

# Quasi-Monte Carlo methods for Bayesian optimal experimental design

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IFIP TC7 System Modeling and Optimization

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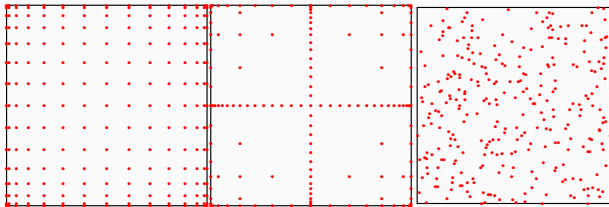
Part II: Bayesian optimal experimental design

# **Part I: Quasi-Monte Carlo methods**

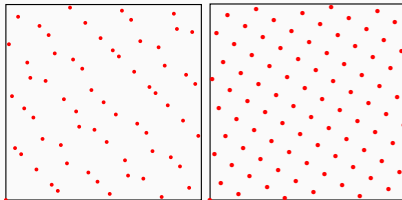
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# High-dimensional numerical integration

$$\int_{[0,1]^s} f(\mathbf{y}) d\mathbf{y} \approx \sum_{i=1}^n w_i f(\mathbf{t}_i)$$



**Figure 1:** Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)



**Figure 2:** Sobol' points, lattice rule (examples of QMC rules)

*Quasi-Monte Carlo (QMC) methods* are a class of *equal weight* cubature rules

$$\int_{[0,1]^s} f(\mathbf{y}) \, d\mathbf{y} \approx \frac{1}{n} \sum_{i=1}^n f(\mathbf{t}_i),$$

where  $(\mathbf{t}_i)_{i=1}^n$  is an ensemble of *deterministic* nodes in  $[0, 1]^s$ .

The nodes  $(\mathbf{t}_i)_{i=1}^n$  are NOT random!! Instead, they are *deterministically chosen*.

QMC methods exploit the smoothness and anisotropy of an integrand in order to achieve better-than-Monte Carlo rates.

# Lattice rules

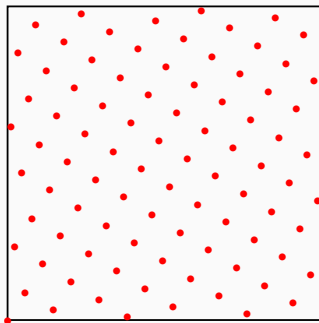
*Rank-1 lattice rules*

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

have the points

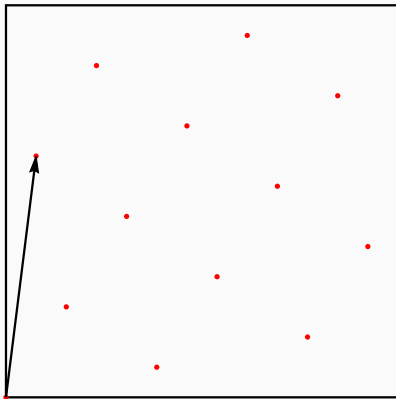
$$\mathbf{t}_i = \text{mod} \left( \frac{i\mathbf{z}}{n}, 1 \right), \quad i \in \{1, \dots, n\},$$

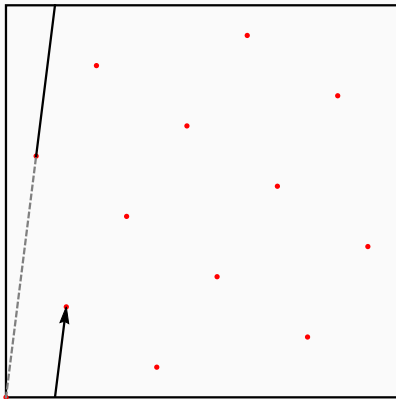
where the entire point set is determined by the *generating vector*  $\mathbf{z} \in \mathbb{N}^s$ , with all components *coprime* to  $n$ .



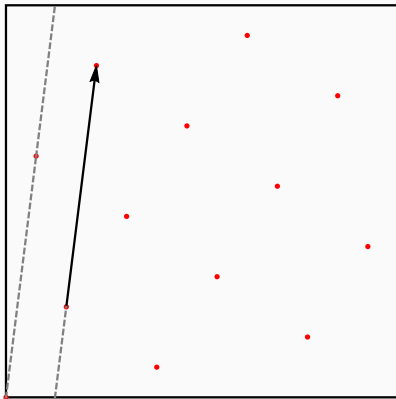
Lattice rule with  $\mathbf{z} = (1, 55)$  and  $n = 89$   
nodes in  $[0, 1]^2$

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

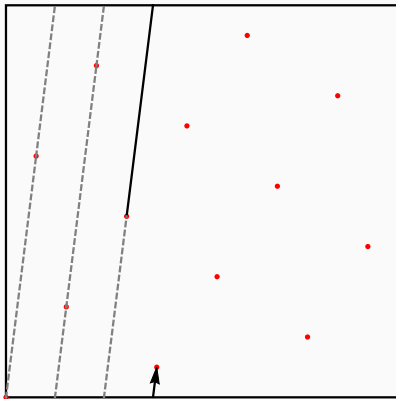


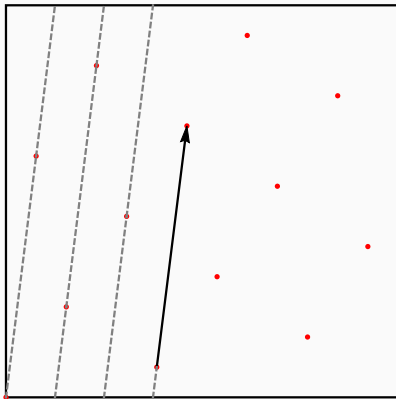


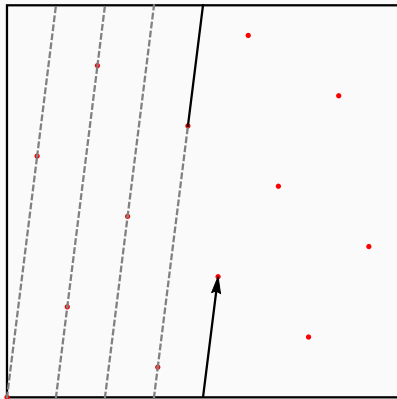


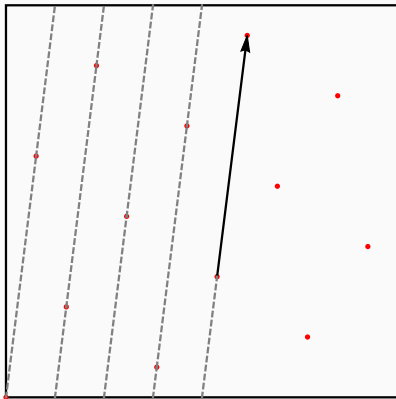


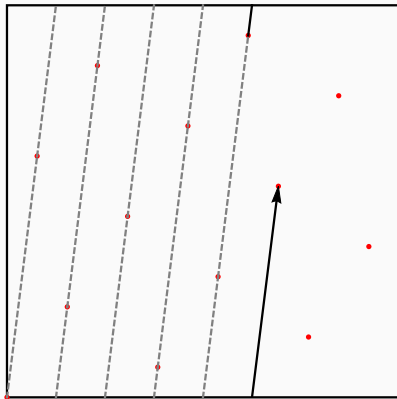


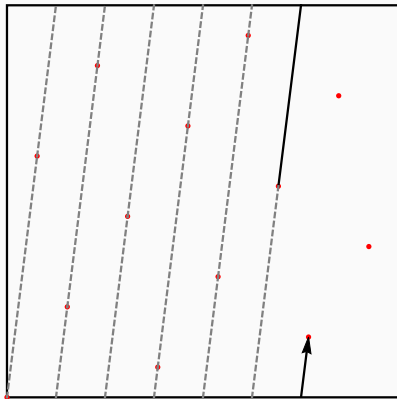




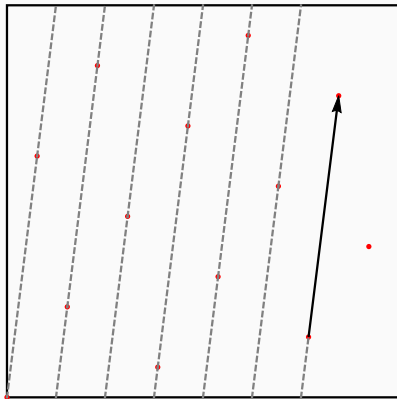


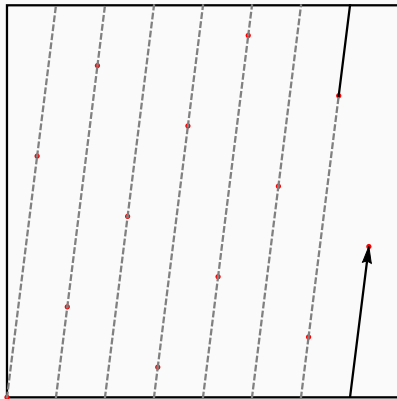












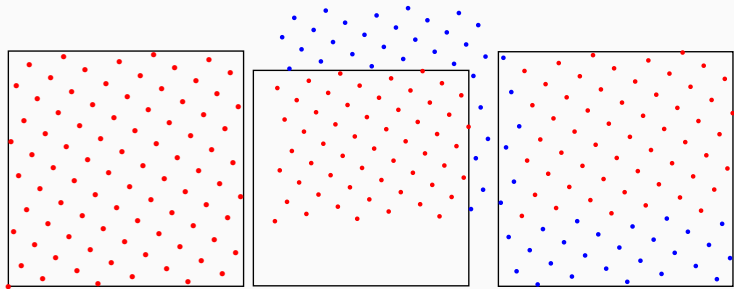
# Randomly shifted lattice rules

Shifted rank-1 lattice rules have points

$$\mathbf{t}_i = \text{mod} \left( \frac{i\mathbf{z}}{n} + \mathbf{\Delta}, 1 \right), \quad i \in \{1, \dots, n\}.$$

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

*Use a number of random shifts for error estimation.*



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

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

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

Then

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

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

Let  $f: [0, 1]^s \rightarrow \mathbb{R}$  be sufficiently smooth.

Error bound (one random shift):

$$|I_s(f) - Q_{s,n}^{\Delta}(f)| \leq e_{s,n,\gamma}^{\Delta}(\mathbf{z}) \|f\|_{\gamma}.$$

R.M.S. error bound (shift-averaged):

$$\sqrt{\mathbb{E}_{\Delta}[|I_s(f) - \bar{Q}_{s,n}(f)|^2]} \leq e_{s,n,\gamma}^{\text{sh}}(\mathbf{z}) \|f\|_{\gamma}.$$

We consider weighted Sobolev spaces with dominating mixed smoothness, equipped with norm

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

and (squared) worst case error

$$P(\mathbf{z}) := e_{s,n,\gamma}^{\text{sh}}(\mathbf{z})^2 = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s\}} \gamma_{\mathbf{u}} \prod_{j \in \mathbf{u}} \omega\left(\left\{\frac{kz_j}{n}\right\}\right)$$

where  $\omega(x) = x^2 - x + \frac{1}{6}$ .

## CBC algorithm (Sloan, Kuo, Joe 2002)

The idea of the *component-by-component* (CBC) algorithm is to find a good generating vector  $\mathbf{z} = (z_1, \dots, z_s)$  by proceeding as follows:

1. Set  $z_1 = 1$ ;
2. With  $z_1$  fixed, choose  $z_2$  to minimize error criterion  $P(z_1, z_2)$ ;
3. With  $z_1$  and  $z_2$  fixed, choose  $z_3$  to minimize error criterion  $P(z_1, z_2, z_3)$
- $\vdots$

Efficient implementation using FFT (QMC4PDE, QMCPy, etc.) if weights have certain structure (e.g., POD weights).

### **Theorem (CBC error bound)**

*The generating vector  $\mathbf{z} \in \mathbb{N}^s$  constructed by the CBC algorithm, minimizing the squared shift-averaged worst-case error  $[e_{s,n,\gamma}^{\text{sh}}(\mathbf{z})]^2$  for the weighted unanchored Sobolev space in each step, satisfies*

$$[e_{s,n,\gamma}^{\text{sh}}(\mathbf{z})]^2 \leq \left( \frac{1}{\varphi(n)} \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s\}} \gamma_{\mathbf{u}}^{\lambda} \left( \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathbf{u}|} \right)^{1/\lambda} \quad \text{for all } \lambda \in (1/2, 1],$$

where  $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$  denotes the Riemann zeta function for  $x > 1$ .

Remarks:

- Optimal rate of convergence  $\mathcal{O}(n^{-1+\delta})$  in weighted Sobolev spaces, independently of  $s$  under an appropriate condition on the weights.
- Cost of algorithm for POD weights is  $\mathcal{O}(s n \log n + s^2 n)$  using FFT.

**Significance:** Suppose that  $f \in H_{s,\gamma}$  for all  $\gamma = (\gamma_u)_{u \subseteq \{1:s\}}$ . Then for any given sequence of weights  $\gamma$ , we can use the CBC algorithm to obtain a generating vector satisfying the error bound

$$\sqrt{\mathbb{E}_{\Delta} |I_s f - Q_{s,n}^{\Delta} f|^2} \leq \left( \frac{1}{\varphi(n)} \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^{\lambda} \left( \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|u|} \right)^{1/(2\lambda)} \|f\|_{s,\gamma} \quad (1)$$

for all  $\lambda \in (1/2, 1]$ . We can use the following strategy:

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



## **Part II: Bayesian optimal experimental design**

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

Measurement model:

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

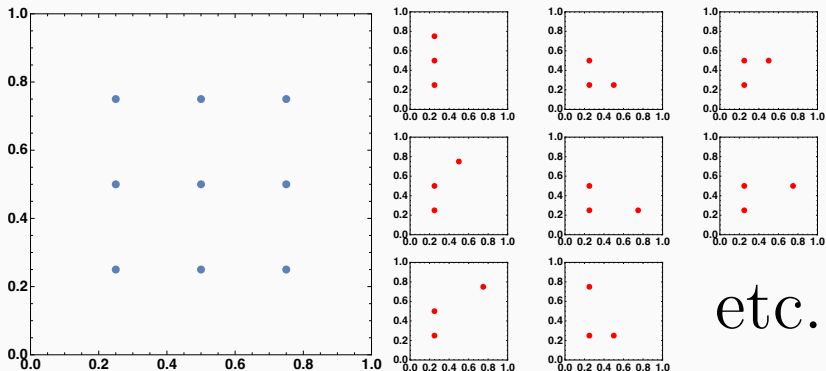
where  $\mathbf{y} \in \mathbb{R}^k$  is the measurement data and  $\eta \in \mathbb{R}^k$  is Gaussian noise such that  $\eta \sim \mathcal{N}(0, \Gamma)$  with positive definite covariance matrix  $\Gamma \in \mathbb{R}^{k \times k}$ .

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

### Example

Suppose we have 9 slots and 3 sensors. Before carrying out the experiment, which 3 slots do we expect to be the most informative for the recovery of the unknown parameter?

→  $\binom{9}{3} = 84$  possible configurations



Left: 9 slots. Right: We have 84 possible ways to place 3 sensors into 9 slots.

*How to rank the 84 different possibilities from most informative to least informative?*

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

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

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

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

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

The posterior is given by Bayes' theorem

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

which means that the expected utility can be written as

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

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

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

where  $\mathbf{b} := (b_j)_{j \geq 1} \in \ell^p$  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  $\Gamma = \sigma^2 I_k$ ,  $0 < \sigma \leq 1$ .

### Example

**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

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

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

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

with  $a_0 \in W^{1,\infty}(D)$  and  $\psi_j \in W^{1,\infty}(D)$ ,  $j \geq 1$ , such that

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

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

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

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

Under these conditions, it is easy to see that

$$\begin{aligned} \text{EIG} &= \int_Y \int_{\Theta} \log \left( \frac{\pi(\mathbf{y}|\boldsymbol{\theta}, \boldsymbol{\xi})}{\pi(\mathbf{y}|\boldsymbol{\xi})} \right) \pi(\mathbf{y}|\boldsymbol{\theta}, \boldsymbol{\xi}) \pi(\boldsymbol{\theta}) \, d\boldsymbol{\theta} \, d\mathbf{y} \\ &= \log C - 1 - \int_Y \log \left( \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} \, d\boldsymbol{\theta} \right) \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} \, d\boldsymbol{\theta} \, d\mathbf{y}. \end{aligned}$$

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

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

- Parametric regularity of the integrand in

$$\int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} d\boldsymbol{\theta}$$

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

$$f(G(\boldsymbol{\theta}, \cdot)), \quad (3)$$

where  $f: \mathbb{R}^k \rightarrow \mathbb{R}$  is a (somewhat) smooth nonlinear quantity of interest<sup>†</sup>, and

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

What can be said about the parametric regularity of (3)?

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<sup>†</sup>E.g.,  $f(\mathbf{x}) = \|\mathbf{y} - \mathbf{x}\|^2$  or  $f(\mathbf{x}) = e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - \mathbf{x}\|^2}$ .

Faà di Bruno's formula:

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

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

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

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

$$\kappa_{\nu + e_j, \lambda}(\theta) = \sum_{\ell \in \text{supp}(\lambda)} \sum_{\mathbf{0} \leq \mathbf{m} \leq \nu} \binom{\nu}{\mathbf{m}} \partial^{\mathbf{m} + e_j} [G(\theta, \cdot)]_{\ell} \kappa_{\nu - \mathbf{m}, \lambda - e_{\ell}}(\theta) \quad \text{otherwise.}$$

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

### Lemma

For all  $1 \leq |\lambda| \leq |\nu|$ , there holds

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

### Proof.

By induction w.r.t. the order of the multi-index  $\nu$ .



For the present problem, plugging the upper bound for  $|\kappa_{\nu,\lambda}(\theta)|$  into the expression

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

and making some simple estimates yields altogether that

$$|\partial_{\theta}^{\nu} e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\theta, \cdot)\|^2}| \leq 3.82^k \cdot C_0^{|\nu|} 2^{|\nu|-1} \sigma^{-|\nu|} |\nu|! \mathbf{b}^{\nu} \quad \text{for all } \nu \neq \mathbf{0}.$$

# Decomposing the high-dimensional integral

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

$$\begin{aligned}
 & \int_{\mathbb{R}^k} \log \left( \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} d\boldsymbol{\theta} \right) \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\tilde{\boldsymbol{\theta}}, \boldsymbol{\xi})\|^2} d\tilde{\boldsymbol{\theta}} d\mathbf{y} \\
 &= \int_{[-K, K]^k} \log \left( \int_{\Theta} C_{k, \sigma} e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} d\boldsymbol{\theta} \right) \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\tilde{\boldsymbol{\theta}}, \boldsymbol{\xi})\|^2} d\tilde{\boldsymbol{\theta}} d\mathbf{y} \\
 &+ \int_{\mathbb{R}^k \setminus [-K, K]^k} \log \left( \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\boldsymbol{\theta}, \boldsymbol{\xi})\|^2} d\boldsymbol{\theta} \right) \int_{\Theta} C e^{-\frac{1}{2\sigma^2} \|\mathbf{y} - G(\tilde{\boldsymbol{\theta}}, \boldsymbol{\xi})\|^2} d\tilde{\boldsymbol{\theta}} d\mathbf{y} \\
 &=: \mathcal{I}_K + \tilde{\mathcal{I}}_K.
 \end{aligned}$$

For  $K \gg 1$ , there holds

$$\begin{aligned}
 |\tilde{\mathcal{I}}_K| &\leq C^{1/2} e^{\frac{\|\bar{G}\|^2}{4\sigma^2}} (4\pi\sigma^2)^{k/2} \\
 &- C^{1/2} e^{\frac{\|\bar{G}\|^2}{4\sigma^2}} (\pi\sigma^2)^{k/2} \prod_{j=1}^k \left( \operatorname{erf} \left( \frac{\bar{G}_j + K}{2\sigma} \right) - \operatorname{erf} \left( \frac{\bar{G}_j - K}{2\sigma} \right) \right),
 \end{aligned}$$

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

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

QMC weights for the **inner integral**:

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

with  $\beta_j := \frac{2C_0}{\sigma} b_j$ ,  $j \in \{1, \dots, s\}$ , 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.

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

QMC weights for the **outer integral**:

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

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

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

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

# The nested integral

**Goal of computation:**

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

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

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

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

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

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

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

# Why full tensor product cubature is a bad idea

Approximating the integral

$$\mathcal{I}_K(f) = \int_{Y_K} g \left( \int_{\Theta} f(\theta, \mathbf{y}, \xi) d\theta \right) d\mathbf{y},$$

by

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

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  $\mathcal{O}(n^{-\alpha}) = \mathcal{O}(N^{-\alpha/2})$   
→ 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

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

**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

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

under some additional technical assumptions.

# Numerical experiment

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

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}, \boldsymbol{\theta}) \nabla u(\mathbf{x}, \boldsymbol{\theta})) = 10x_1, & \mathbf{x} \in D, \boldsymbol{\theta} \in [-1/2, 1/2]^{100}, \\ u(\cdot, \boldsymbol{\theta})|_{\partial D} = 0, & \boldsymbol{\theta} \in [-1/2, 1/2]^{100}, \end{cases}$$

equipped with the parametric diffusion coefficient

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

# Numerical experiment

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

$$\Xi = \{(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \in \Upsilon^3 \mid \mathbf{x}_i \neq \mathbf{x}_j \text{ for } i \neq j\},$$

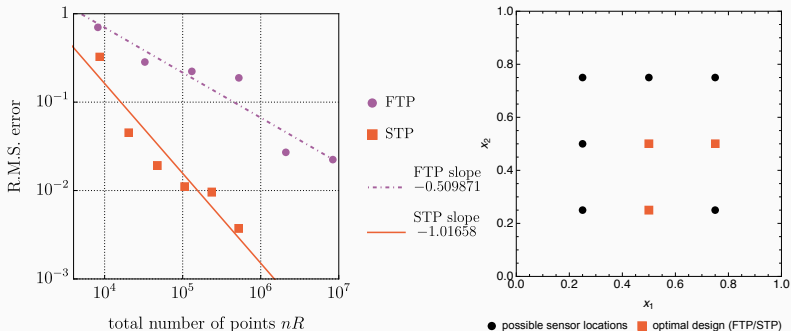
where

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

maximizing the expected information gain subject to the observation operator


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

# Numerical experiment



Left: R.M.S. errors for the full tensor product (FTP) and sparse tensor product (STP) cubatures of the nested integral subject to affine and uniform parameterization of the input random field with  $R = 8$  random shifts.

Right: the optimal design corresponding to the cubature rule with the largest number of points.

- QMC for DOE: sparse approach can recover almost the optimal rate.
- Preprint:
  -  V. Kaarnioja and C. Schillings. Quasi-Monte Carlo for Bayesian design of experiment problems governed by parametric PDEs. Preprint 2024. arXiv:2405.03529 [math.NA]

**Thank you for your attention!**