



# **Modeling domain uncertainty using periodic random variables with application to elliptic PDEs**

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

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# High-dimensional numerical integration

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

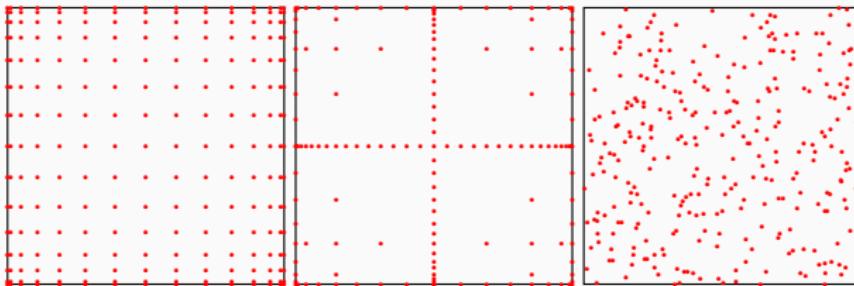


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

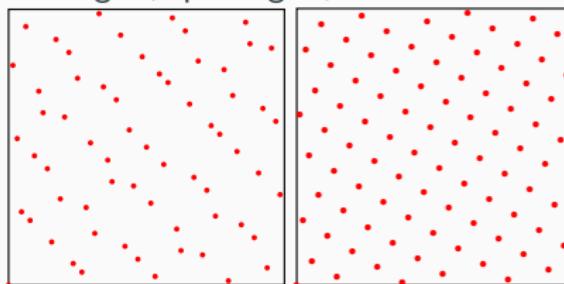


Figure 2: Sobol' points, lattice rule (examples of QMC rules)

*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.

How to choose  $\mathbf{t}_1, \dots, \mathbf{t}_n \in [0, 1]^s$  in a QMC rule?

- Non-periodic case: *Low discrepancy points*
  - Koksma, Hlawka, Sobol', Faure, Niederreiter, Dick, ...
- Periodic case: Korobov, Zaremba, Hua, ...

Periodic means

$$f(y_1, y_2, \dots, y_s) = f(y_1 + 1, y_2, \dots, y_s) = f(y_1, y_2 + 1, \dots, y_s) = \dots$$

# Lattice rules

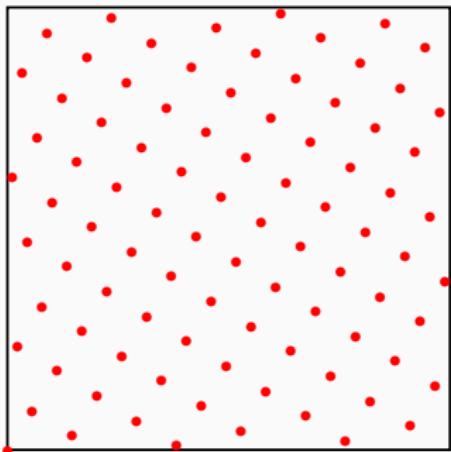
Rank-1 lattice rules

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

have the points

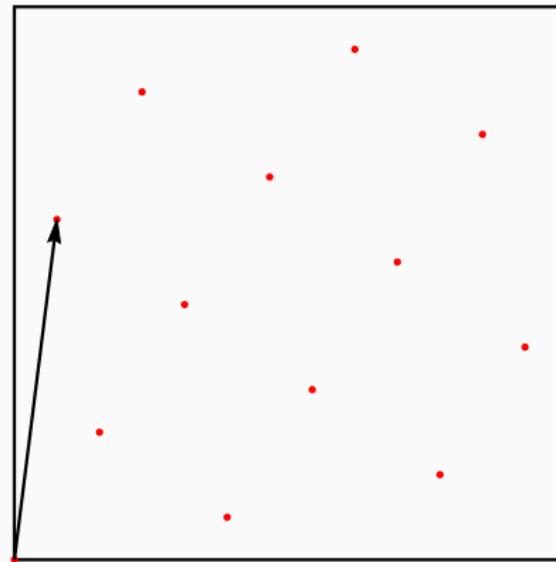
$$\mathbf{t}_i = \text{mod}\left(\frac{i\mathbf{z}}{n}, 1\right), \quad i \in \{1, \dots, n\},$$

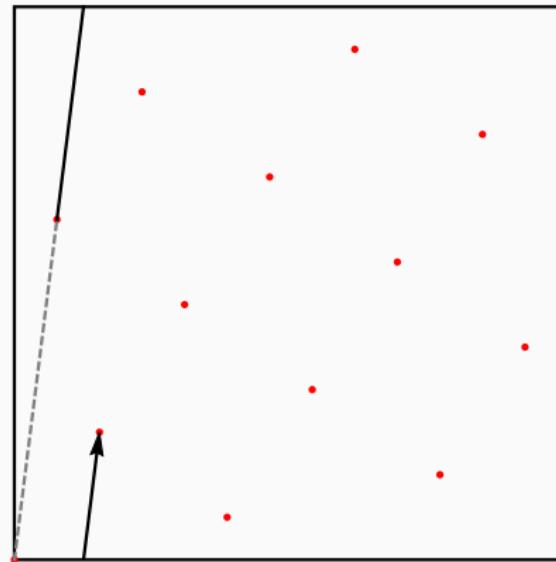
where the entire point set is determined by the *generating vector*  $\mathbf{z} \in \mathbb{N}^s$ , with all components *coprime* to  $n$ .

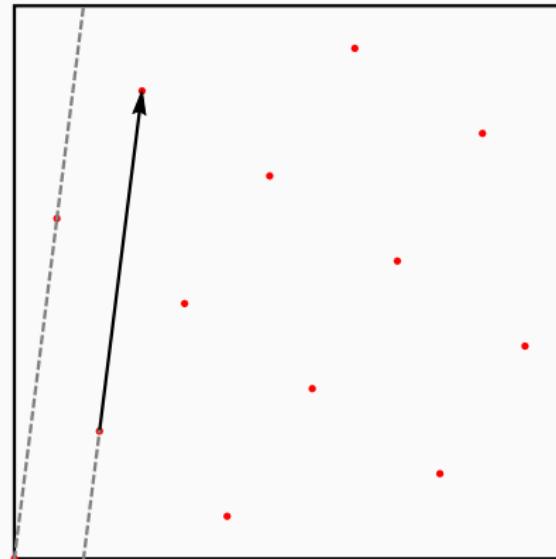


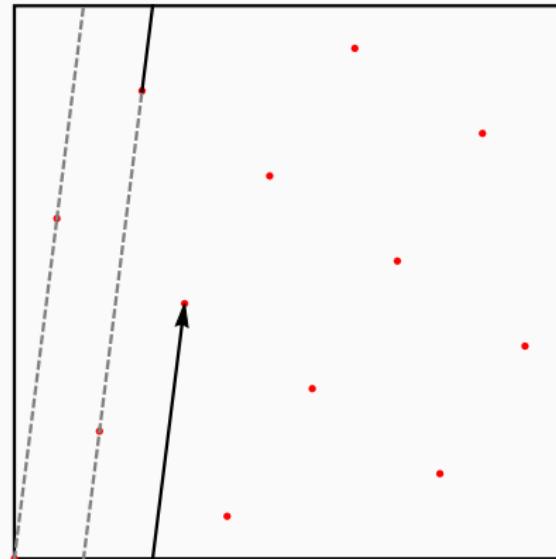
Lattice rule with  $\mathbf{z} = (1, 55)$  and  $n = 89$   
nodes in  $[0, 1]^2$

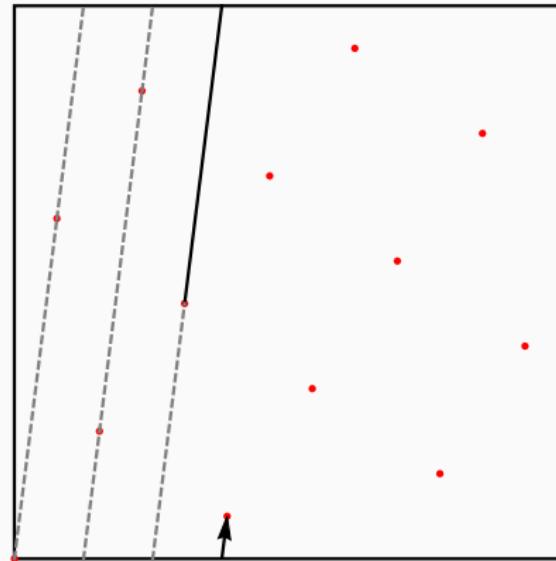
*Lattice rules and periodic functions are a match made in heaven!*

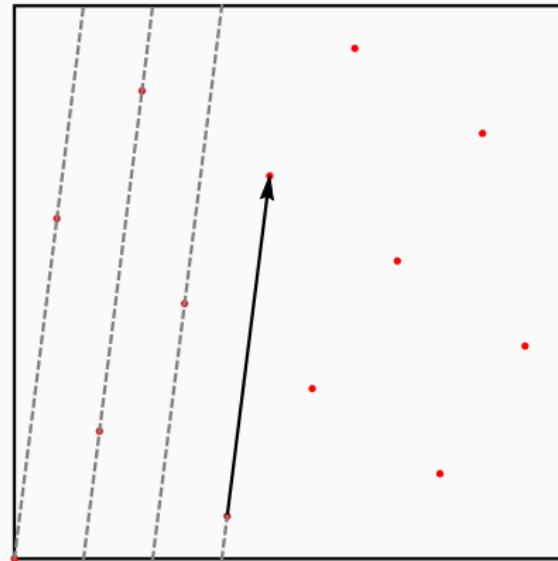


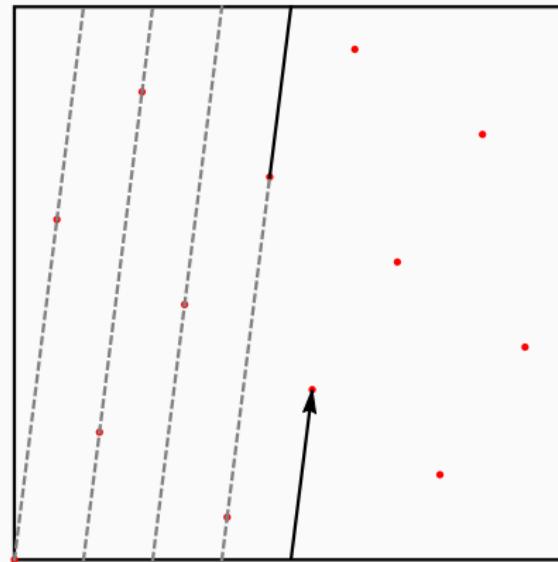


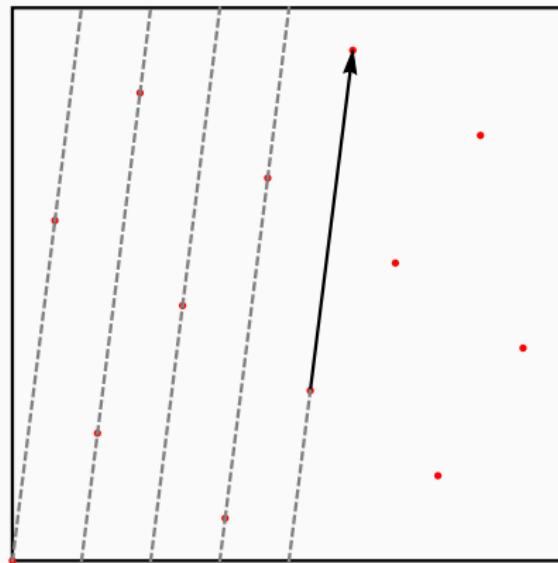


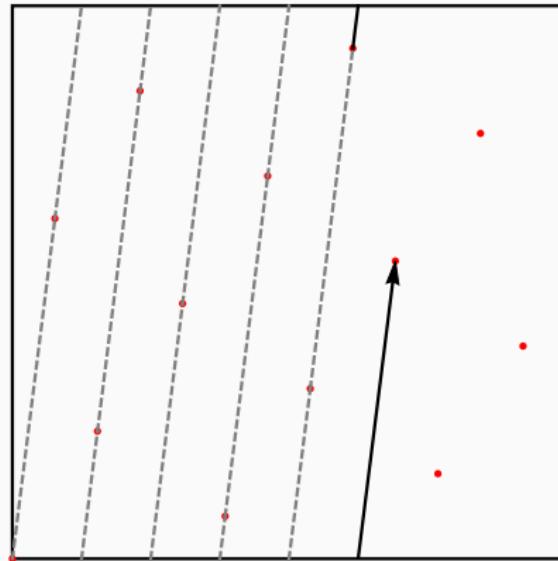


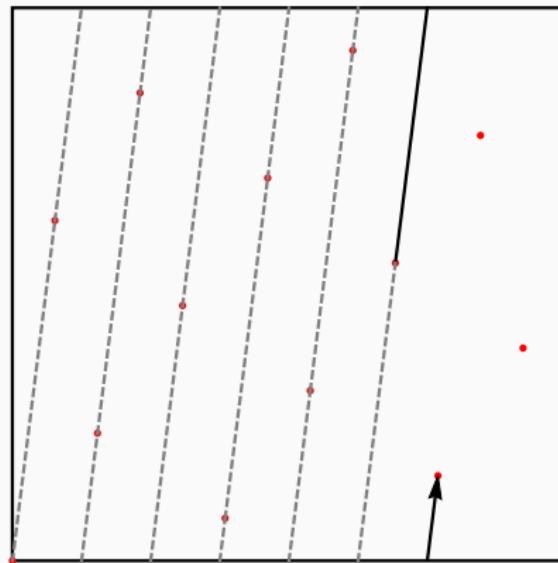


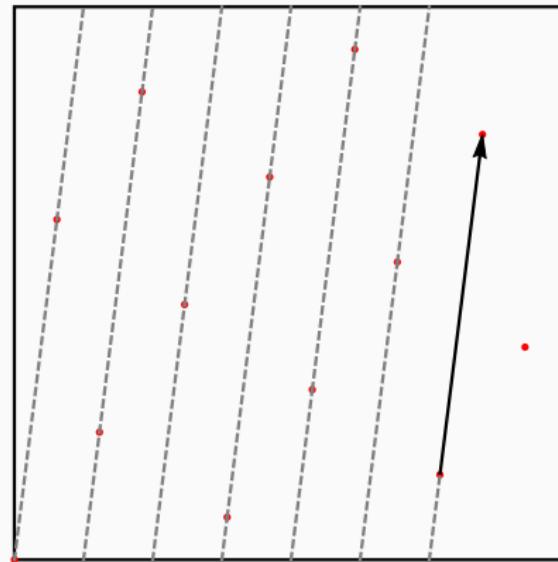


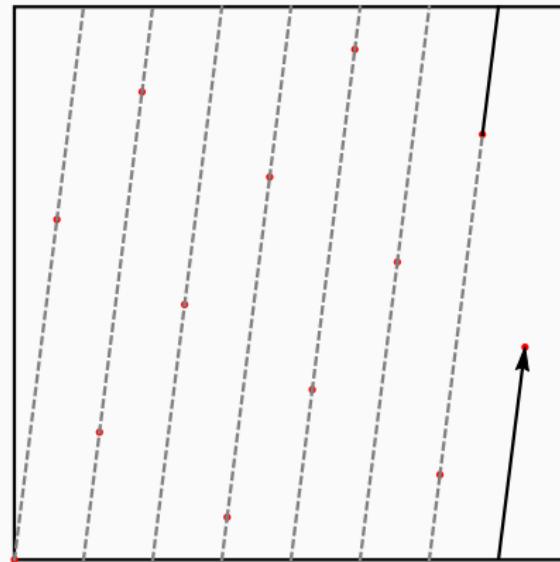












## Dimension $s = 1$ : the only lattice is the left-Riemann rule

For  $z \in \{1, \dots, n - 1\}$ ,  $\gcd(z, n) = 1$ , there holds

$$Q_{1,n}(f) = \frac{1}{n} \sum_{k=1}^n f\left(\text{mod}\left(\frac{kz}{n}, 1\right)\right) = \frac{1}{n} \sum_{k=1}^n f\left(\frac{k}{n}\right).$$

Suppose  $f: [0, 1] \rightarrow \mathbb{R}$  is  $p$  times continuously differentiable and periodic.

Let  $h = \frac{1}{n}$ . Then the Euler–Maclaurin summation formula gives

$$\begin{aligned} \sum_{k=0}^{n-1} hf(kh) &= \int_0^1 f(x) dx + \sum_{k=1}^{\lfloor p/2 \rfloor} \frac{B_{2k}}{(2k)!} (f^{(2k-1)}(1) - f^{(2k-1)}(0)) \\ &\quad - (-1)^p h^p \int_0^1 \tilde{B}_p(x) f^{(p)}(x) dx \end{aligned}$$



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$$\left| \int_0^1 f(x) dx - \sum_{k=1}^{\lfloor p/2 \rfloor} \frac{B_{2k}}{(2k)!} (f^{(2k-1)}(1) - f^{(2k-1)}(0)) \right| = O(n^{-p})$$

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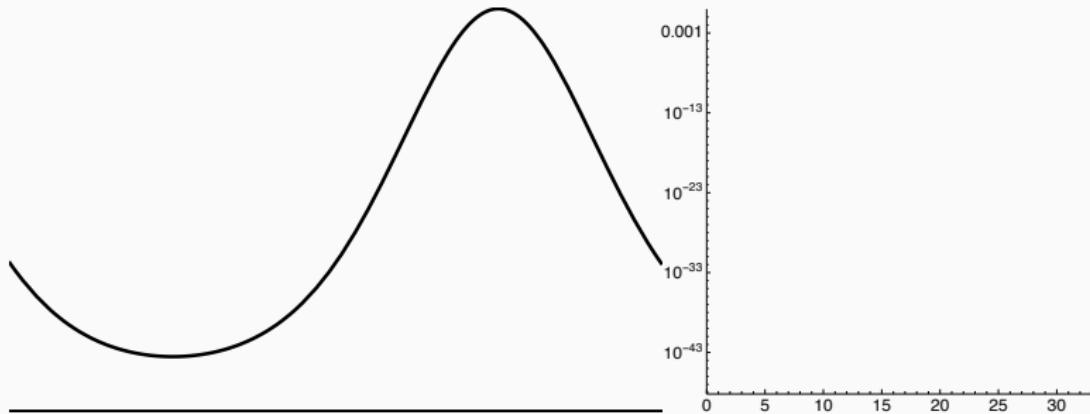
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$$\therefore \left| \int_0^1 f(x) dx - \frac{1}{n} \sum_{k=0}^{n-1} f\left(\frac{k}{n}\right) \right| = \mathcal{O}(n^{-p}).$$

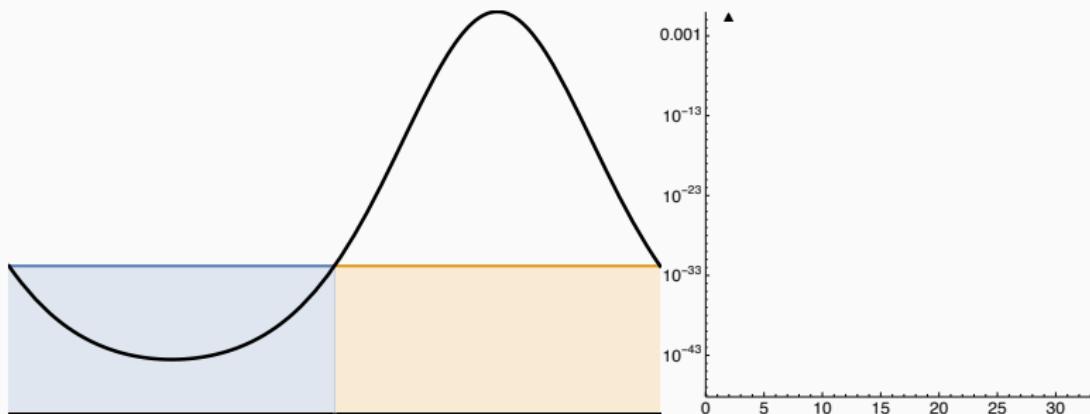
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$$\int_0^1 \exp(-\sin(2\pi x)) dx$$



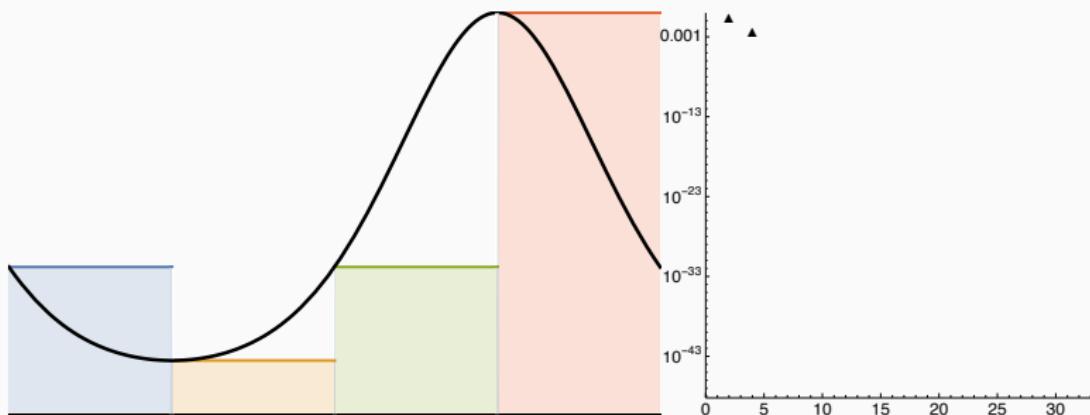
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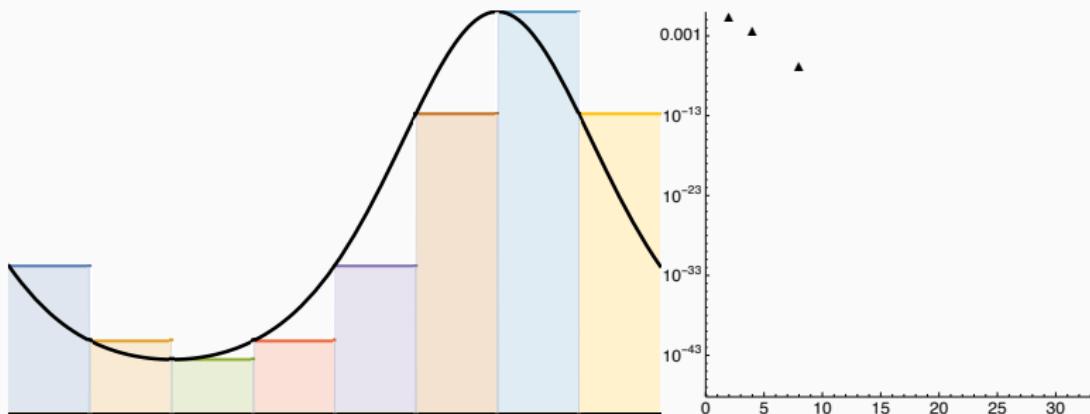
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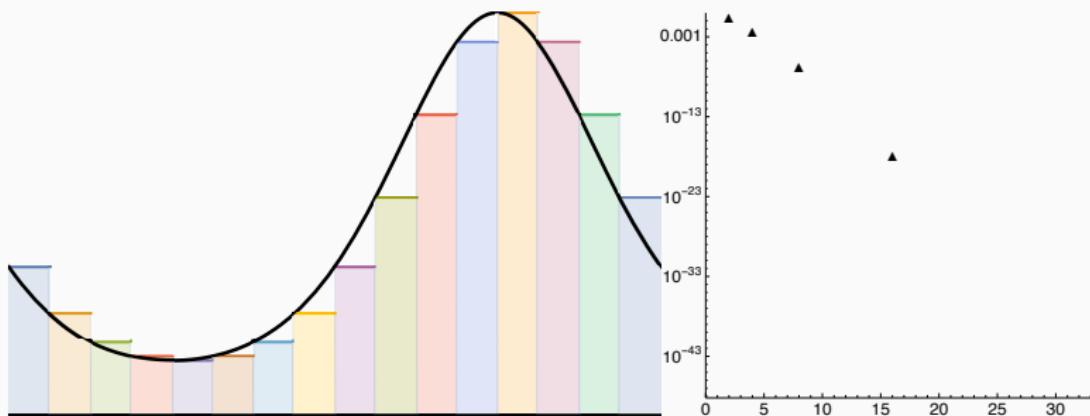
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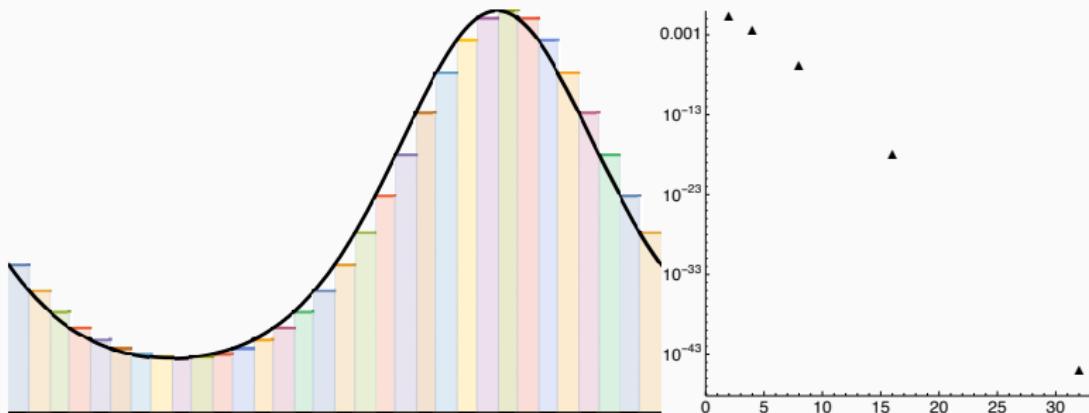
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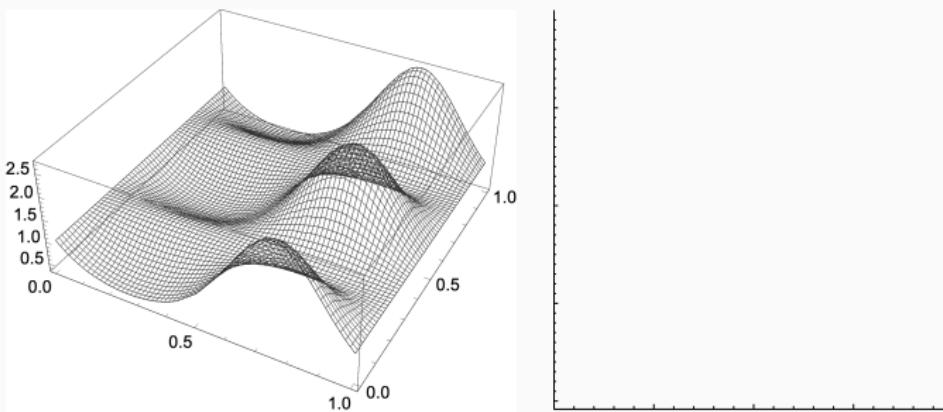
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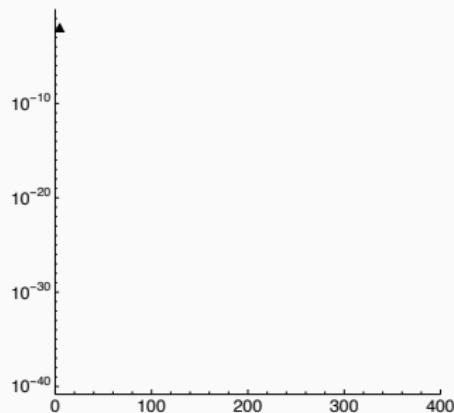
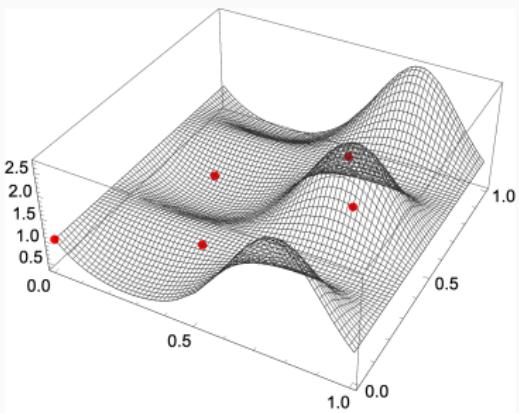
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

$$\int_0^1 \int_0^1 \exp(-\sin(2\pi x) \cos(2\pi y)^2) dx dy$$



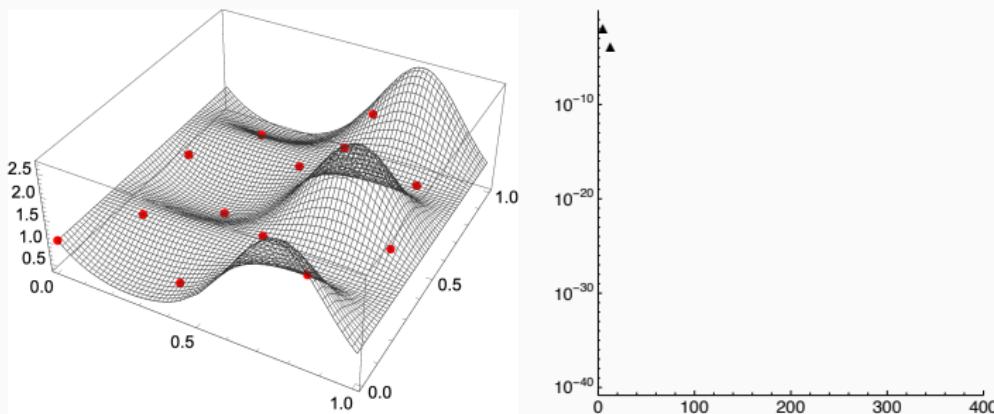
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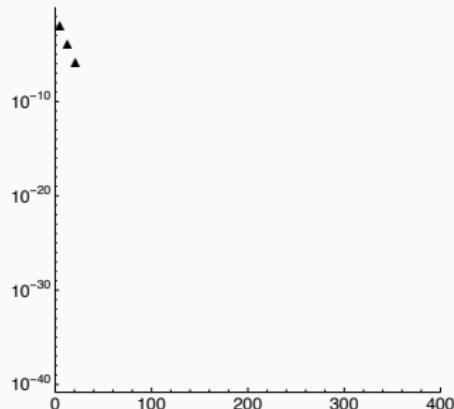
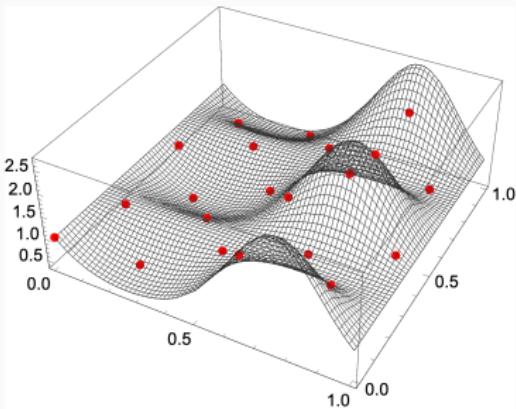
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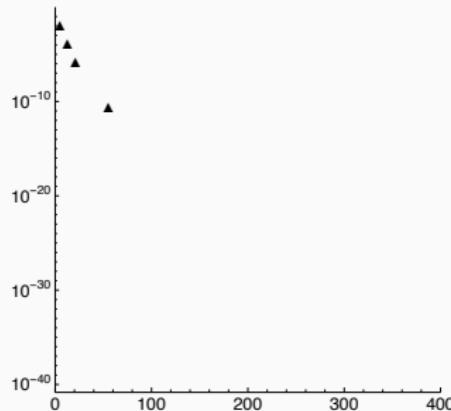
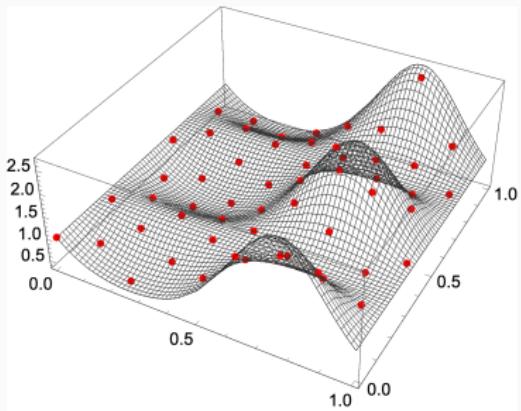
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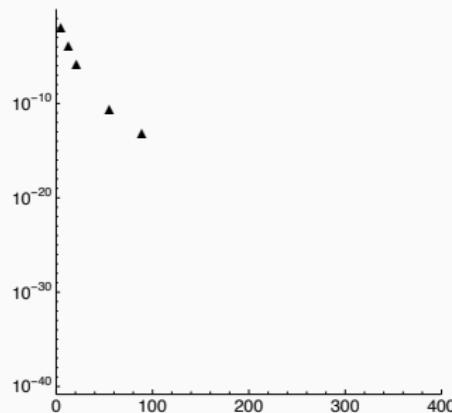
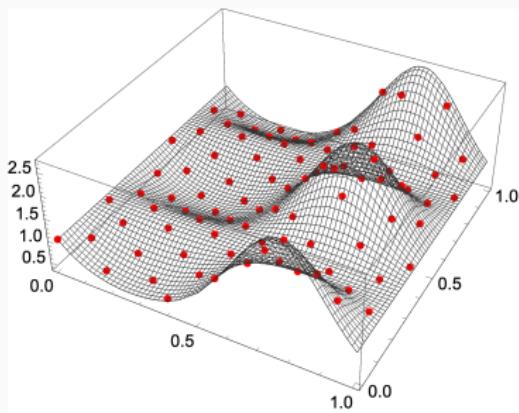
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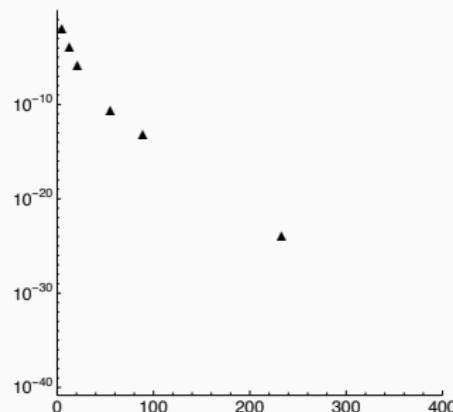
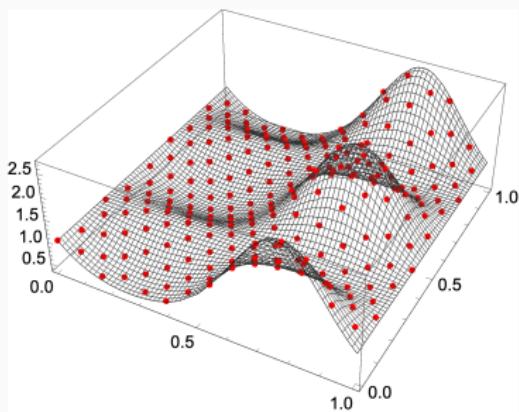
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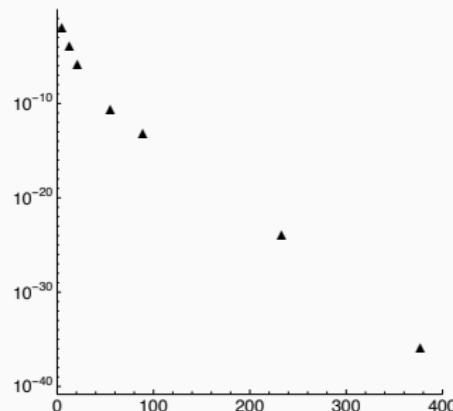
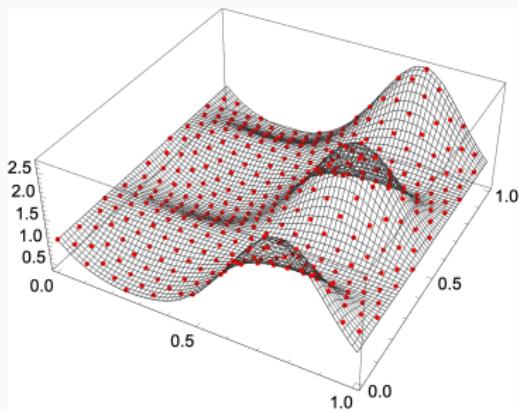
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For continuous 1-periodic functions with absolutely convergent Fourier series, the lattice rule error is precisely (Sloan and Kachoyan 1987):

$$Q_{s,n}(f) - I_s(f) = \sum_{\mathbf{h} \in \Lambda^\perp \setminus \{\mathbf{0}\}} \hat{f}(\mathbf{h}),$$

where  $\hat{f}(\mathbf{h}) := \int_{[0,1]^s} f(\mathbf{y}) e^{-2\pi i \mathbf{y} \cdot \mathbf{h}} d\mathbf{y}$  for  $\mathbf{h} \in \mathbb{Z}^s$  and the *dual lattice*  $\Lambda^\perp = \Lambda^\perp(\mathbf{z}) = \{\mathbf{h} \in \mathbb{Z}^s : \mathbf{h} \cdot \mathbf{z} \equiv 0 \pmod{n}\}$  is defined with respect to the generating vector  $\mathbf{z}$  of the rank-1 lattice rule.

Let  $\alpha \geq 2$  be an integer,  $\gamma := (\gamma_u)_{u \subseteq \{1:s\}}$  a collection of positive weights, and set  $r_\alpha(\gamma, \mathbf{h}) := \gamma_{\text{supp}(\mathbf{h})}^{-1} \prod_{j \in \text{supp}(\mathbf{h})} |h_j|^\alpha$  for  $\mathbf{h} \in \mathbb{Z}^s$  with  $\text{supp}(\mathbf{h}) := \{j \in \{1:s\} : h_j \neq 0\}$ . Using the error formula, we can write

$$|I_s(f) - Q_{s,n}(f)| = \left| \sum_{\mathbf{h} \in \Lambda^\perp \setminus \{\mathbf{0}\}} \hat{f}(\mathbf{h}) \frac{r_\alpha(\gamma, \mathbf{h})}{r_\alpha(\gamma, \mathbf{h})} \right| \leq \underbrace{\left( \sum_{\mathbf{h} \in \Lambda^\perp \setminus \{\mathbf{0}\}} \frac{1}{r_\alpha(\gamma, \mathbf{h})} \right)}_{=: P_\alpha(\mathbf{z})} \|f\|_\alpha,$$

where  $\|f\|_\alpha := \sup_{\mathbf{h} \in \mathbb{Z}^s} |\hat{f}(\mathbf{h})| r_\alpha(\gamma, \mathbf{h})$  and (if  $\alpha$  is even) it turns out that

$$P_\alpha(\mathbf{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u \prod_{j \in u} \omega\left(\left\{ \frac{kz_j}{n} \right\}\right), \quad \omega(x) := (2\pi)^\alpha \frac{B_\alpha(x)}{(-1)^{\alpha/2+1} \alpha!}. \quad 13$$

## 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  $z_1 = 1$  (this is a freebie since  $P(1) = P(z)$  for all  $z \in \mathbb{N}$ );
  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  
 $P(z_1, z_2, z_3)$
- ⋮

Notes:

- The CBC algorithm is a *greedy algorithm*: in general, it will not find the generating vector  $\mathbf{z}$  that minimizes  $P(\mathbf{z})$ . However, it can be shown that the generating vector obtained by the CBC algorithm satisfies an error bound (more on this later).
- For generic  $\boldsymbol{\gamma} = (\gamma_u)_{u \subseteq \{1:s\}}$ , evaluating  $P(\mathbf{z}) = P(\boldsymbol{\gamma}, \mathbf{z})$  takes  $\mathcal{O}(2^s)$  operations. For an efficient implementation, it is desirable that the weights  $\boldsymbol{\gamma}$  can be characterized by an expression that does not contain too many degrees of freedom.

## CBC with POD weights

Suppose that we have QMC weights in *product and order dependent* (POD) form

$$\gamma_{\mathfrak{u}} := \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j, \quad \emptyset \neq \mathfrak{u} \subseteq \{1 : s\},$$

for some positive scalars  $(\Gamma_k)_{k \geq 1}$  and  $(\gamma_j)_{j=1}^s$ .

In this case, it turns out that the error criterion

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

can be written in the dimensionally recursive form

$$P(z_1, \dots, z_s) = P(z_1, \dots, z_{s-1}) + \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\ell=1}^s p_{s,\ell}(k),$$

where  $p_{s,\ell}(k) = p_{s-1,\ell}(k) + \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_s \omega\left(\left\{\frac{kz_s}{n}\right\}\right) p_{s-1,\ell-1}(k)$  together with  $p_{s,0}(k) = 1$  for all  $k$ .

For simplicity, let  $n$  be prime. We note that the CBC algorithm can be implemented using the recurrence on the previous page, i.e.,

$$P(z_1, \dots, z_d) = P(z_1, \dots, z_{d-1}) + \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\ell=1}^d p_{d,\ell}(k),$$

where  $p_{d,\ell}(k) = p_{d-1,\ell}(k) + \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_d \omega\left(\left\{\frac{kz_d}{n}\right\}\right) p_{d-1,\ell-1}(k)$  together with  $p_{d,0}(k) = 1$  for all  $k$ , as follows:

1. Define the matrix  $\Omega_n = [\omega\left(\left\{\frac{kz}{n}\right\}\right)]_{\substack{z \in \{1, \dots, n-1\} \\ k \in \{0, \dots, n-1\}}}$  and initialize vectors

$\mathbf{p}_{0,\ell} = \mathbf{1}_n$  for  $\ell = 1, \dots, s$ .

**for**  $d = 1, \dots, s$ , **do**

2. Pick the value of  $z_d \in \{1, \dots, n-1\}$  corresponding to the smallest entry in the matrix-vector product

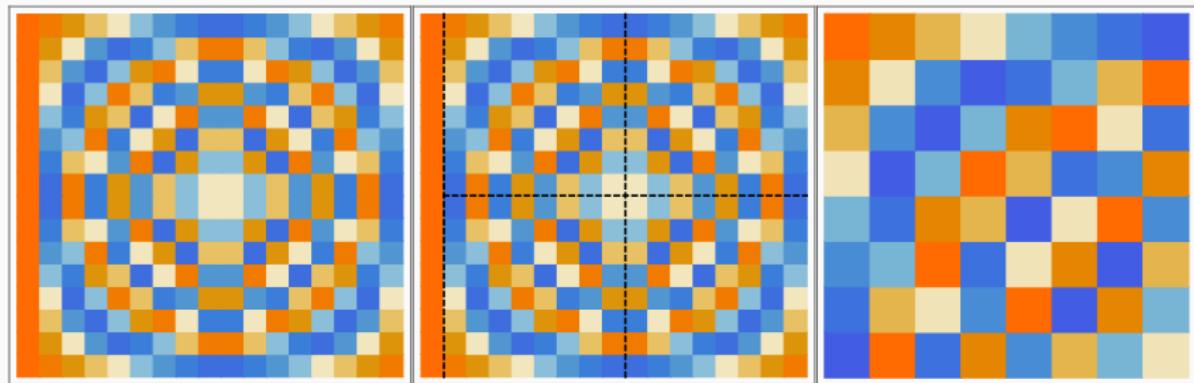
$$\Omega_n \mathbf{x}, \quad \text{with } \mathbf{x} := \sum_{\ell=1}^d \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_d \mathbf{p}_{d-1,\ell-1}.$$

3. Update  $\mathbf{p}_{d,\ell} := \mathbf{p}_{d-1,\ell} + \Omega_n(z_d) * \left( \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_d \mathbf{p}_{d-1,\ell-1} \right)$ .

**end for**

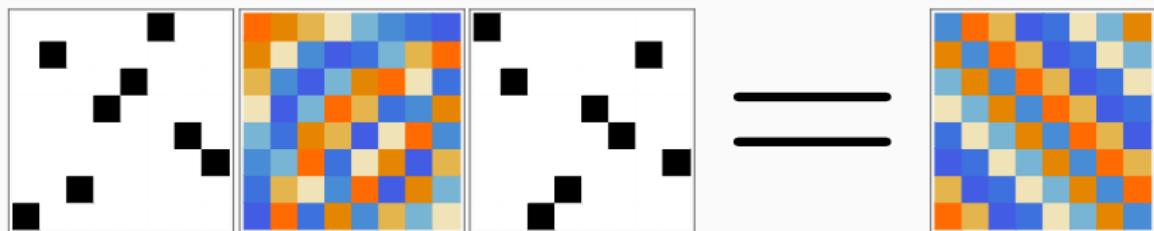
## What makes fast CBC fast?

Note that the matrix-vector product  $\Omega_n \mathbf{x}$  in the CBC loop costs  $\mathcal{O}(n^2)$  operations. However, it was shown by Kuo, Nuyens, and Cools (2006) that the blocks of  $\Omega_n$  can be permuted into circulant form  $\rightarrow$  the matrix-vector product can be implemented in  $\mathcal{O}(n \log n)$  operations using FFT.



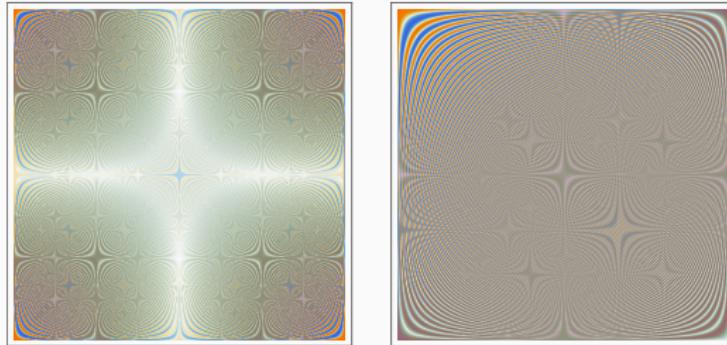
**Figure 3:** Example with  $\Omega_{17}$ . Note that the first column is a constant and can be left out (the components of  $\Omega_n \mathbf{x}$  are shifted by a constant  $\rightarrow$  the smallest component stays invariant). Noting the obvious symmetries in the remaining four blocks, we can focus on the top left block.

When  $n$  is prime, it is possible to use the so-called Rader transformation to permute the block matrices into circulant form. (The permutation matrices can be easily generated by computing the “generator”, i.e., primitive root modulo  $n$ .)

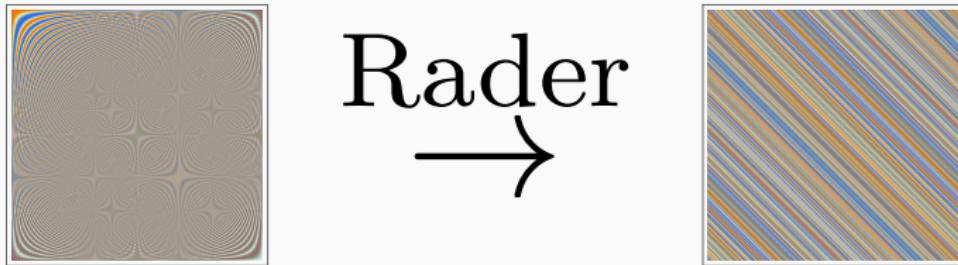


**Figure 4:** The original block matrix is multiplied from both sides by Rader permutation matrices (the black elements indicate the value 1 and white elements indicate the value 0) to obtain a circulant matrix.

## Example with $n = 1009$



**Figure 5:** LHS: Original  $\Omega_{1009}$ . RHS: top left block of  $\Omega_{1009}$  (sans first column).



**Figure 6:** Rader transformation turns the top left block matrix circulant.

- Cost of algorithm for POD weights is  $\mathcal{O}(s n \log n + s^2 n)$  using FFT.
- CBC works for any (composite) number  $n \geq 2$ , but the implementation is more involved when  $n$  is not prime.

**Lemma (J. Dick, I. H. Sloan, X. Wang, H. Woźniakowski (2006))**  
*A generating vector  $z \in \{1, \dots, n-1\}^s$  can be constructed by the CBC algorithm such that*

$$|I_s(f) - Q_{s,n}(f)| \leq \left( \frac{2}{n} \sum_{\emptyset \neq u \subseteq \{1, \dots, s\}} \gamma_u^\lambda (2\zeta(\alpha\lambda))^{|u|} \right)^{1/\lambda} \|f\|_\alpha$$

for  $\lambda \in (1/\alpha, 1]$ ,  $\alpha > 1$ ,  $n$  is any prime power,  $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$ ,  $x > 1$ .

Application of QMC theory:

- Estimate the norm (critical step)
- Choose the weights
- Weights as input to the CBC construction

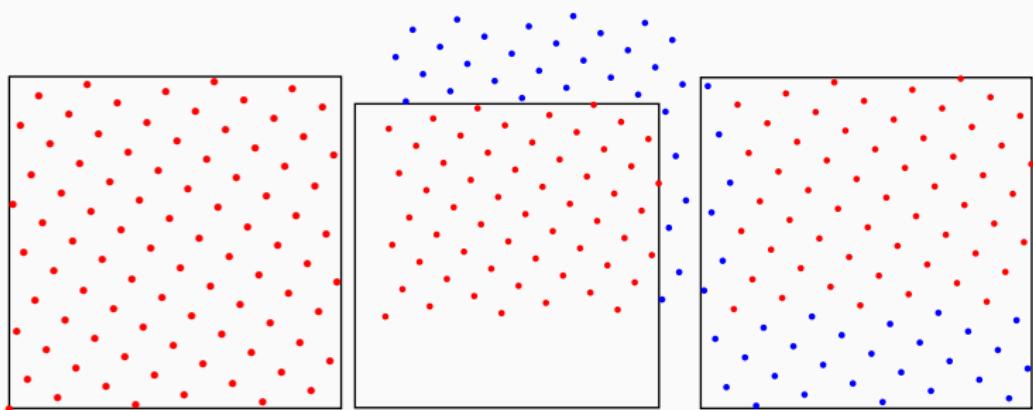
## Non-periodic setting: randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

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

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



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

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

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

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):

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

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

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

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

$$P(z) := e_{s,n,\gamma}^{\text{sh}}(z)^2 = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\emptyset \neq \mathbf{u} \subseteq \{1:s\}} \gamma_{\mathbf{u}} \prod_{j \in \mathbf{u}} \omega \left( \left\{ \frac{kz_j}{n} \right\} \right), \quad \omega(x) = x^2 - x + \frac{1}{6}.$$

Optimal rate of convergence  $\mathcal{O}(n^{-1+\varepsilon})$  in weighted Sobolev spaces (corresponds to  $\alpha = 2$  in periodic setting), CBC construction with error criterion  $P(z)$ . For details, cf. [Dick, Kuo, Sloan, **Acta Numer.** 2013].

## **Part II: The periodic model of uncertainty quantification for PDEs**

---

Consider the elliptic PDE problem:

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}) \nabla u(\mathbf{x})) = f(\mathbf{x}) & \text{for } \mathbf{x} \in D, \\ +\text{boundary conditions.} \end{cases}$$

In practice, one or several of the material/system parameters may be uncertain or incompletely known and modeled as random fields:

- PDE coefficient  $a$  may be uncertain;
- Source term  $f$  may be uncertain;
- Boundary conditions may be uncertain;
- The domain  $D$  itself may be uncertain (main topic of today's talk).

In forward uncertainty quantification, one is interested in assessing how uncertainties in the inputs of a mathematical model affect the output.

⇒ If the uncertain inputs are modeled as random fields, then the output of the PDE is also a random field. One may be interested in assessing the statistical response of the system, for example, the expectation or variance of the PDE solution (or some other quantity of interest thereof).

## Background

A popular model in the literature: the uniform and affine model

Let  $(\Omega, \Gamma, \mathbb{P})$  be a probability space. For  $\mathbf{x} \in D$  and  $\omega \in \Omega$ ,

$$a(\mathbf{x}, \omega) = \bar{a}(\mathbf{x}) + \sum_{j \geq 1} Y_j(\omega) \psi_j(\mathbf{x}), \quad Y_j \text{ i.i.d. uniform on } [-\frac{1}{2}, \frac{1}{2}].$$

Computing  $\mathbb{E}[u(\mathbf{x}, \cdot)]$  (or some quantity of interest  $\mathbb{E}[G(u)]$ ) using

- Rank-1 lattice cubature rules with random shifts  
⇒ cubature error  $\mathcal{O}(n^{-1+\varepsilon})$  at best. (Kuo, Schwab, Sloan 2012)
- Interlaced polynomial lattice rules  
⇒ higher order convergence  $\mathcal{O}(n^{-1/p})$  for some  $0 < p < 1$  ( $p$  is a summability exponent s.t.  $(\|\psi_j\|_{L^\infty})_{j \geq 1} \in \ell^p$ ). (Dick, Kuo, Le Gia, Nuyens, Schwab 2014)

## Periodic model of UQ

In this talk, we instead model the uncertainty in the diffusion coefficient as follows.

Let  $(\Omega, \Gamma, \mathbb{P})$  be a probability space. For  $\mathbf{x} \in D$  and  $\omega \in \Omega$ ,

$$a(\mathbf{x}, \omega) = \bar{a}(\mathbf{x}) + \sum_{j \geq 1} \Theta(Y_j(\omega)) \psi_j(\mathbf{x}), \quad Y_j \text{ i.i.d. uniform on } [-\frac{1}{2}, \frac{1}{2}]$$

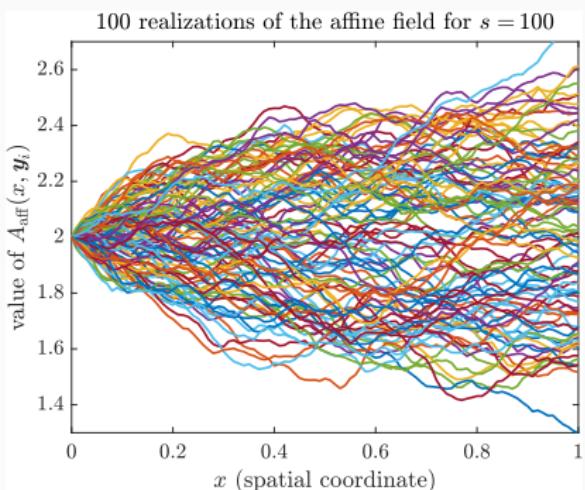
with the special choice  $\Theta(y) = \frac{1}{\sqrt{6}} \sin(2\pi y)$ .

- Note that  $Z(\omega) := \sin(2\pi Y(\omega))$  has the probability density  $\frac{1}{\pi} \frac{1}{\sqrt{1-z^2}}$  on  $[-1, 1]$ , i.e,  $Z \sim \text{Arcsine}(-1, 1)$ .
- We can match the mean and covariance of  $a$  with the “uniform model”.
- Note that the periodicity is only assumed for the *random/uncertain* variable!

# Affine vs. periodic

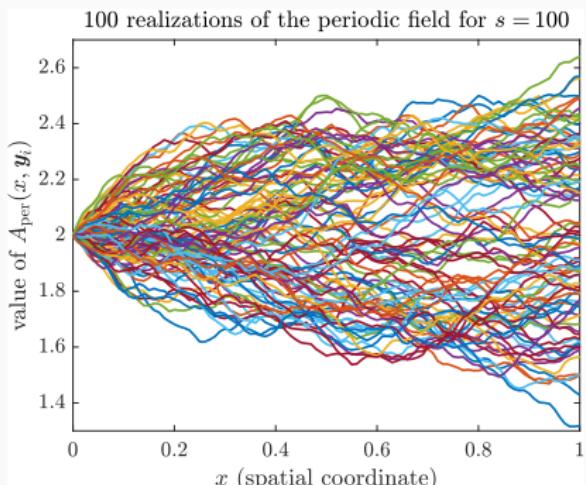
Affine

$$a(x, \mathbf{y}) = \bar{a}(x) + \sum_{j=1}^{100} y_j \psi_j(x)$$



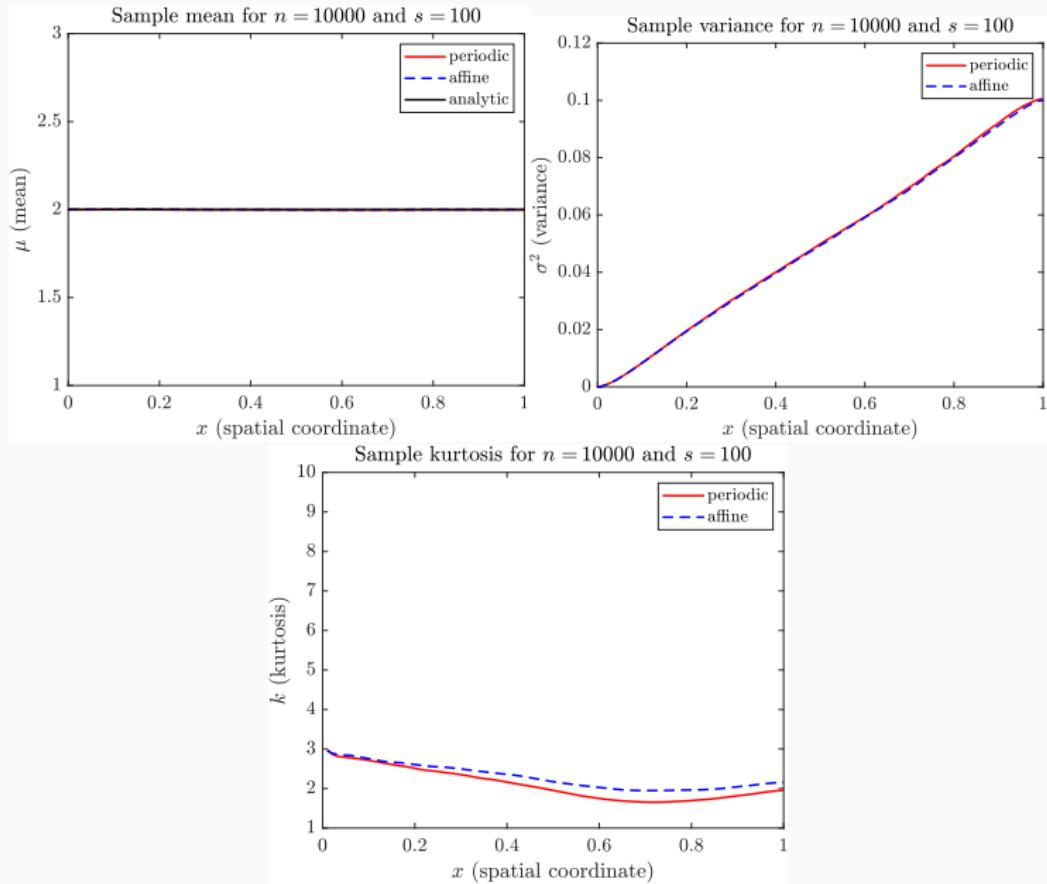
Periodic

$$a(x, \mathbf{y}) = \bar{a}(x) + \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j) \psi_j(x)$$



$$\bar{a}(x) = 2, \quad \psi_j(x) = j^{-3/2} \sin((j - \frac{1}{2})\pi x), \quad x \in [0, 1]$$

# Affine vs. periodic



## **Part III: Domain uncertainty quantification for elliptic PDEs**

---

Consider the Poisson problem

$$\begin{cases} -\Delta u(\mathbf{x}, \omega) = f(\mathbf{x}) & \text{for } \mathbf{x} \in D(\omega), \\ u(\mathbf{x}, \omega) = 0 & \text{for } \mathbf{x} \in \partial D(\omega), \end{cases}$$

where the bounded domain  $D(\omega) \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ , is assumed to be *uncertain*.

**Domain mapping method:** Let  $D_{\text{ref}} \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ , be a fixed reference domain. Define perturbation field  $\mathbf{V}(\omega): \overline{D_{\text{ref}}} \rightarrow \mathbb{R}^d$ , which we assume is given explicitly.

Uncertain domains studied by many authors in the literature: Harbrecht, Peters, Siebenmorgen, Schwab, Zech...

## Parameterization of domain uncertainty

Let  $U := [0, 1]^{\mathbb{N}}$  and let  $\mathbf{V}: \overline{D_{\text{ref}}} \times U \rightarrow \mathbb{R}^d$  be a vector field such that

$$\mathbf{V}(\mathbf{x}, \mathbf{y}) := \mathbf{x} + \frac{1}{\sqrt{6}} \sum_{i=1}^{\infty} \sin(2\pi y_i) \psi_i(\mathbf{x}), \quad \mathbf{x} \in D_{\text{ref}}, \quad \mathbf{y} \in U,$$

with *stochastic fluctuations*  $\psi_i: D_{\text{ref}} \rightarrow \mathbb{R}^d$ . Denoting the Jacobian matrix of  $\psi_i$  by  $\psi'_i$ , the Jacobian matrix  $J(\cdot, \mathbf{y}): D_{\text{ref}} \rightarrow \mathbb{R}^{d \times d}$  of vector field  $\mathbf{V}$  is

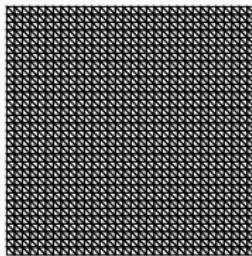
$$J(\mathbf{x}, \mathbf{y}) = I + \frac{1}{\sqrt{6}} \sum_{i=1}^{\infty} \sin(2\pi y_i) \psi'_i(\mathbf{x}), \quad \mathbf{x} \in D_{\text{ref}}, \quad \mathbf{y} \in U.$$

The family of *admissible domains*  $\{D(\mathbf{y})\}_{\mathbf{y} \in U}$  is parameterized by

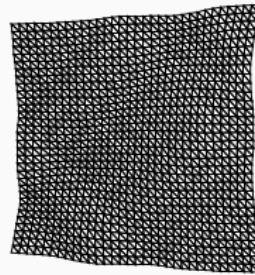
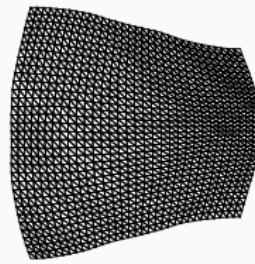
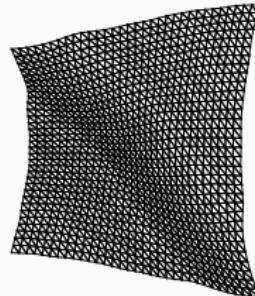
$$D(\mathbf{y}) := \mathbf{V}(D_{\text{ref}}, \mathbf{y}), \quad \mathbf{y} \in U,$$

and we define the *hold-all domain* by setting

$$\mathcal{D} := \bigcup_{\mathbf{y} \in U} D(\mathbf{y}).$$



**Figure 7:** Reference domain



**Figure 8:** Three realizations of the random domain

## Notations and assumptions

The reference domain  $D_{\text{ref}} \subset \mathbb{R}^d$ ,  $d \in \{2, 3\}$ , is bounded with Lipschitz boundary.

(A1) For each  $\mathbf{y} \in U$ ,  $\mathbf{V}(\cdot, \mathbf{y}) : \overline{D_{\text{ref}}} \rightarrow \mathbb{R}^d$  is an invertible, twice continuously differentiable vector field.

(A2) For some  $C > 0$ , there holds

$$\|\mathbf{V}(\cdot, \mathbf{y})\|_{C^2(\overline{D_{\text{ref}}})} \leq C \quad \text{and} \quad \|\mathbf{V}^{-1}(\cdot, \mathbf{y})\|_{C^2(\overline{D(\mathbf{y})})} \leq C \quad \text{for all } \mathbf{y} \in U.$$

(A3) There exist constants  $0 < \sigma_{\min} \leq 1 \leq \sigma_{\max} < \infty$  such that

$$\sigma_{\min} \leq \min \sigma(J(\mathbf{x}, \mathbf{y})) \leq \max \sigma(J(\mathbf{x}, \mathbf{y})) \leq \sigma_{\max} \quad \text{for all } \mathbf{x} \in D_{\text{ref}}, \mathbf{y} \in U,$$

where  $\sigma(J(\mathbf{x}, \mathbf{y}))$  denotes the set of all singular values of matrix  $J(\mathbf{x}, \mathbf{y})$ ,

(A4) There holds  $\|\psi_i\|_{W^{1,\infty}(D_{\text{ref}}; \mathbb{R}^d)} < \infty$  for all  $i \in \mathbb{N}$  and  $\sum_{i=1}^{\infty} \|\psi_i\|_{W^{1,\infty}(D_{\text{ref}}; \mathbb{R}^d)} < \infty$ .

(A5) For some  $p \in (0, 1)$ , there holds

$$\sum_{i=1}^{\infty} \|\psi_i\|_{W^{1,\infty}(D_{\text{ref}}; \mathbb{R}^d)}^p < \infty.$$

The variational formulation of the model problem can be stated as follows: for  $\mathbf{y} \in U$ , find  $u(\cdot, \mathbf{y}) \in H_0^1(D(\mathbf{y}))$  such that

$$\int_{D(\mathbf{y})} \nabla u(\mathbf{x}, \mathbf{y}) \cdot \nabla v(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} = \int_{D(\mathbf{y})} f(\mathbf{x}) v(\mathbf{x}, \mathbf{y}) \, d\mathbf{x} \quad \forall v \in H_0^1(D(\mathbf{y})), \quad (1)$$

where  $f \in \mathcal{C}^\infty(\mathcal{D})$  is assumed to be an analytic function.

We can transport the variational formulation (1) to the reference domain by a change of variable. Let us define

$$A(\mathbf{x}, \mathbf{y}) := (J(\mathbf{x}, \mathbf{y})^T J(\mathbf{x}, \mathbf{y}))^{-1} \det J(\mathbf{x}, \mathbf{y})$$

$$f_{\text{ref}}(\mathbf{x}, \mathbf{y}) := f(V(\mathbf{x}, \mathbf{y})) \det J(\mathbf{x}, \mathbf{y}),$$

for  $\mathbf{x} \in D_{\text{ref}}$ ,  $\mathbf{y} \in U$ . Then we can recast the problem (1) on the reference domain as follows: for  $\mathbf{y} \in U$ , find  $\widehat{u}(\cdot, \mathbf{y}) \in H_0^1(D_{\text{ref}})$  such that

$$\int_{D_{\text{ref}}} (A(\mathbf{x}, \mathbf{y}) \nabla \widehat{u}(\mathbf{x}, \mathbf{y})) \cdot \nabla \widehat{v}(\mathbf{x}) \, d\mathbf{x} = \int_{D_{\text{ref}}} f_{\text{ref}}(\mathbf{x}, \mathbf{y}) \widehat{v}(\mathbf{x}) \, d\mathbf{x} \quad \forall \widehat{v} \in H_0^1(D_{\text{ref}}). \quad (2)$$

The solutions to problems (1) and (2) are connected to one another by

$$u(\cdot, \mathbf{y}) = \widehat{u}(V^{-1}(\cdot, \mathbf{y}), \mathbf{y}) \quad \Leftrightarrow \quad \widehat{u}(\cdot, \mathbf{y}) = u(V(\cdot, \mathbf{y}), \mathbf{y}), \quad \mathbf{y} \in U.$$

**Theorem (Hakula–Harbrecht–K–Kuo–Sloan 2022)**  
 There holds for all  $\mathbf{y} \in U$  and all multi-indices  $\nu \neq \mathbf{0}$  that

$$\|\partial_{\mathbf{y}}^{\nu} \widehat{u}(\cdot, \mathbf{y})\|_{H_0^1(D_{\text{ref}})} \lesssim (2\pi \widetilde{C})^{|\nu|} \sum_{\mathbf{m} \leq \nu} \frac{(|\mathbf{m}| + d - 1)!}{(d - 1)!} \prod_{i \geq 1} (m_i! \beta_i^{m_i} S(\nu_i, m_i)),$$

where  $\rho \geq 1$  satisfies  $\|\partial_{\mathbf{x}}^{\nu} f\|_{L^{\infty}(\mathcal{D})} \leq C_f \nu! \rho^{|\nu|}$ ,  $\widetilde{C} := \frac{2d! (1+\sigma_{\max})^d \sigma_{\max}^3}{\sigma_{\min}^{d+4}}$ ,

$\beta_j := \frac{2+\sqrt{2}}{\sqrt{6}} \max(1 + \sqrt{3}, \rho) \|\psi_j\|_{W^{1,\infty}(D_{\text{ref}})}$ , and  $S(n, k)$  denotes the Stirling number of the second kind.

Plugging the above into the QMC error bound suggests choosing the (SPOD) weights

$$\gamma_{\mathbf{u}} := \sum_{\mathbf{m}_{\mathbf{u}} \in \{1:\alpha\}^{|\mathbf{u}|}} \frac{(|\mathbf{m}_{\mathbf{u}}| + d - 1)!}{(d - 1)!} \prod_{j \in \mathbf{u}} (\widetilde{C}^{\alpha} m_j! \beta_j^{m_j} S(\alpha, m_j)), \quad \emptyset \neq \mathbf{u} \subseteq \{1 : s\},$$

and by setting  $\lambda := p$  and  $\alpha := \lfloor \frac{1}{p} \rfloor + 1$ , we obtain QMC convergence rate  $\|I_s(\widehat{u}_s) - Q_{s,n}(\widehat{u}_s)\|_{L^1(D_{\text{ref}})} = \mathcal{O}(n^{-1/p})$  where the implied coefficient can be shown to be independent of the dimension  $s$ .

*Remark.* The fast CBC construction cost to obtain the generating vector with SPOD weights is  $\mathcal{O}(s n \log n + \alpha^2 s^2 n)$  operations.

## Numerical experiment

Let us consider the domain parameterization

$$D(\mathbf{y}) := \{(x_1, x_2) \in \mathbb{R}^2 : 0 \leq x_1 \leq 1, 0 \leq x_2 \leq a(x_1, \mathbf{y})\}, \quad \mathbf{y} = (y_j)_{j=1}^s \in [0, 1]^s,$$

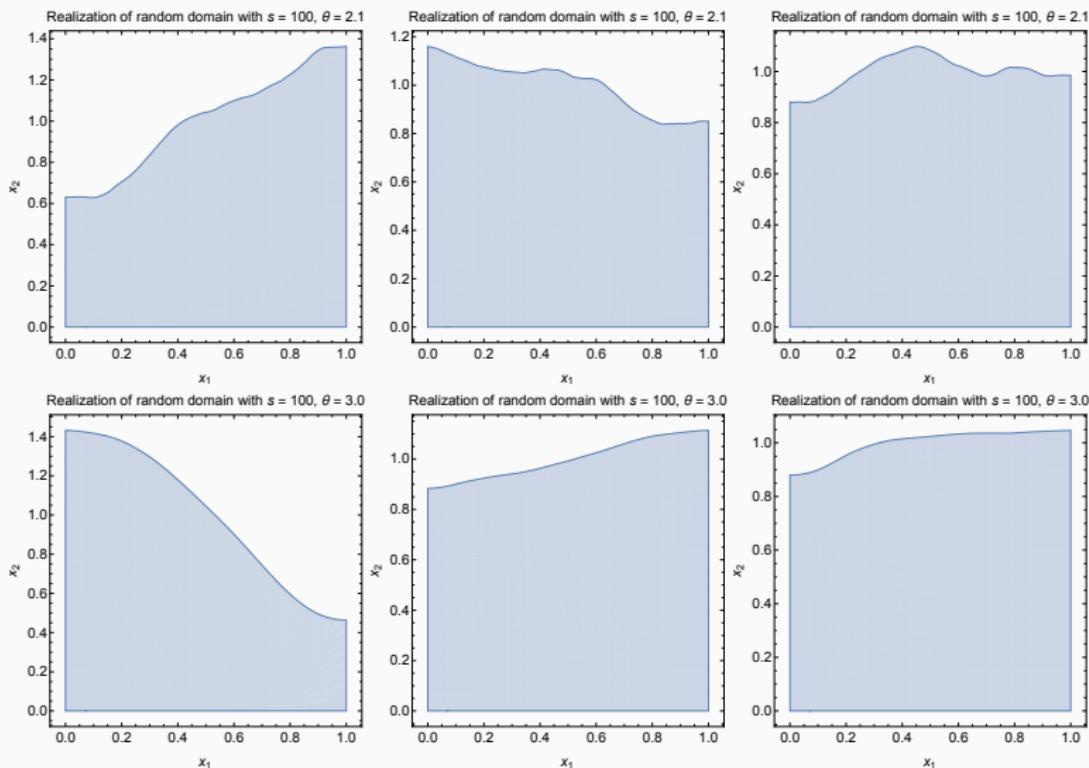
where

$$a(x, \mathbf{y}) := 1 + \frac{c}{\sqrt{6}} \sum_{j=1}^s \sin(2\pi y_j) \psi_j(x), \quad x \in [0, 1] \text{ and } \mathbf{y} \in [0, 1]^s$$

with  $c := \sqrt{3/2}$  and  $\psi_j(x) := j^{-\theta} \cos(j\pi x)$ ,  $\theta > 2$ . Thus the reference domain in this case is the unit square, and the uncertain boundary is confined to the upper edge of the square. We set  $f(\mathbf{x}) := x_2$ . It is possible to write  $D(\mathbf{y}) = V(D(\mathbf{0}), \mathbf{y})$  with the vector-valued expansion

$$\mathbf{V}(\mathbf{x}, \mathbf{y}) := \mathbf{x} + \frac{1}{\sqrt{6}} \sum_{j=1}^s \sin(2\pi y_j) \psi_j(\mathbf{x}), \quad \psi_j(\mathbf{x}) := c j^{-\theta} \begin{bmatrix} 0 \\ x_2 \cos(j\pi x_1) \end{bmatrix}.$$

It can be shown that  $\|\psi_j\|_{W^{1,\infty}} = c\pi j^{1-\theta}$  and  $\sigma_{\max} = 1 + \frac{c\pi}{\sqrt{6}} \zeta(\theta - 1)$ . The expected rate of QMC convergence is  $\mathcal{O}(n^{-\theta+1})$ . Transported PDE problem discretized using piecewise linear FEM with mesh size  $h = 2^{-5}$ .

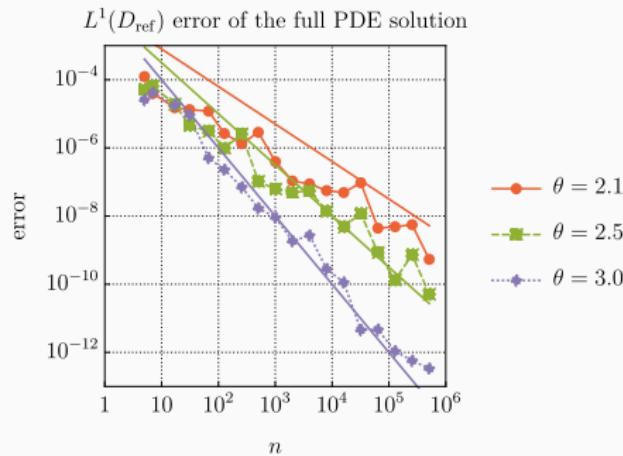


**Figure 9:** Realizations of the random domains in the numerical experiments. Here, we set  $s = 100$  and  $\theta \in \{2.1, 3.0\}$ . Recall that the reference domain is  $D_{\text{ref}} = (0, 1)^2$ .

# QMC error of the full PDE solution

We considered the QMC error of the full PDE solution

$$\left\| \int_{[0,1]^s} \widehat{u}_{s,h}(\cdot, \mathbf{y}) d\mathbf{y} - \frac{1}{n} \sum_{i=1}^n \widehat{u}_{s,h}(\cdot, \mathbf{t}_i) \right\|_{L^1(D_{\text{ref}})}.$$

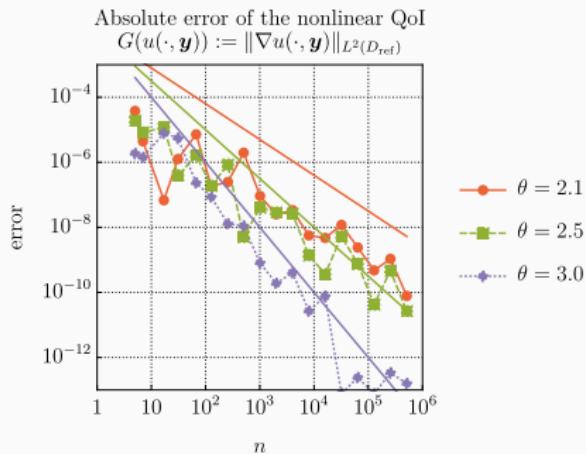


**Figure 10:** QMC cubature errors with increasing  $n$ , varying decay rate  $\theta \in \{2.1, 2.5, 3.0\}$ , and fixed dimension  $s = 100$ . The theoretically expected convergence rates are 1.1, 1.5, and 2.0, respectively. As the reference solution, we use a QMC approximation computed using  $n = 1\,024\,207$  nodes.

# QMC error for nonlinear quantity of interest

We also considered the QMC error of a nonlinear quantity of interest

$$\left| \int_{[0,1]^s} G(\hat{u}_{s,h}(\cdot, \mathbf{y})) d\mathbf{y} - \frac{1}{n} \sum_{i=1}^n G(\hat{u}_{s,h}(\cdot, \mathbf{t}_i)) \right|, \quad G: H_0^1(D_{\text{ref}}) \rightarrow \mathbb{R}.$$



**Figure 11:** QMC cubature errors with increasing  $n$ , varying decay rate  $\theta \in \{2.1, 2.5, 3.0\}$ , and fixed dimension  $s = 100$ . The expected convergence rates are 1.1, 1.5, and 2.0, respectively. As the reference solution, we use a QMC approximation computed using  $n = 1\,024\,207$  nodes.

# Conclusions

- We propose a periodic model for modeling uncertain/random domains. From a modeling point of view, there does not seem to be any reason to prefer the affine model over the periodic model.
- Periodicity yields higher order convergence for QMC quadrature, without the use of, e.g., interlaced polynomial lattice rules (which have higher CBC construction cost).
- Potential applications for inverse UQ problems such as domain shape recovery from measurement data.

**Thank you for your attention!**

# Some QMC resources

Surveys on QMC for PDE problems:

-  J. Dick, F. Y. Kuo, and I. H. Sloan.  
High-dimensional integration: The quasi-Monte Carlo way. *Acta Numer.* **22**:133–288, 2013.
-  F. Y. Kuo and D. Nuyens. Application of quasi-Monte Carlo methods to elliptic PDEs with random diffusion coefficients: A survey of analysis and implementation. *Found. Comput. Math.* **16**:1631–1696, 2016.
-  F. Y. Kuo and D. Nuyens. Application of quasi-Monte Carlo methods to PDEs with random coefficients – An overview and tutorial. *MCQMC 2016 proceedings*, pp. 53–71, 2018.
- Software:**
  -  F. Y. Kuo and D. Nuyens.  
QMC4PDE software.  
<https://people.cs.kuleuven.be/~dirk.nuyens/qmc4pde/>
  -  D. Nuyens. Magic point shop.  
<https://people.cs.kuleuven.be/~dirk.nuyens/qmc-generators/>
  -  F. Y. Kuo. Lattice rule generating vectors. <https://web.maths.unsw.edu.au/~fkuo/lattice/index.html>
  -  R. N. Gantner. Tools for Higher-Order Quasi-Monte Carlo.  
[www.sam.math.ethz.ch/HOQMC/](http://www.sam.math.ethz.ch/HOQMC/)
  -  F. J. Hickernell et al. QMCPy. <https://arxiv.org/abs/2102.07833>