsymbol{y}) = 0, & \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in U, \\ -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{y})\nabla q(\boldsymbol{x},\boldsymbol{y})) = u(\boldsymbol{x},\boldsymbol{y}), & \boldsymbol{x} \in D,\ \boldsymbol{y} \in U, \\ q(\boldsymbol{x},\boldsymbol{y}) = 0, & \boldsymbol{x} \in \partial D,\ \boldsymbol{y} \in U, \end{cases}$$

where $f\colon D \to \mathbb{R}$ is a fixed source term.

The weak formulation of this problem is to find, for all $\boldsymbol{y} \in U$, $u(\cdot,\boldsymbol{y}) \in H_0^1(D)$ and $q(\cdot,\boldsymbol{y}) \in H_0^1(D)$ such that

$$\int_D a(\boldsymbol{x},\boldsymbol{y})\nabla u(\boldsymbol{x},\boldsymbol{y}) \cdot \nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_D f(\boldsymbol{x})v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \text{for all } v \in H_0^1(D),$$
$$\int_D a(\boldsymbol{x},\boldsymbol{y})\nabla q(\boldsymbol{x},\boldsymbol{y}) \cdot \nabla v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_D u(\boldsymbol{x},\boldsymbol{y})v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \quad \text{for all } v \in H_0^1(D),$$

where we assume that $f \in L^2(D)$.

Find a parametric regularity bound for $\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} q(\cdot,\boldsymbol{y})\|_{H_0^1(D)}$, where $\boldsymbol{y} \in U$ and $\boldsymbol{\nu} \in \mathscr{F}$.

*Hint:* The result proved in task 7 may be helpful.

9. Let $q_s(\cdot,(y_1,\ldots,y_s)) := q(\cdot,(y_1,\ldots,y_s,0,0,\ldots))$, where $q$ is defined as in task 8. Let

$$I_s(f) := \int_{[0,1]^s} f(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \quad \text{and} \quad Q_{n,s}^{\boldsymbol{\Delta}}(f) := \frac{1}{n}\sum_{k=1}^n f\bigg(\bigg\{\frac{k\boldsymbol{z}}{n} + \boldsymbol{\Delta}\bigg\} - \frac{\mathbf{1}}{\mathbf{2}}\bigg),$$

i.e., $Q_{n,s}^{\boldsymbol{\Delta}}$ denotes a shifted lattice rule with generating vector $\boldsymbol{z} \in \mathbb{N}^s$ and shift $\boldsymbol{\Delta} \in [0,1]^s$.

Let $n$ be either prime or $n = 2^k$, $k \in \mathbb{N}$, and let $G \in H^{-1}(D)$. Show that there exists a generating vector that can be constructed using the CBC algorithm such that

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}|I_s(G(q_s)) - Q_{n,s}^{\boldsymbol{\Delta}}(G(q_s))|^2} \le Cn^{\max\{-1/p+1/2,-1+\delta\}}, \tag{5}$$

where $\delta \in (0,1/2)$ is arbitrary and the constant $C > 0$ is independent of the dimension $s$.

10. The QMC cubature convergence rate (5) remains of course invariant when we replace $q_s$ by a discrete approximation solved from the coupled PDE system in task 8 using a conforming finite element method. Validate the convergence rate in task 9 numerically by solving $q_s$ approximately using the finite element

method and fixed dimension $s = 100$. As the quantity of interest $G \in H^{-1}(D)$, take

$$G(v) := \int_D v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \quad v \in H_0^1(D).$$

(You can have a look at exercise sheet 11 to get an idea of how to compute $G(v_h)$ numerically when $v_h$ is an element of a finite element space!)

You can choose the parameterization of the diffusion coefficient freely. You can try, for example, $a_0(x_1, x_2) = 1$ and $\psi_j(x_1, x_2) = j^{-2}\sin(j\pi x_1)\sin(j\pi x_2)$.

To solve the coupled PDE numerically using the finite element method, you can use the routine you wrote in task 1, the MATLAB code available on the course webpage or you can download the file `FEM5.mat` from the course webpage. The file contains FE matrices as well as other FEM objects corresponding to a FE discretization of the computational domain $D = (0, 1)^2$. The file contains the stiffness tensor `grad`, mass matrix `mass`, FE nodes `nodes`, mesh element connectivity array `element`, a vector containing indices of the interior FE nodes `interior`, element center points `centers`, the number of FE coordinates `ncoord`, and the number of FE elements `nelem`. These were generated by the `FEMdata.m` MATLAB routine. In MATLAB, you can import the data using the command `load FEM5.mat`. In Python, this can be achieved via

```
import numpy as np
import scipy.io
mat = scipy.io.loadmat('FEM5.mat')
```

The contents can be accessed via `mat['grad']`, `mat['mass']`, `mat['nodes']`, etc.

As the generating vector, you can use an off-the-shelf lattice rule which you can download from the address `https://vesak90.userpage.fu-berlin.de/offtheshelf.txt`. Alternatively, you can use either the `fastcbc.m` routine available on the course webpage or, e.g., the Python routines available at `https://people.cs.kuleuven.be/~dirk.nuyens/qmc4pde/`. Note that if you use tailored generating vectors instead of the off-the-shelf lattice, you will need to recompute the generating vector for each value of $n$. (The off-the-shelf lattice rule has been designed to work for $n = 2^k$ cubature nodes with $k = 10, \ldots, 20$, whereas the `fastcbc.m` and QMC4PDE codes only work for a single value of $n$.) Note that if you use a tailored QMC rule, then you are theoretically guaranteed to get a dimensionally-independent QMC convergence rate (although in practice, the off-the-shelf lattice usually has comparable performance).