Quasi-Monte Carlo approach to Bayesian optimal experimental design

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Part I: Quasi-Monte Carlo methods

Lattice rules

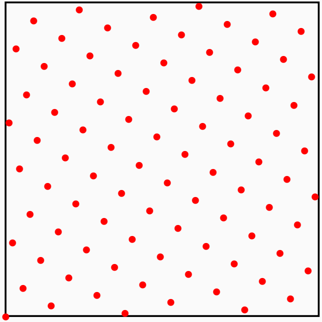
Rank-1 lattice rules

$$Q_{s,n}(f) = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{t}_i)$$

have the points

$$\boldsymbol{t}_i = \operatorname{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.



Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

The quality of the lattice rule is determined by the choice of $\boldsymbol{z}$.

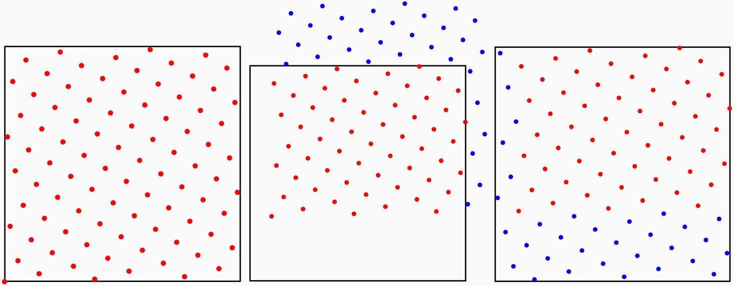
Randomly shifted lattice rules

Shifted rank-1 lattice rules have points

$$\boldsymbol{t}_i = \operatorname{mod}\left(\frac{i\boldsymbol{z}}{n} + \boldsymbol{\Delta}, 1\right), \quad i \in \{1, \ldots, n\}.$$

$\boldsymbol{\Delta} \in [0,1)^s$ is the *shift*

Use a number of random shifts for error estimation.



Lattice rule shifted by $\boldsymbol{\Delta} = (0.1, 0.3)$.

Let $\mathbf{\Delta}^{(r)}$, $r = 1, \ldots, R$, be independent random shifts drawn from $U([0,1]^s)$ and define

$$Q_{s,n}^{(r)}(f) := \frac{1}{n} \sum_{i=1}^{n} f(\mathrm{mod}(\boldsymbol{t}_i + \mathbf{\Delta}^{(r)}, 1)). \text{ (QMC rule with 1 random shift)}$$

Then

$$\overline{Q}_{s,n}(f) = \frac{1}{R} \sum_{r=1}^{R} Q_{s,n}^{(r)} f \qquad \text{(QMC rule with } R \text{ random shifts)}$$

is an unbiased estimator of $I_s(f)$.

Tailoring QMC cubatures: Suppose that $f \in H_{s,\boldsymbol{\gamma}}$ for all $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$, where $H_{s,\boldsymbol{\gamma}}$ denotes a weighted Sobolev space with dominating mixed smoothness, equipped with norm

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

Then for any given sequence of weights $\boldsymbol{\gamma}$, we can use the CBC algorithm to obtain a generating vector satisfying the error bound

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} |I_s f - Q_{s,n}^{\boldsymbol{\Delta}} f|^2} \le \left(\frac{1}{\varphi(n)} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathfrak{u}|} \right)^{1/(2\lambda)} \|f\|_{s,\boldsymbol{\gamma}} \tag{1}$$

for all $\lambda \in (1/2, 1]$. Here, φ is the Euler totient function and ζ is the Riemann zeta function. We can play the following game:

- For a given integrand f, estimate the norm $\|f\|_{s,\boldsymbol{\gamma}}$.
- Find weights $\boldsymbol{\gamma}$ which *minimize* the error bound (1).
- Using the optimized weights $\boldsymbol{\gamma}$ as input, use the CBC algorithm to find a generating vector which *satisfies* the error bound (1).

(Cf., e.g., the survey by Kuo and Nuyens in FoCM 2016 or the tutorial by the same authors in MCQMC 2016 proceedings, and references therein.)

Part II: Bayesian optimal experimental design

Let $G\colon \Theta \times \Xi \to \mathbb{R}^k$ be a forward mapping depending on a true parameter $\boldsymbol{\theta} \in \Theta$ and a design parameter $\boldsymbol{\xi} \in \Xi$.

Measurement model:

$$\boldsymbol{y} = G(\boldsymbol{\theta}, \boldsymbol{\xi}) + \boldsymbol{\eta},$$

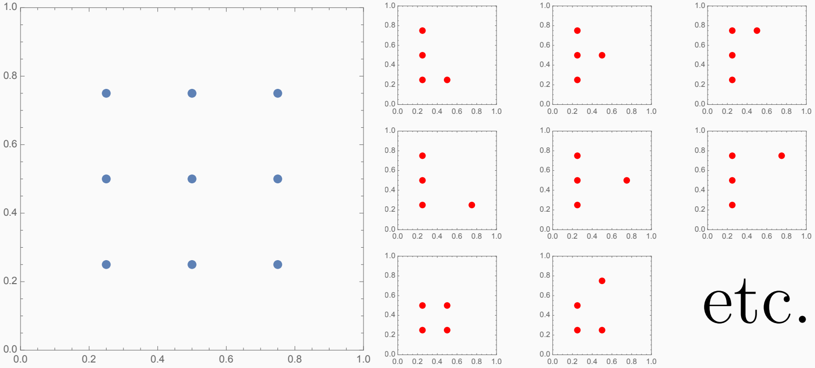
where $\boldsymbol{y} \in \mathbb{R}^k$ is the measurement data and $\boldsymbol{\eta} \in \mathbb{R}^k$ is Gaussian noise such that $\boldsymbol{\eta} \sim \mathcal{N}(0, \Gamma)$ with positive definite covariance matrix $\Gamma \in \mathbb{R}^{k \times k}$.

Goal in Bayesian optimal experimental design: Recover the design parameter $\boldsymbol{\xi}$ for the Bayesian inference of $\boldsymbol{\theta}$, which we model as a random variable endowed with prior distribution $\pi(\boldsymbol{\theta})$.

Example

Suppose we have 9 slots and 4 sensors. Before carrying out the experiment, which 4 slots do we expect to be the most informative for the recovery of the unknown parameter?

$\rightarrow \binom{9}{4} = 126$ possible configurations



Left: 9 slots. Right: We have 126 possible ways to place 4 sensors into 9 slots.

How to rank the 126 different possibilities from most informative to least informative?

A measure of the information gain for a given design $\boldsymbol{\xi}$ and data $\boldsymbol{y}$ is given by the Kullback–Leibler divergence

$$D_{\mathrm{KL}}(\pi(\cdot|\boldsymbol{y},\boldsymbol{\xi})\|\pi(\cdot)) := \int_{\Theta} \log\left(\frac{\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\theta})}\right)\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}. \tag{2}$$

We wish to maximize the expected utility (2) over the design space Ξ with respect to the data $\boldsymbol{y}$ and model parameters $\boldsymbol{\theta}$:

$$\max_{\boldsymbol{\xi}\in\Xi} \underbrace{\int_{Y}\int_{\Theta} \log\left(\frac{\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\theta})}\right)\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})\pi(\boldsymbol{y}|\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}}_{=:\mathrm{EIG}},$$

where $\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})$ corresponds to the posterior distribution of the parameter $\boldsymbol{\theta}$ and $\pi(\boldsymbol{y}|\boldsymbol{\xi}) = \int_{\Theta} \pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})\pi(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}$ is the marginal distribution of the data $\boldsymbol{y}$.

The posterior is given by Bayes' theorem

$$\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi}) = \frac{\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})\pi(\boldsymbol{\theta})}{\pi(\boldsymbol{y}|\boldsymbol{\xi})},$$

which means that the expected utility can be written as

$$\begin{aligned}
\mathrm{EIG} &= \int_Y \int_\Theta \log\left(\frac{\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})}{\pi(\boldsymbol{\theta})}\right)\pi(\boldsymbol{\theta}|\boldsymbol{y},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}\,\pi(\boldsymbol{y}|\boldsymbol{\xi})\mathrm{d}\boldsymbol{y} \\
&= \int_\Theta \left[\int_Y \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})}{\pi(\boldsymbol{y}|\boldsymbol{\xi})}\right)\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})\mathrm{d}\boldsymbol{y}\right]\pi(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}.
\end{aligned}$$

Approaches taken in the literature:

- Double-loop Monte Carlo (Beck, Mansour, Espath, Long, Tempone)
- MCLA (Beck, Mansour, Espath, Long, Tempone)
- DLMCIS (Beck, Mansour, Espath, Long, Tempone)

Let us assume the following:

A1 The forward model $\boldsymbol{y} = G(\boldsymbol{\theta}, \boldsymbol{\xi}) + \boldsymbol{\eta}$ satisfies

$$\|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} G(\boldsymbol{\theta}, \boldsymbol{\xi})\| \leq C_0 |\boldsymbol{\nu}|! \boldsymbol{b}^{\boldsymbol{\nu}},$$

where $\boldsymbol{b} := (b_j)_{j \geq 1} \in \ell^p$ are nonnegative real numbers for some $p \in (0,1)$ and $C_0 \geq 1$ is independent of $\boldsymbol{\xi} \in \Xi$.

A2 $\Theta = [-\frac{1}{2}, \frac{1}{2}]^s$ and $\pi(\boldsymbol{\theta}) = 1$ for $\boldsymbol{\theta} \in \Theta$ and 0 otherwise.

A3 The noise covariance is $\Gamma = \sigma^2 I_k$, $0 < \sigma \leq 1$.

Model problem: Let $D \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, be a nonempty, bounded, and convex Lipschitz domain and $z \in L^2(D)$. For each $\boldsymbol{\theta} \in \Theta$, there exists a strong solution $u(\cdot, \boldsymbol{\theta}) \in H^2(D) \cap H_0^1(D)$ to

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

where we assume that $\boldsymbol{\theta} = (\boldsymbol{\theta}_j)_{j \geq 1}$ i.i.d. uniformly distributed in $[-1/2, 1/2]$,

$$a(\boldsymbol{x}, \boldsymbol{\theta}) = a_0(\boldsymbol{x}) + \sum_{j \geq 1} \theta_j \psi_j(\boldsymbol{x}), \quad \boldsymbol{x} \in D,\ \boldsymbol{\theta} \in [-1/2, 1/2]^{\mathbb{N}},$$

with $a_0 \in W^{1,\infty}(D)$ and $\psi_j \in W^{1,\infty}(D)$, $j \geq 1$, such that $\sum_{j \geq 1} \|\psi_j\|_{W^{1,\infty}(D)} < \infty$, $0 < a_{\min} \leq a(\boldsymbol{x}, \boldsymbol{\theta}) \leq a_{\max} < \infty$ for all $\boldsymbol{x} \in D$, $\boldsymbol{\theta} \in [-1/2, 1/2]^{\mathbb{N}}$, and $b_j := \|\psi_j\|_{L^\infty(D)} / a_{\min}$.

Then $G(\boldsymbol{\theta}, \boldsymbol{\xi}) := (u(\boldsymbol{x}, \boldsymbol{\theta}))_{\boldsymbol{x} \in \boldsymbol{\xi}}$, where $\boldsymbol{\xi} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\} \subset D$, satisfies A1.

If $\boldsymbol{\theta} \perp \boldsymbol{\eta}$, then the likelihood is given by

$$\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi}) = C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}, \quad C = \frac{1}{(2\pi\sigma^2)^{k/2}}.$$

Under these conditions, it is easy to see that

$$\mathrm{EIG} = \int_Y \int_\Theta \log\left(\frac{\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})}{\pi(\boldsymbol{y}|\boldsymbol{\xi})}\right)\pi(\boldsymbol{y}|\boldsymbol{\theta},\boldsymbol{\xi})\pi(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}$$

$$= \log C - 1 - \int_Y \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}.$$

Observations:

- The **inner integral** can be approximated *independently* of the dimension s using QMC.
- In general, the data dimension k affects the QMC cubature error bound of the **outer integral**.
- How to efficiently approximate the nested integrals?

Consider

$$\int_Y \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}.$$

- Parametric regularity of the integrand in
$$\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}$$
is well-understood (as long as the parametric regularity of G can be quantified); straightforward modification of Herrmann–Keller–Schwab (2021).
- More generally, in many applications of UQ, we are interested in parametric integrals of quantities of the general form
$$f(G(\boldsymbol{\theta},\cdot)), \tag{3}$$
where $f:\mathbb{R}^k\to\mathbb{R}$ is a (somewhat) smooth nonlinear quantity of interest[†], and
$$\|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}}G(\boldsymbol{\theta},\cdot)\|\leq C_0|\boldsymbol{\nu}|!\boldsymbol{b}^{\boldsymbol{\nu}}.$$
What can be said about the parametric regularity of (3)?

[†]E.g., $f(\boldsymbol{x})=\|\boldsymbol{y}-\boldsymbol{x}\|^2$ or $f(\boldsymbol{x})=\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-\boldsymbol{x}\|^2}$.

Faà di Bruno's formula:

$$\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} f(G(\boldsymbol{\theta},\cdot)) = \sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \partial_{\boldsymbol{x}}^{\boldsymbol{\lambda}} f(\boldsymbol{x})\Big|_{\boldsymbol{x}=G(\boldsymbol{\theta},\cdot)} \kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}}(\boldsymbol{\theta}), \quad \boldsymbol{\nu}\neq\boldsymbol{0},$$

where the sequence $(\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}})$ depends only on G via

$\kappa_{\boldsymbol{\nu},\boldsymbol{0}} \equiv \delta_{\boldsymbol{\nu},\boldsymbol{0}},$

$\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}} \equiv 0 \quad$ if $|\boldsymbol{\nu}| < |\boldsymbol{\lambda}|$ or $\boldsymbol{\lambda} \not\geq \boldsymbol{0}$ (i.e., if $\boldsymbol{\lambda}$ contains negative entries),

$$\kappa_{\boldsymbol{\nu}+\boldsymbol{e}_j,\boldsymbol{\lambda}}(\boldsymbol{\theta}) = \sum_{\ell\in\mathrm{supp}(\boldsymbol{\lambda})} \sum_{\boldsymbol{0}\le\boldsymbol{m}\le\boldsymbol{\nu}} \binom{\boldsymbol{\nu}}{\boldsymbol{m}} \partial^{\boldsymbol{m}+\boldsymbol{e}_j}[G(\boldsymbol{\theta},\cdot)]_\ell \kappa_{\boldsymbol{\nu}-\boldsymbol{m},\boldsymbol{\lambda}-\boldsymbol{e}_\ell}(\boldsymbol{\theta}) \quad \text{otherwise.}$$

Since $\|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} G(\boldsymbol{\theta},\cdot)\| \le C_0|\boldsymbol{\nu}|!\boldsymbol{b}^{\boldsymbol{\nu}}$, we obtain the following *uniform* bound.

Lemma
For all $1 \le |\boldsymbol{\lambda}| \le |\boldsymbol{\nu}|$, there holds

$$|\kappa_{\boldsymbol{\nu},\boldsymbol{\lambda}}(\boldsymbol{\theta})| \le C_0^{|\boldsymbol{\lambda}|} \frac{|\boldsymbol{\nu}|!(|\boldsymbol{\nu}|-1)!}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!} \boldsymbol{b}^{\boldsymbol{\nu}}.$$

Proof.
By induction w.r.t. the order of the multi-index $\boldsymbol{\nu}$. □

For the present problem, we obtain

$$
\begin{aligned}
&|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\cdot)\|^2}| \\
&\le \left(\frac{C_0}{\sigma}\right)^{|\boldsymbol{\nu}|} \sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} |\partial_{\boldsymbol{x}}^{\boldsymbol{\lambda}} \mathrm{e}^{-\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}|\Big|_{\boldsymbol{x}=\sigma^{-1}(\boldsymbol{y}-G(\boldsymbol{\theta},\cdot))} \frac{|\boldsymbol{\nu}|!(|\boldsymbol{\nu}|-1)!}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}\boldsymbol{b}^{\boldsymbol{\nu}}.
\end{aligned}
$$

Cramér's inequality:

$$
\left|\frac{\mathrm{d}^\lambda}{\mathrm{d}x^\lambda}\mathrm{e}^{-x^2/2}\right| \le 1.1\sqrt{\lambda!} \quad \Rightarrow \quad |\partial_{\boldsymbol{x}}^{\boldsymbol{\lambda}} \mathrm{e}^{-\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}| \le 1.1^k\sqrt{\boldsymbol{\lambda}!}
$$

and thus

$$
\begin{aligned}
&|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\cdot)\|^2}| \\
&\le 1.1^k\left(\frac{C_0}{\sigma}\right)^{|\boldsymbol{\nu}|}\boldsymbol{b}^{\boldsymbol{\nu}}|\boldsymbol{\nu}|!(|\boldsymbol{\nu}|-1)! \sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \frac{\sqrt{\boldsymbol{\lambda}!}}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!}.
\end{aligned}
$$

It remains to estimate the multi-index sum, but fortunately this is not too difficult:

$$\sum_{\substack{1\le|\boldsymbol{\lambda}|\le|\boldsymbol{\nu}|\\ \boldsymbol{\lambda}\in\mathbb{N}_0^k}} \frac{\sqrt{\boldsymbol{\lambda}!}}{\boldsymbol{\lambda}!(|\boldsymbol{\nu}|-|\boldsymbol{\lambda}|)!(|\boldsymbol{\lambda}|-1)!} = \sum_{\ell=1}^{|\boldsymbol{\nu}|} \frac{1}{(|\boldsymbol{\nu}|-\ell)!(\ell-1)!} \sum_{\substack{\boldsymbol{\lambda}\in\mathbb{N}_0^k\\ |\boldsymbol{\lambda}|=\ell}} \frac{1}{\sqrt{\boldsymbol{\lambda}!}}$$

$$\le \sum_{\ell=1}^{|\boldsymbol{\nu}|} \frac{1}{(|\boldsymbol{\nu}|-\ell)!(\ell-1)!} \left(\sum_{\lambda=0}^{\infty} \frac{1}{\sqrt{\lambda!}}\right)^k$$

$$\le 3.47^k \cdot \frac{2^{|\boldsymbol{\nu}|-1}}{(|\boldsymbol{\nu}|-1)!},$$

where we made use of $\sum_{\lambda=0}^{\infty} \frac{1}{\sqrt{\lambda!}} = 3.469506\ldots$ and the summation identity $\sum_{\ell=1}^{\nu} \frac{1}{(\nu-\ell)!(\ell-1)!} = \frac{2^{\nu-1}}{(\nu-1)!}$.

Summa summarum:

Lemma
For all $\boldsymbol{\nu}\neq\mathbf{0}$, there holds

$$|\partial_{\boldsymbol{\theta}}^{\boldsymbol{\nu}} \mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\cdot)\|^2}| \le 3.82^k \cdot C_0^{|\boldsymbol{\nu}|} 2^{|\boldsymbol{\nu}|-1}\sigma^{-|\boldsymbol{\nu}|}|\boldsymbol{\nu}|!\boldsymbol{b}^{\boldsymbol{\nu}}.$$

Decomposing the high-dimensional integral

Suppose that $Y = \mathbb{R}^k$. Then

$$\int_{\mathbb{R}^k} \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\widetilde{\boldsymbol{\theta}},\boldsymbol{\xi})\|^2}\,\mathrm{d}\widetilde{\boldsymbol{\theta}}\,\mathrm{d}\boldsymbol{y}$$

$$= \int_{[-K,K]^k} \log\left(\int_\Theta C_{k,\sigma}\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\widetilde{\boldsymbol{\theta}},\boldsymbol{\xi})\|^2}\,\mathrm{d}\widetilde{\boldsymbol{\theta}}\,\mathrm{d}\boldsymbol{y}$$

$$+ \int_{\mathbb{R}^k\setminus[-K,K]^k} \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\widetilde{\boldsymbol{\theta}},\boldsymbol{\xi})\|^2}\,\mathrm{d}\widetilde{\boldsymbol{\theta}}\,\mathrm{d}\boldsymbol{y}$$

$$=: \mathcal{I}_K + \widetilde{\mathcal{I}}_K.$$

For $K \gg 1$, there holds

$$|\widetilde{\mathcal{I}}_K| \le C^{1/2}\mathrm{e}^{\frac{\|\overline{G}\|^2}{4\sigma^2}}(4\pi\sigma^2)^{k/2} - C^{1/2}\mathrm{e}^{\frac{\|\overline{G}\|^2}{4\sigma^2}}(\pi\sigma^2)^{k/2}\prod_{j=1}^k\left(\mathrm{erf}\left(\frac{\overline{G}_j+K}{2\sigma}\right)-\mathrm{erf}\left(\frac{\overline{G}_j-K}{2\sigma}\right)\right),$$

where $\overline{G} := (\overline{G}_j)_{j=1}^k := G(\boldsymbol{\theta}^*,\boldsymbol{\xi}^*)$, $(\boldsymbol{\theta}^*,\boldsymbol{\xi}^*) := \arg\max_{(\boldsymbol{\theta},\boldsymbol{\xi})\in(\Theta,\Xi)}\|G(\boldsymbol{\theta},\boldsymbol{\xi})\|$.

$$\int_{[-K,K]^k} \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}$$

QMC weights for the **inner integral**:

$$\gamma_{\mathfrak{u}} = \left(|\mathfrak{u}|!\prod_{j\in\mathfrak{u}}\frac{\beta_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^\lambda}}\right)^{\frac{2}{1+\lambda}}, \quad \lambda = \begin{cases}\frac{p}{2-p} & \text{if } p\in(2/3,1),\\ \frac{1}{2-2\delta} & \text{if } p\in(0,2/3],\end{cases}$$

with $\beta_j := \frac{2C_0}{\sigma}b_j$, $j\in\{1,\ldots,s\}$, and $\delta>0$ arbitrary, yields the QMC convergence rate

$$\mathcal{O}(\varphi(n)^{\max\{-1/p+1/2,-1+\delta\}})$$

independently of the dimension s with $\varphi(n)$ denoting the Euler totient function.

$$\int_{[-K,K]^k} \log\left(\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\right)\int_\Theta C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}\,\mathrm{d}\boldsymbol{\theta}\,\mathrm{d}\boldsymbol{y}$$

QMC weights for the **outer integral**:

$$\widetilde{\gamma}_{\mathfrak{u}} = \left(|\mathfrak{u}|!\prod_{j\in\mathfrak{u}}\frac{1.1^k k\sigma^{-1}\mathrm{e}^{\frac{1}{2\sigma^2}(kK^2+2\sqrt{k}KC+C^2)}}{\log(2)\sqrt{2\zeta(2\widetilde{\lambda})/(2\pi^2)^{\widetilde{\lambda}}}}\right)^{\frac{2}{1+\widetilde{\lambda}}}, \quad \widetilde{\lambda} = \frac{1}{2-2\widetilde{\delta}},$$

with $\widetilde{\delta} > 0$ arbitrary, yields the QMC convergence rate

$$\mathcal{O}(\varphi(n)^{-1+\widetilde{\delta}})$$

with $\varphi(n)$ denoting the Euler totient function. Note that the implied coefficient depends on k.

The nested integral

Goal of computation:

$$\mathcal{I}_K(f) = \int_{Y_K} g\bigg(\int_{\Theta} f(\boldsymbol{\theta}, \boldsymbol{y}, \boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}\bigg)\,\mathrm{d}\boldsymbol{y},$$

where $g(x) := x\log x$, $Y_K = [-K, K]^k$, and $f(\boldsymbol{\theta}, \boldsymbol{y}, \boldsymbol{\xi}) := C\mathrm{e}^{-\frac{1}{2\sigma^2}\|\boldsymbol{y}-G(\boldsymbol{\theta},\boldsymbol{\xi})\|^2}$.

Define a hierarchy of QMC cubature operators for the **outer integral**, i.e.,

$$I^{(1)}F := \int_{Y_K} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \approx 2^{-\ell}\sum_{k=1}^{2^\ell} F(\boldsymbol{y}_k^{(\ell)}) =: Q_\ell^{(1)}F,\ \ell = \ell_0^{(1)}, \ell_0^{(1)}+1, \ell_0^{(1)}+2, \ldots,$$

for a given function $F \in \widetilde{H}_{k,\widetilde{\gamma}}$, and likewise for the **inner integral**

$$I^{(2)}F := \int_{\Theta} F(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta} \approx 2^{-\ell}\sum_{k=1}^{2^\ell} F(\boldsymbol{\theta}_k^{(\ell)}) =: Q_\ell^{(2)}F,\ \ell = \ell_0^{(2)}, \ell_0^{(2)}+1, \ell_0^{(2)}+2, \ldots,$$

for a given function $F \in H_{s,\boldsymbol{\gamma}}$.

Why full tensor product cubature is a bad idea

Approximating the integral

$$\mathcal{I}_K(f) = \int_{Y_K} g\bigg(\int_\Theta f(\boldsymbol{\theta},\boldsymbol{y},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\theta}\bigg)\,\mathrm{d}\boldsymbol{y},$$

by

$$\mathcal{I}_K(f) \approx Q_\ell^{(1)} g(Q_\ell^{(2)} f) \tag{4}$$

is inefficient. A hand-wavy argument would be as follows:

- Suppose that we have the approximation rates (recall $n = 2^\ell$)

$$|I^{(1)}F - Q_\ell^{(1)}F| \asymp n^{-\alpha} \quad \text{and} \quad |I^{(2)}F - Q_\ell^{(2)}F| \asymp n^{-\alpha}.$$

- Evaluating (4) takes $N = n^2$ function calls, but the cubature accuracy will not be better than $\mathcal{O}(n^{-\alpha}) = \mathcal{O}(N^{-\alpha/2})$
  $\rightarrow$ the convergence rate is effectively halved! ("Curse of dimensionality")

Sparse tensor product cubature in the vein of Gilch, Griebel, Oettershagen (2022)

Define the difference cubature operator corresponding to the **outer integral**

$$\Delta_\ell^{(1)} F := \begin{cases} Q_\ell^{(1)} F - Q_{\ell-1}^{(1)} F & \text{if } \ell \geq 1, \\ Q_0^{(1)} F & \text{if } \ell = 0, \end{cases}$$

as well as the *generalized* difference cubature operators corresponding to the **inner integral**

$$\Delta_\ell^{(2)} F := \begin{cases} g(Q_\ell^{(2)} F) - g(Q_{\ell-1}^{(2)} F) & \text{if } \ell \geq 1, \\ g(Q_0^{(2)} F) & \text{if } \ell = 0. \end{cases}$$

Generalized sparse grid cubature operator:

$$\mathcal{Q}_{L,\varsigma}(f) := \sum_{\varsigma \ell_1 + \frac{\ell_2}{\varsigma} \leq L} \Delta_{\ell_1}^{(1)} \Delta_{\ell_2}^{(2)}(f) = \sum_{\ell_1=0}^{L/\varsigma} \Delta_{\ell_1}^{(1)} g(Q_{\varsigma L - \varsigma^2 \ell_1}^{(2)} f).$$

Sparse tensor product cubature

$$\mathcal{Q}_{L,\varsigma}(f) := \sum_{\varsigma\ell_1+\frac{\ell_2}{\varsigma}\leq L} \Delta^{(1)}_{\ell_1}\Delta^{(2)}_{\ell_2}(f) = \sum_{\ell_1=0}^{L/\varsigma} \Delta^{(1)}_{\ell_1} g(Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f).$$

$$\begin{aligned}
&\|\mathcal{I}_K(f) - \mathcal{Q}_{L,\varsigma}(f)\|_{\boldsymbol{\Delta}} := \sqrt{\mathbb{E}_{\boldsymbol{\Delta}}[|\mathcal{I}_K(f) - \mathcal{Q}_{L,\varsigma}(f)|^2]} \\
&\leq \|(I^{(1)} - Q^{(1)}_{L/\varsigma})g(I^{(2)}f)\|_{\boldsymbol{\Delta}} \\
&\quad + \left\| \sum_{\ell_1=0}^{L/\varsigma} \Delta^{(1)}_{\ell_1}(I^{(2)}f - Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f)\log(I^{(2)}f) \right\|_{\boldsymbol{\Delta}} \\
&\quad + \left\| \sum_{\ell_1=0}^{L/\varsigma} \Delta^{(1)}_{\ell_1}\left(\frac{Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f - I^{(2)}f}{Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f} \right) Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f \right\|_{\boldsymbol{\Delta}} \\
&\quad + \left\| \sum_{\ell_1=0}^{L/\varsigma} \Delta^{(1)}_{\ell_1}\left(\log\left(\frac{I^{(2)}f}{Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f} \right) - \left(\frac{I^{(2)}f}{Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f} - 1 \right) \right) Q^{(2)}_{\varsigma L-\varsigma^2\ell_1} f \right\|_{\boldsymbol{\Delta}}.
\end{aligned}$$

Sparse tensor product cubature

$$\mathcal{Q}_{L,\varsigma}(f) := \sum_{\varsigma\ell_1 + \frac{\ell_2}{\varsigma} \leq L} \Delta_{\ell_1}^{(1)} \Delta_{\ell_2}^{(2)}(f) = \sum_{\ell_1=0}^{L/\varsigma} \Delta_{\ell_1}^{(1)} g(Q_{\varsigma L - \varsigma^2 \ell_1}^{(2)} f).$$

Sparse grid error: Our **inner** and **outer** QMC cubatures have essentially linear convergence rates, i.e.,

$$|I^{(1)}f - Q_\ell^{(1)}f| \lesssim 2^{-(1-\delta)\ell} \quad \text{and} \quad |I^{(2)}f - Q_\ell^{(2)}f| \lesssim 2^{-(1-\delta)\ell}.$$

For an *isotropic* ($\varsigma = 1$) sparse tensor product cubature operator, we obtain

$$\|\mathcal{I}_K(f) - \mathcal{Q}_{L,\varsigma}(f)\|_{\boldsymbol{\Delta}} \lesssim 2^{-(1-\delta)L}(L+1)$$

under some additional technical assumptions.

Numerical experiment

Let $D = (0,1)^2$. We consider the elliptic PDE

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x},\boldsymbol{\theta})\nabla u(\boldsymbol{x},\boldsymbol{\theta})) = x_1, & \boldsymbol{x} \in D,\ \boldsymbol{\theta} \in [-1/2, 1/2]^{100}, \\ u(\cdot,\boldsymbol{\theta})|_{\partial D} = 0, & \boldsymbol{\theta} \in [-1/2, 1/2]^{100}, \end{cases}$$

equipped with the parametric diffusion coefficient

$$a(\boldsymbol{x},\boldsymbol{\theta}) = 2 + 0.1 \sum_{j=1}^{100} j^{-2}\theta_j \sin(\pi j x_1)\sin(\pi j x_2), \boldsymbol{\theta} \in [-1/2, 1/2]^{100}.$$

Numerical experiment

The goal is to find a design $\boldsymbol{\xi}^*$ from the set

$$\Xi = \{(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4) \in \Upsilon^4 \mid \boldsymbol{x}_i \neq \boldsymbol{x}_j \text{ for } i \neq j\},$$

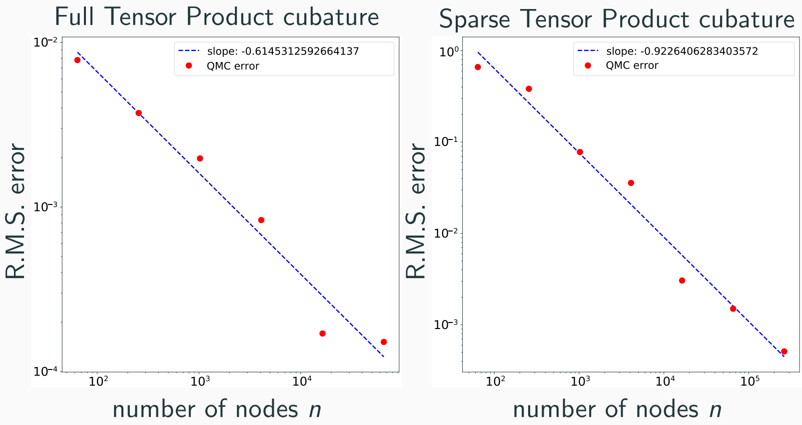
where

$$\begin{aligned}\Upsilon =&\{(0.25, 0.25), (0.25, 0.50), (0.25, 0.75),\\ &(0.50, 0.25), (0.50, 0.50), (0.50, 0.75),\\ &(0.75, 0.25), (0.75, 0.50), (0.75, 0.75)\},\end{aligned}$$

maximizing the expected information gain subject to the observation operator

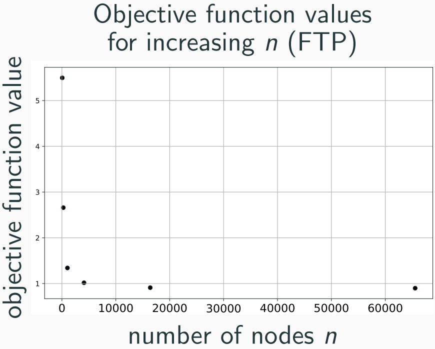
$$G(\boldsymbol{\theta}, \boldsymbol{\xi}) = (u(\boldsymbol{x}, \boldsymbol{\theta}))_{\boldsymbol{x}\in\boldsymbol{\xi}}, \quad \boldsymbol{\theta} \in [-1/2, 1/2]^{100},\ \boldsymbol{\xi} \in \Xi.$$

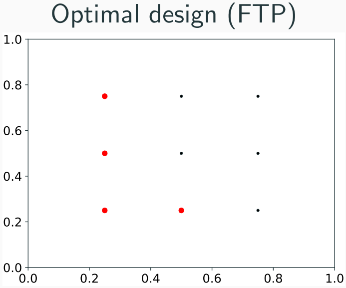
Numerical experiment



Left: Full tensor product (FTP) cubature of the nested integral subject to affine and uniform parameterization of the input random field. Right: Sparse tensor product (STP) cubature of the nested integral subject to affine and uniform parameterization of the input random field.

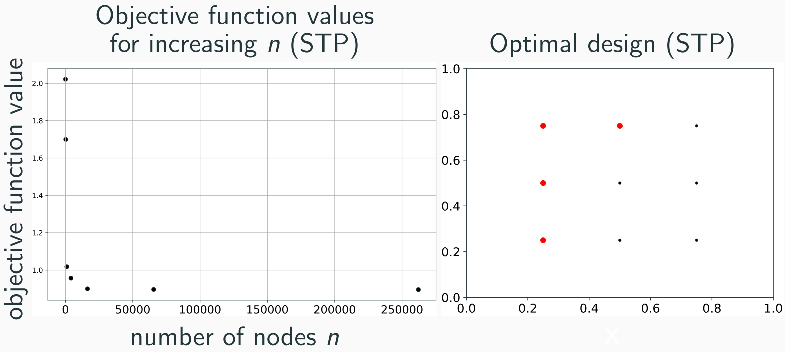
Numerical experiment





The value of the objective function using the full tensor product (FTP) scheme for an increasing number of cubature points (left) and the optimal design corresponding to the cubature rule with the largest number of points (right).

Numerical experiment



The value of the objective function using the sparse tensor product (STP) scheme for an increasing number of cubature points (left) and the optimal design corresponding to the cubature rule with the largest number of points (right).

Conclusions and outlook

- QMC for DOE: sparse approach can recover almost the optimal rate.
- Related QMC analysis for PDE-constrained optimal control under uncertainty (including also the optimization process):

P. A. Guth, K., F. Y. Kuo, C. Schillings, and I. H. Sloan. A Quasi-Monte Carlo Method for Optimal Control Under Uncertainty. *SIAM/ASA J. Uncertain. Quantif.* **9**(2):354–383, 2021

P. A. Guth, K., F. Y. Kuo, C. Schillings, and I. H. Sloan. *Parabolic PDE-Constrained Optimal Control Under Uncertainty With Entropic Risk Measure Using Quasi-Monte Carlo Integration*. Preprint 2022, arXiv:2208.02767 [math.NA]

Preprint coming soon!