Fast kernel interpolation over lattice point sets with application to uncertainty quantification

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Joint work with Yoshihito Kazashi (Uni. Heidelberg), Frances Kuo (UNSW Sydney), Fabio Nobile (EPFL), and Ian Sloan (UNSW Sydney)

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Part I: Quasi-Monte Carlo cubature

High-dimensional numerical integration

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

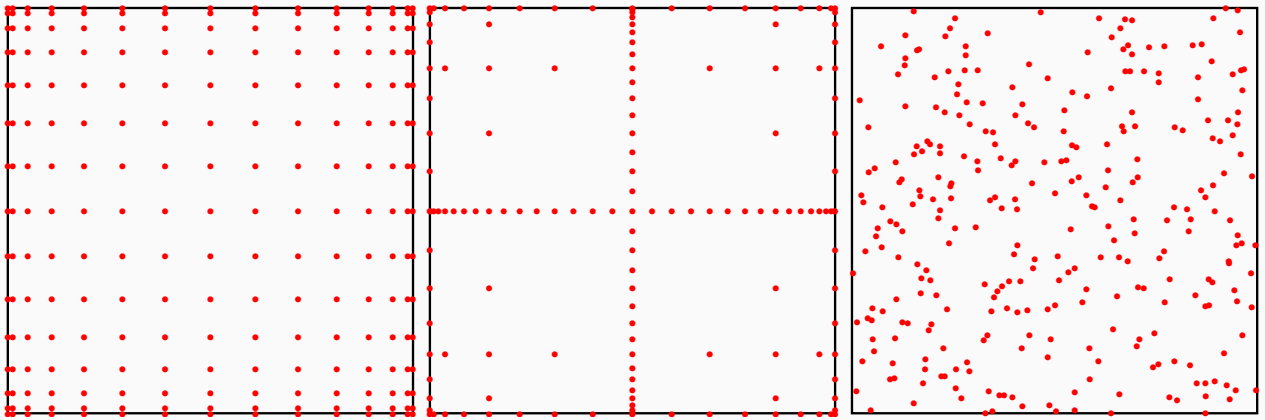


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

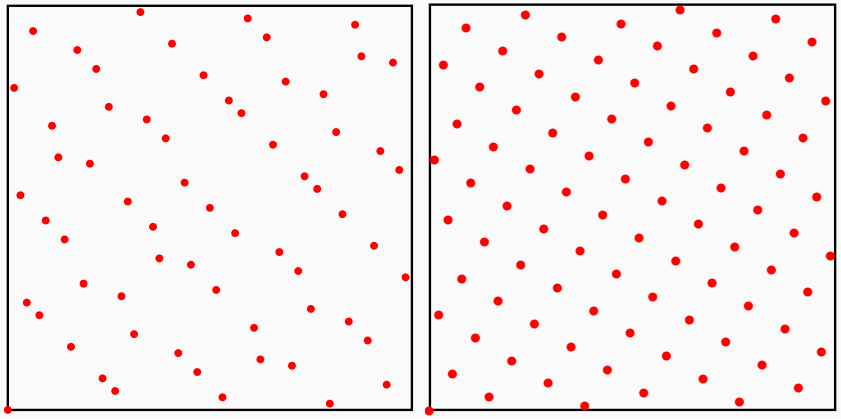


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

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

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

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

The nodes $(\boldsymbol{t}_i)_{i=1}^n$ 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

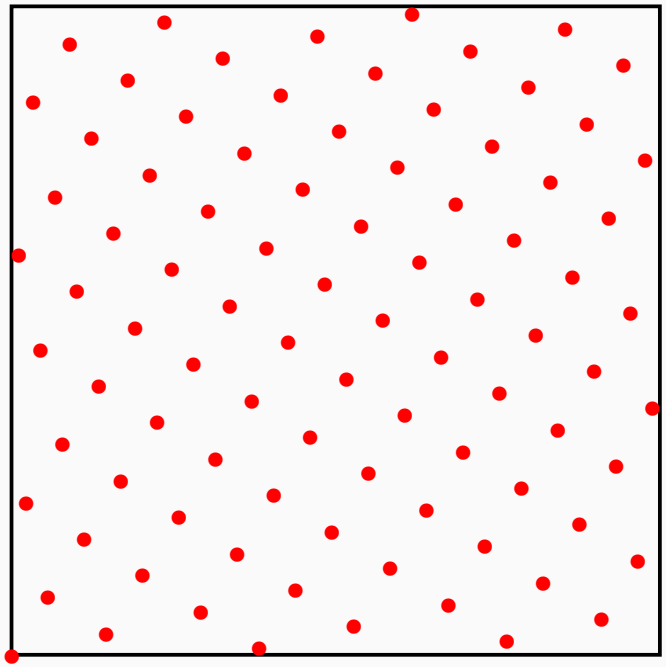
Rank-1 lattice rules

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

have the points

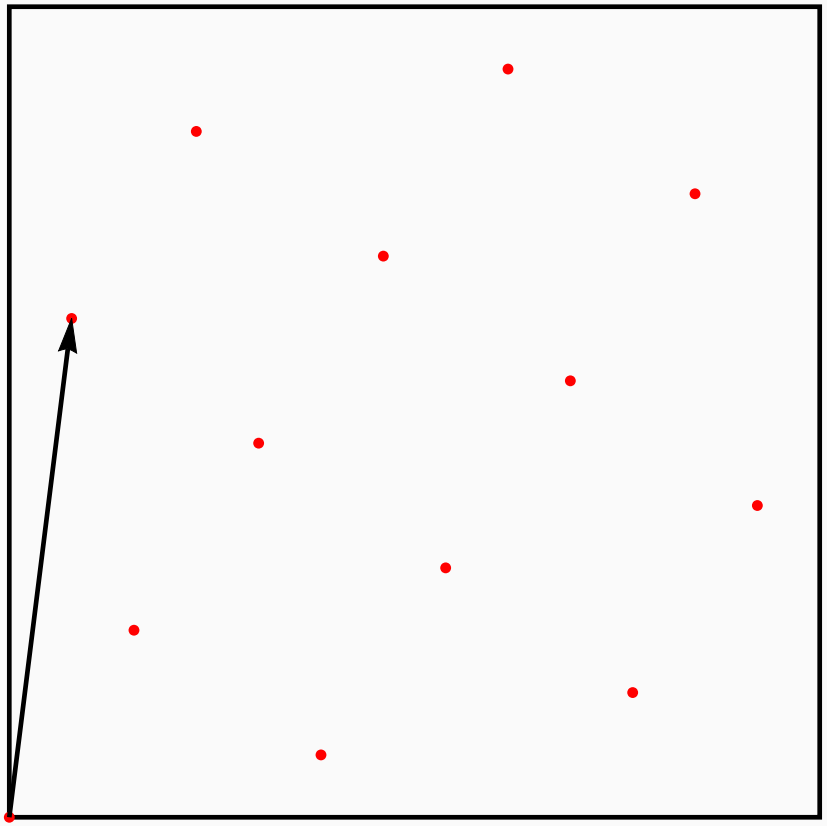
$$\boldsymbol{t}_i = \operatorname{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

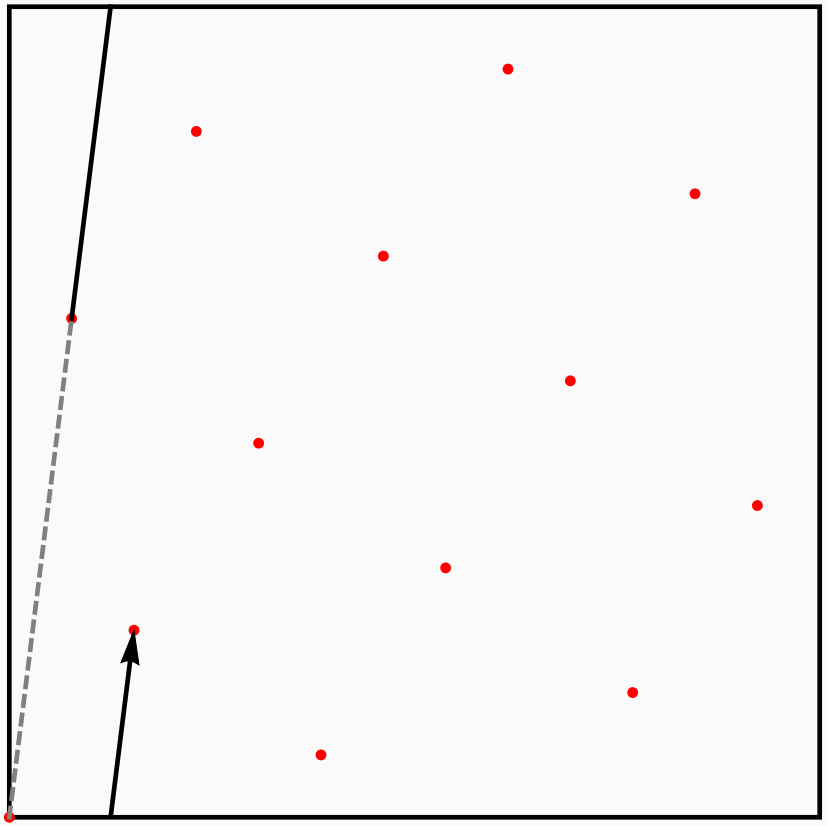
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

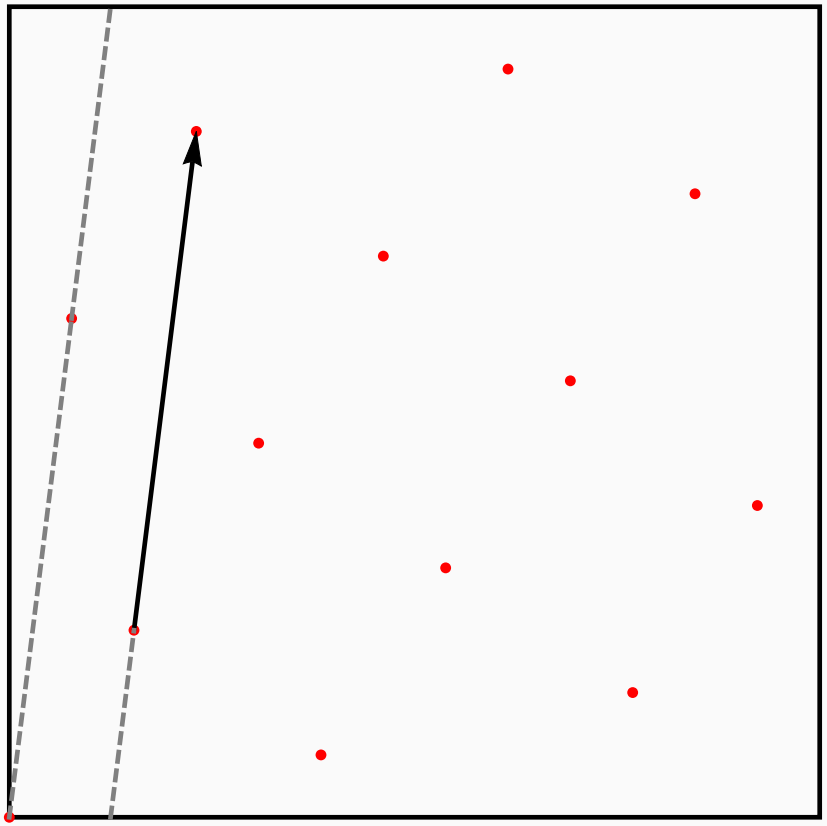


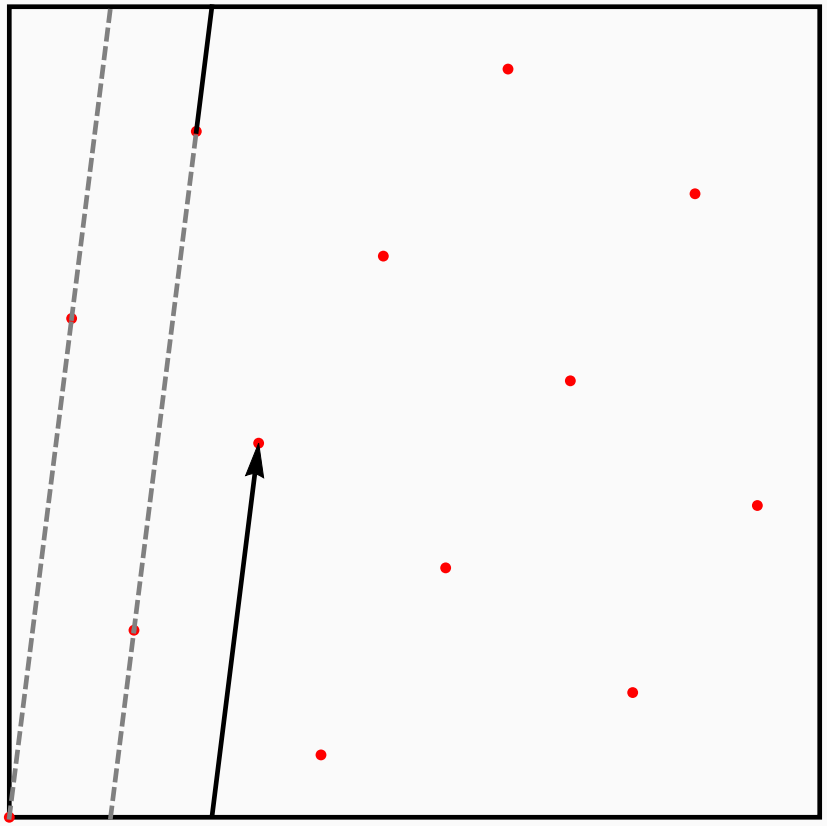
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

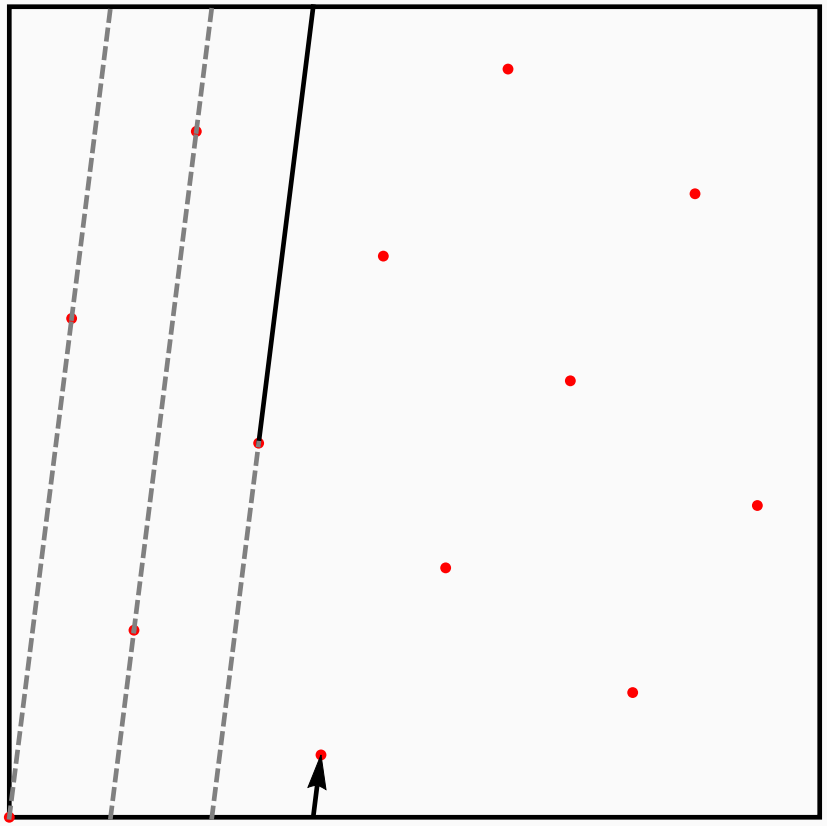
Lattice rules and periodic functions are a match made in heaven!

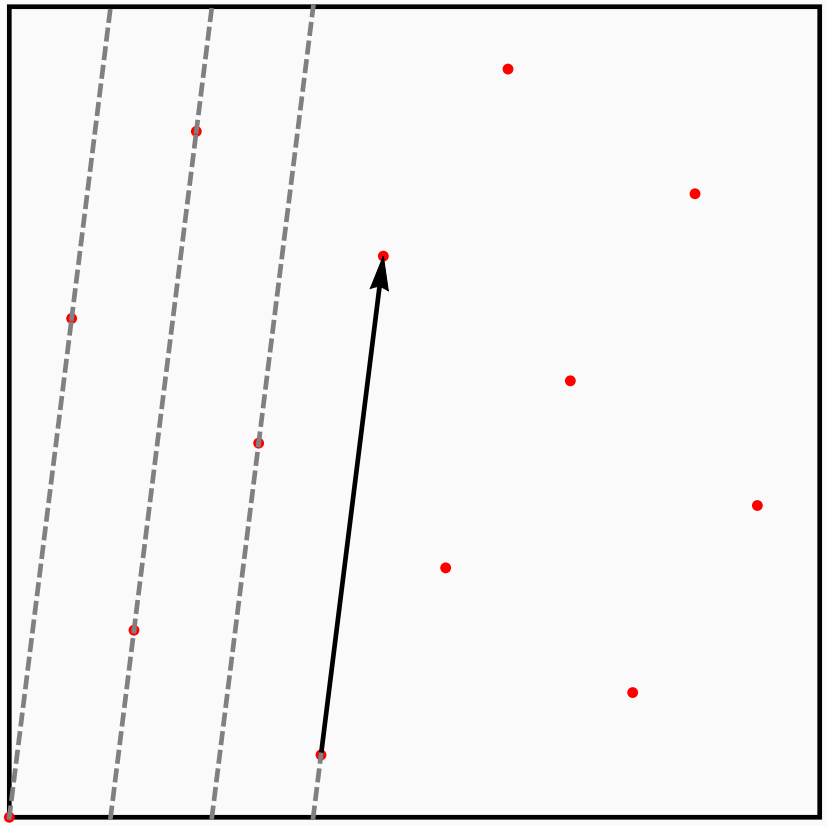


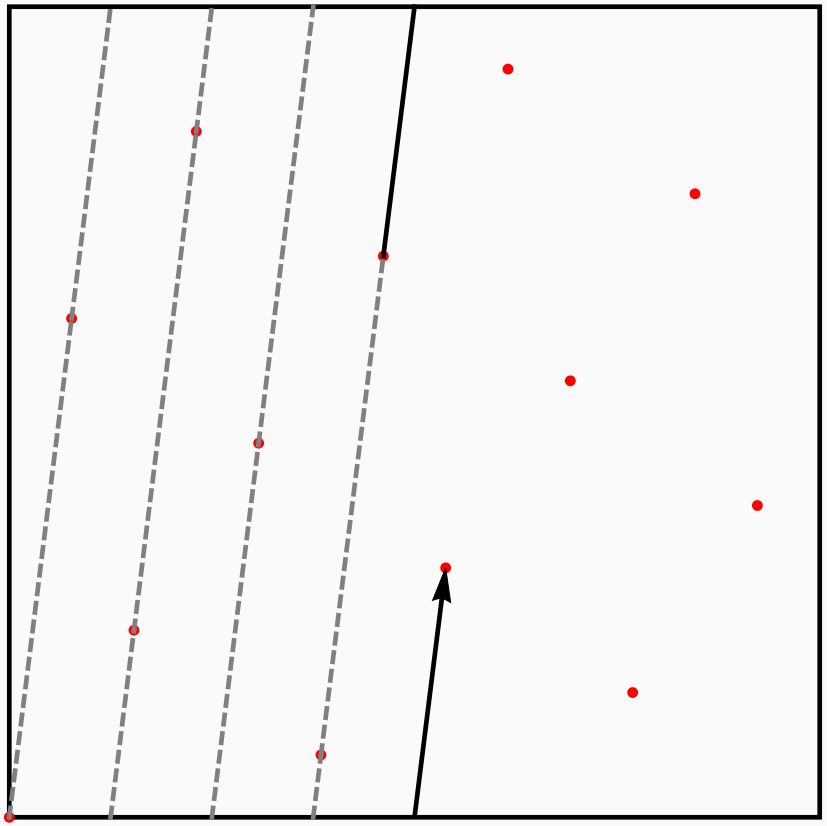


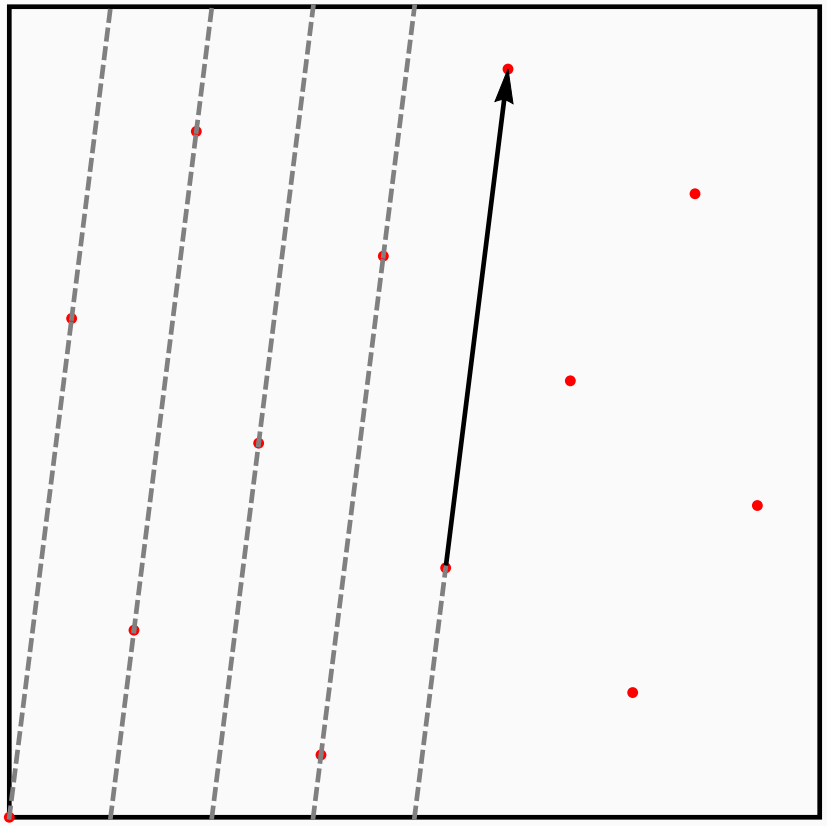


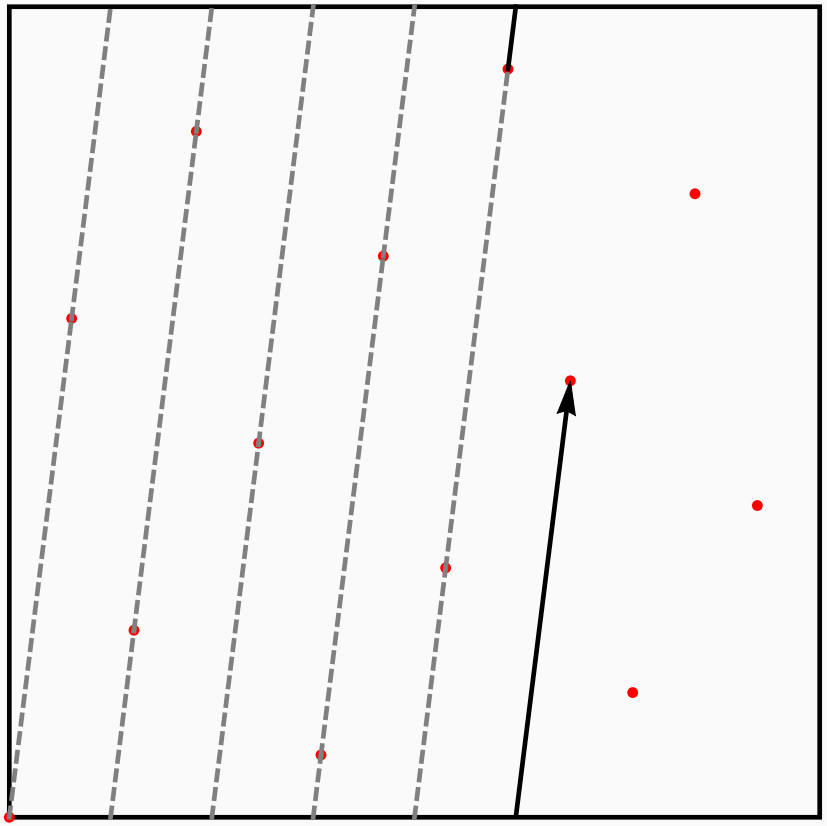


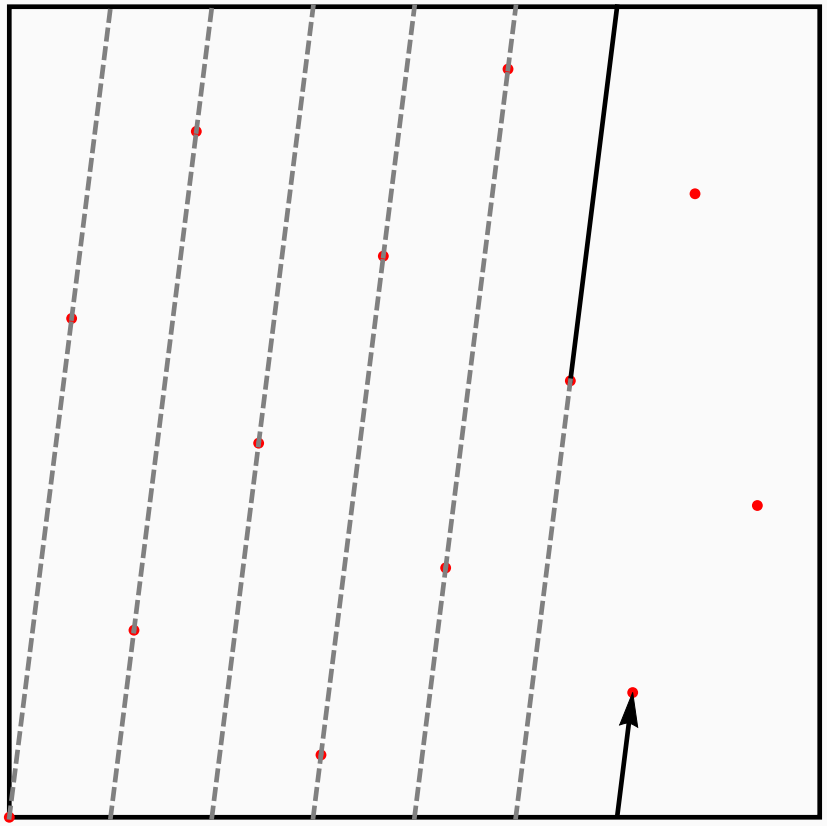


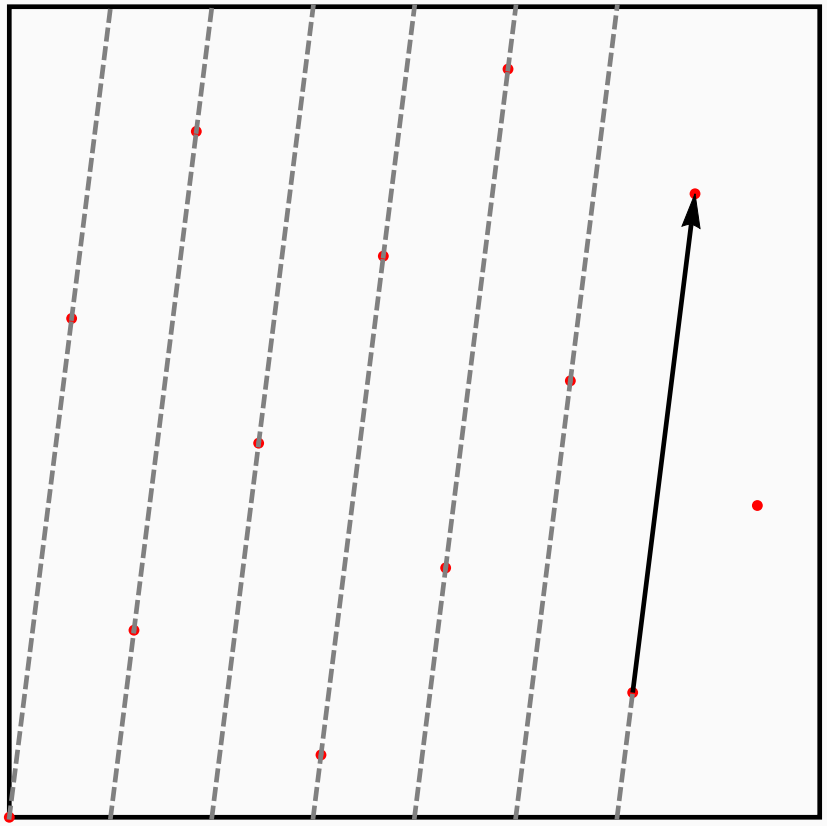


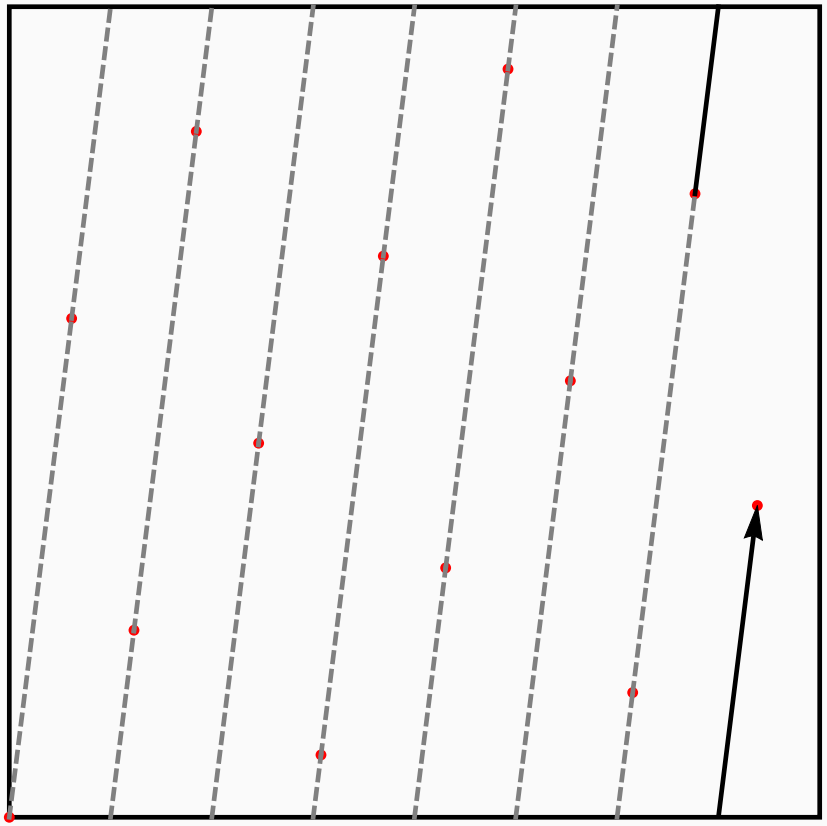












Dimension $s = 1$: the only lattice is the left-Riemann rule

For $z \in \{1, \ldots, n-1\}$, $\gcd(z, n) = 1$, it holds that

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

Suppose $f : [0, 1) \to \mathbb{R}$ is p times continuously differentiable and periodic. Let $h = \frac{1}{n}$. Then the Euler–Maclaurin summation formula gives

$$\sum_{k=0}^{n-1} hf(kh) = \int_0^1 f(x)\,\mathrm{d}x + \sum_{k=1}^{\lfloor p/2 \rfloor} \frac{B_{2k}}{(2k)!}(f^{(2k-1)}(1) - f^{(2k-1)}(0)) - (-1)^p h^p \int_0^1 \widetilde{B}_p(x) f^{(p)}(x)\,\mathrm{d}x$$

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

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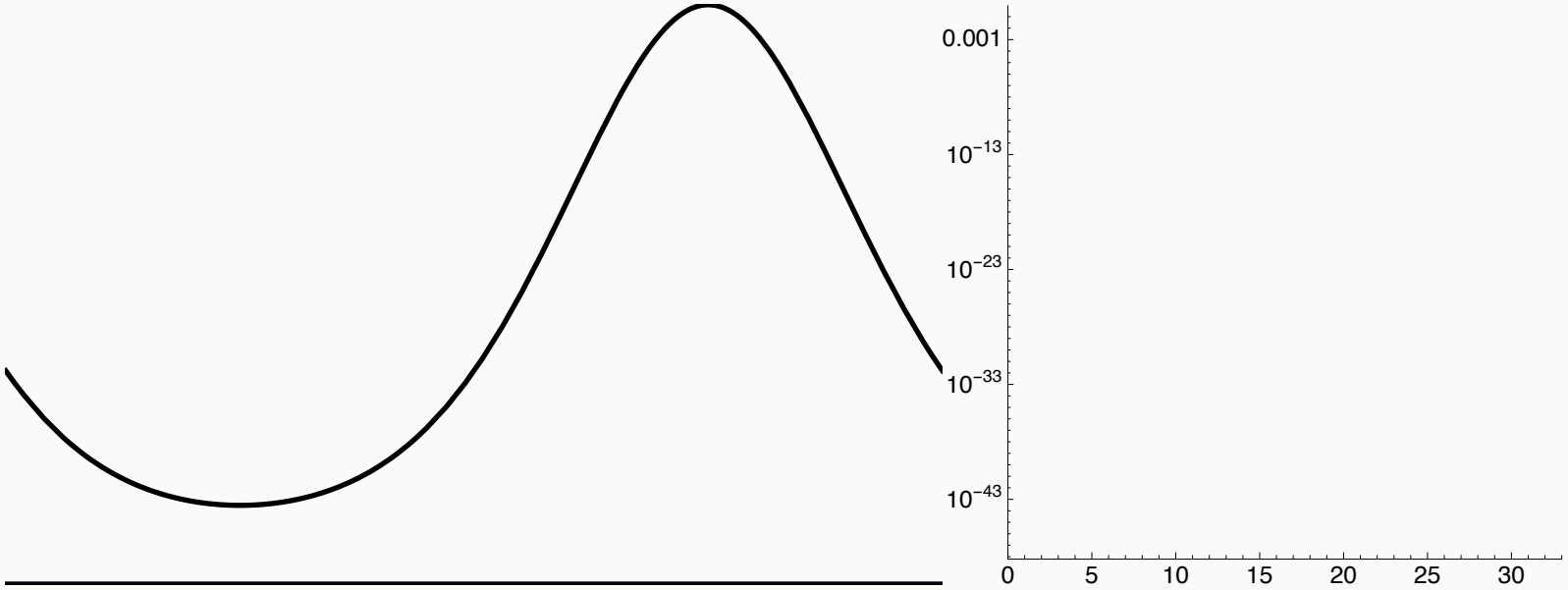
$$\int_0^1 \exp(-\sin(2\pi x))\,\mathrm{d}x$$



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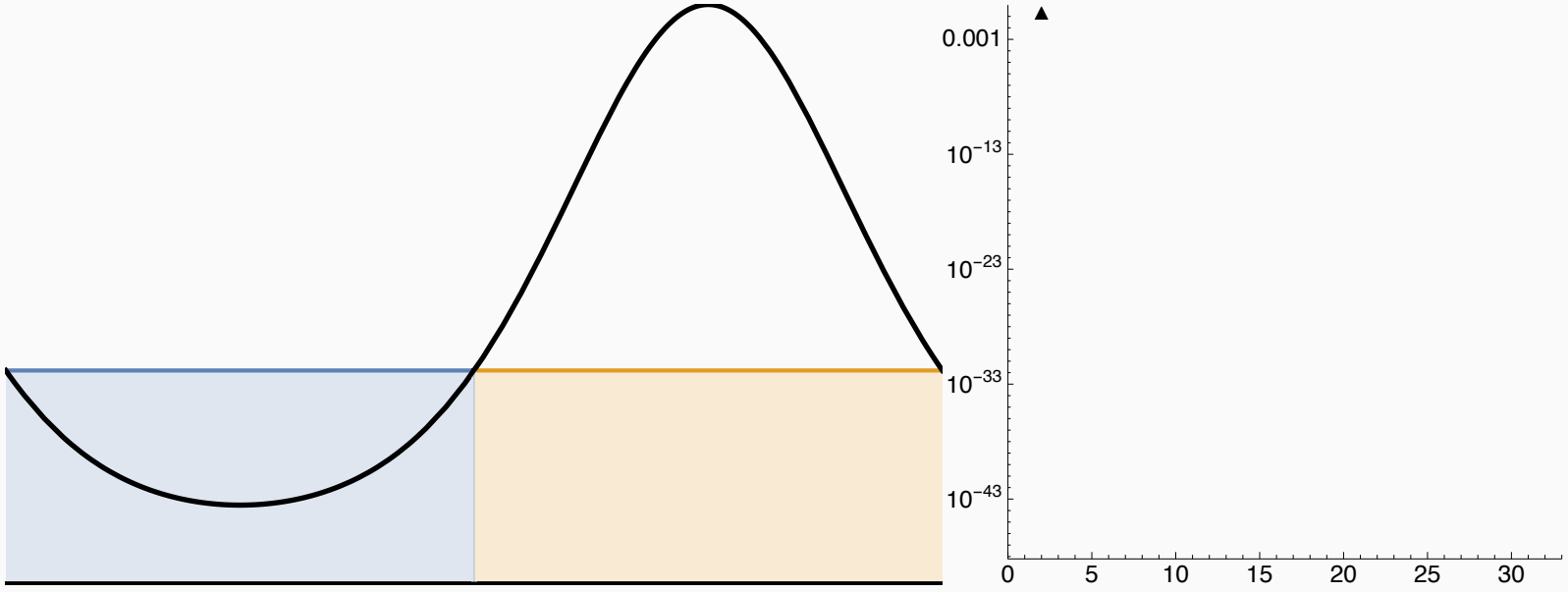

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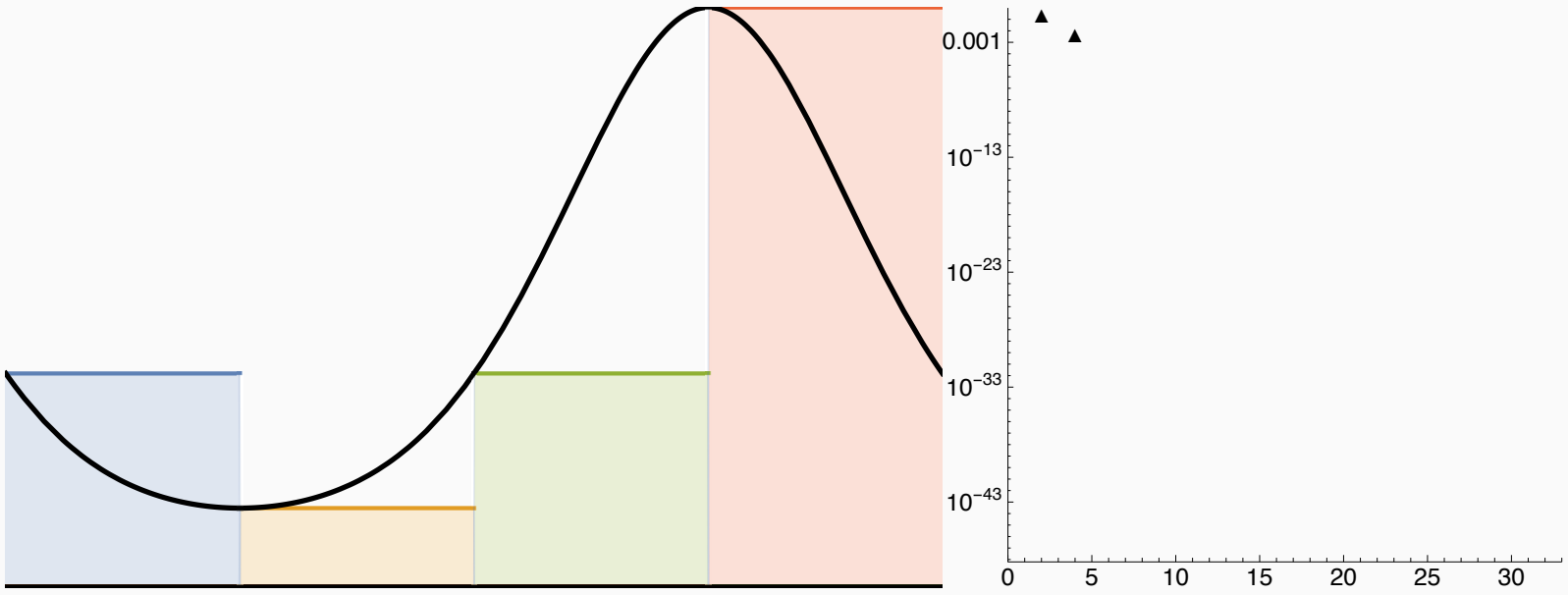

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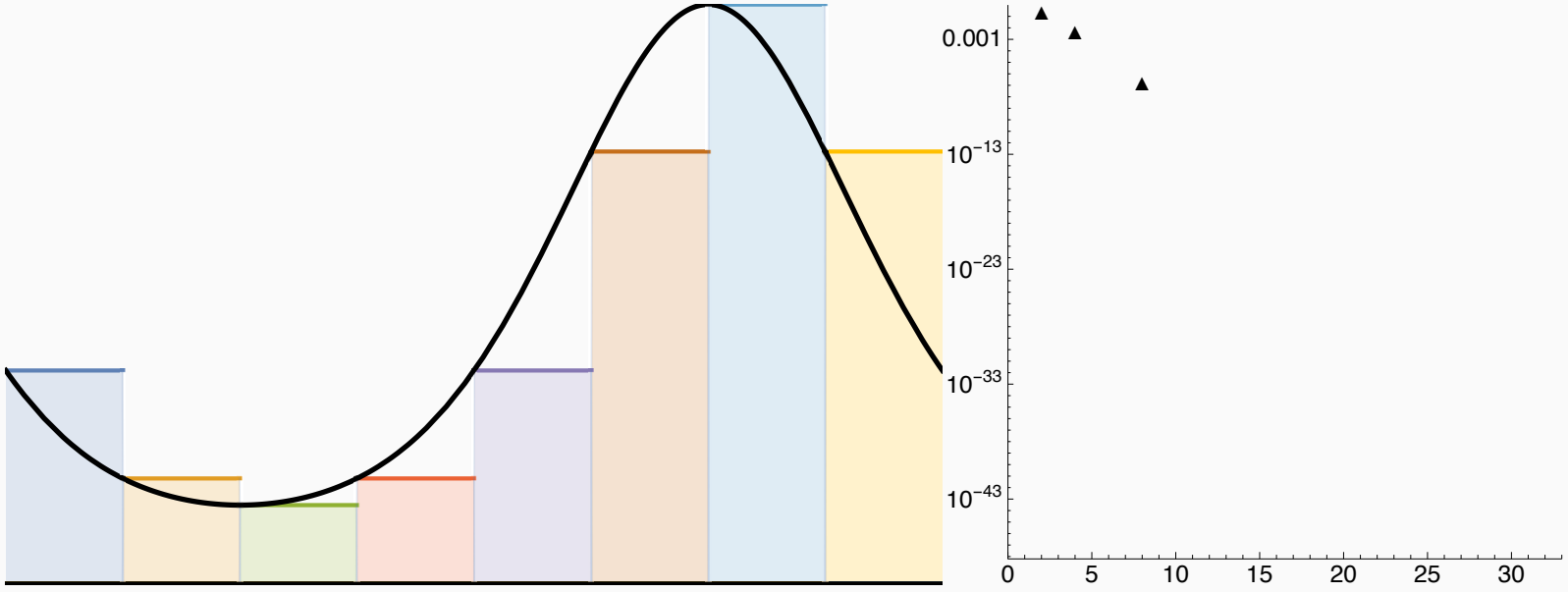

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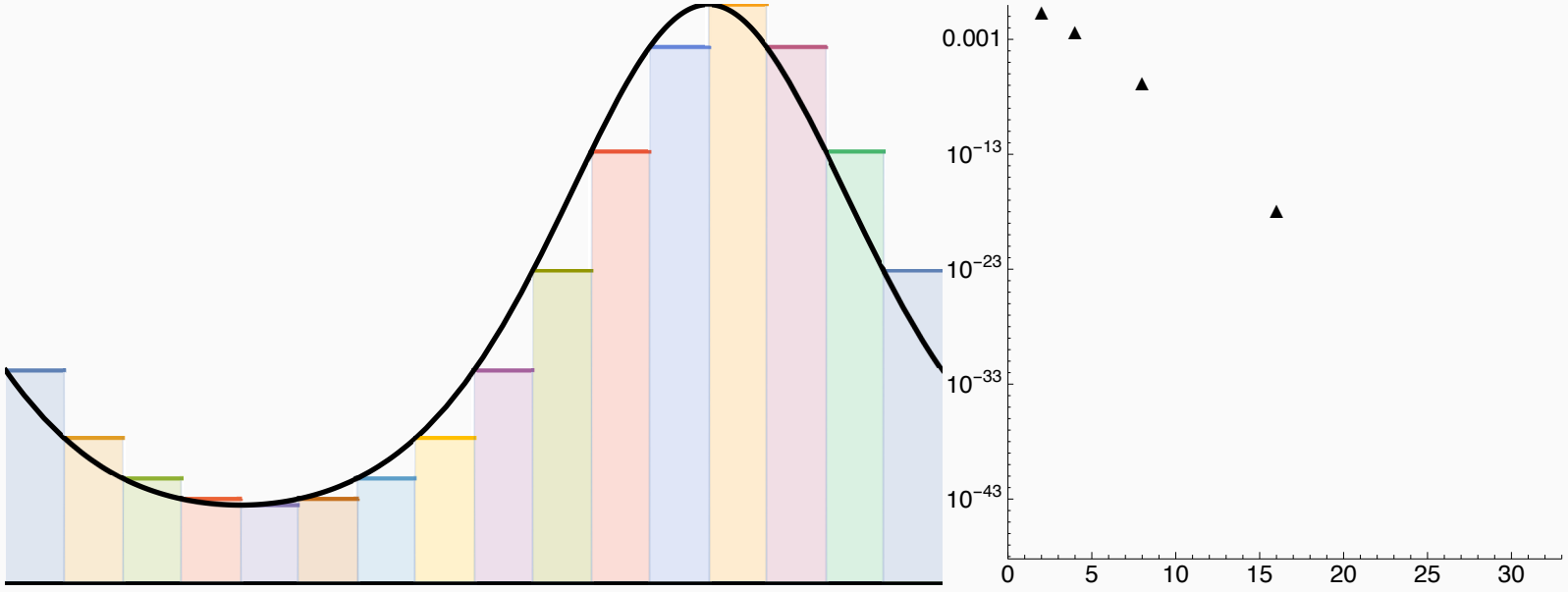

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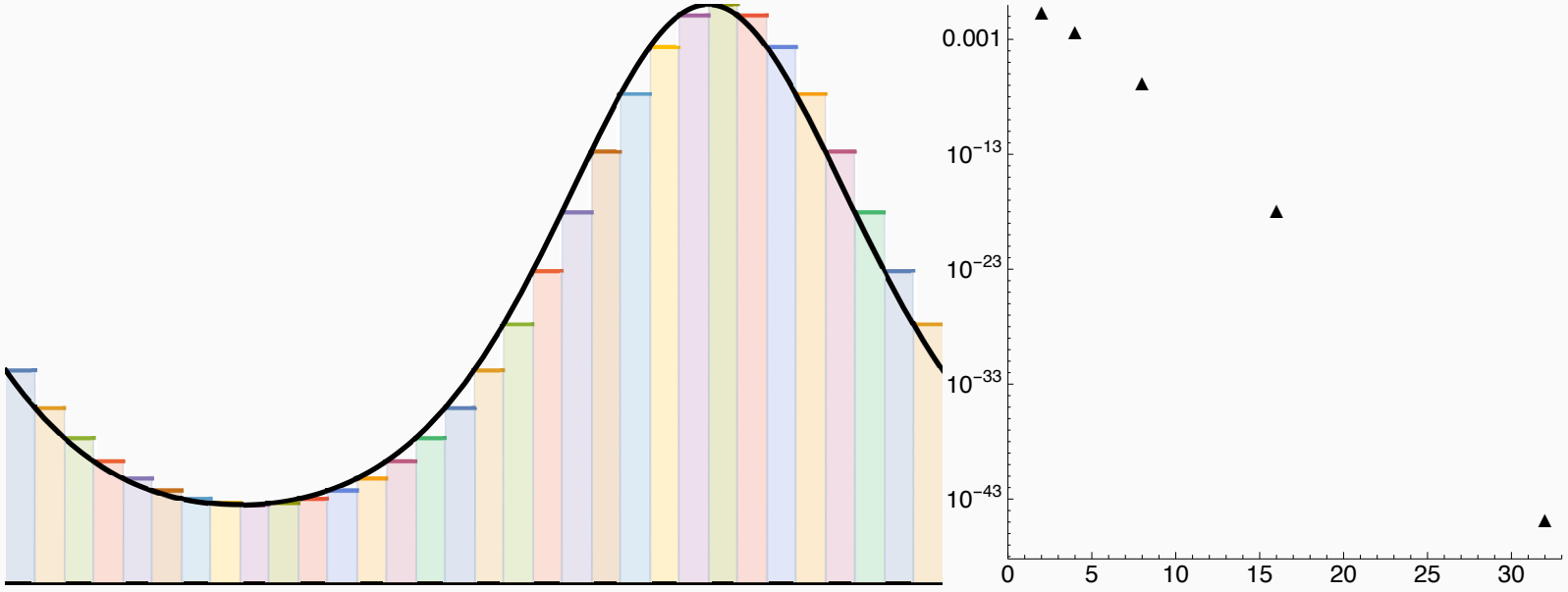

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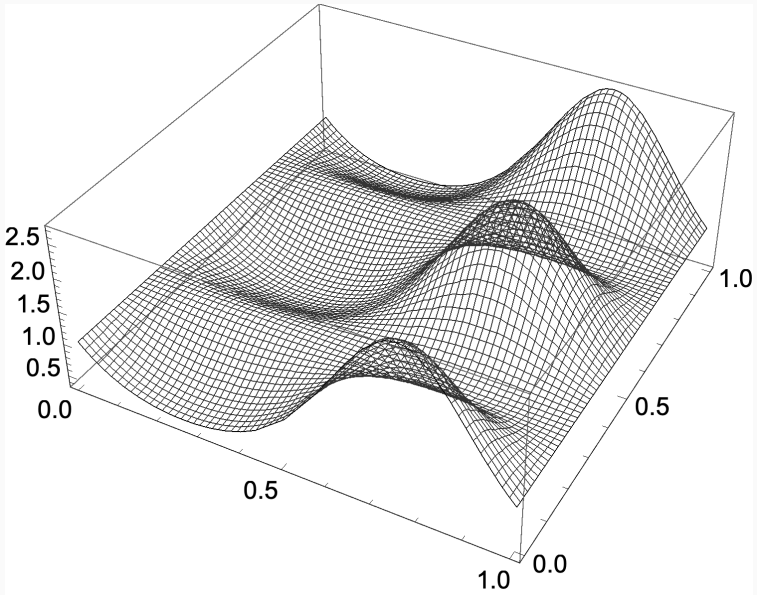

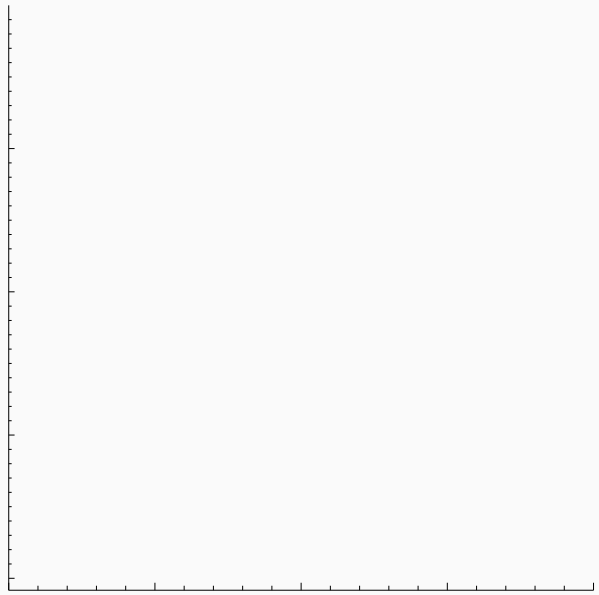

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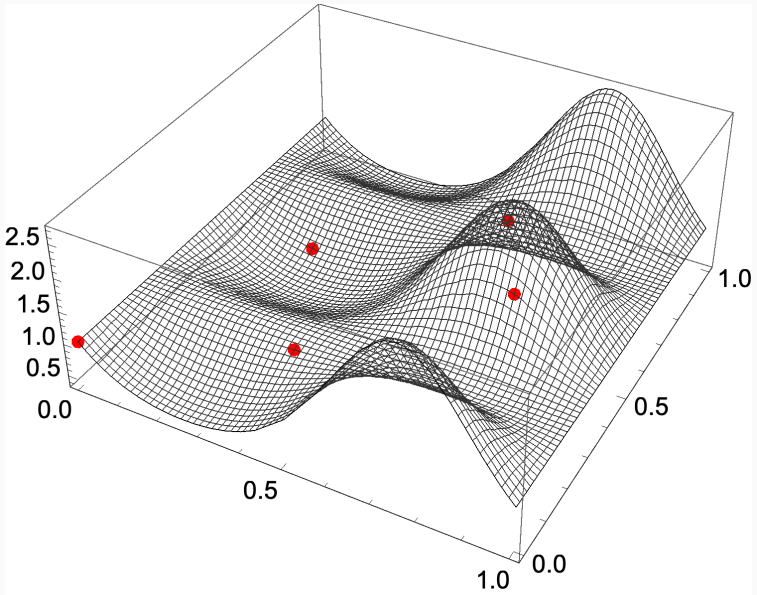

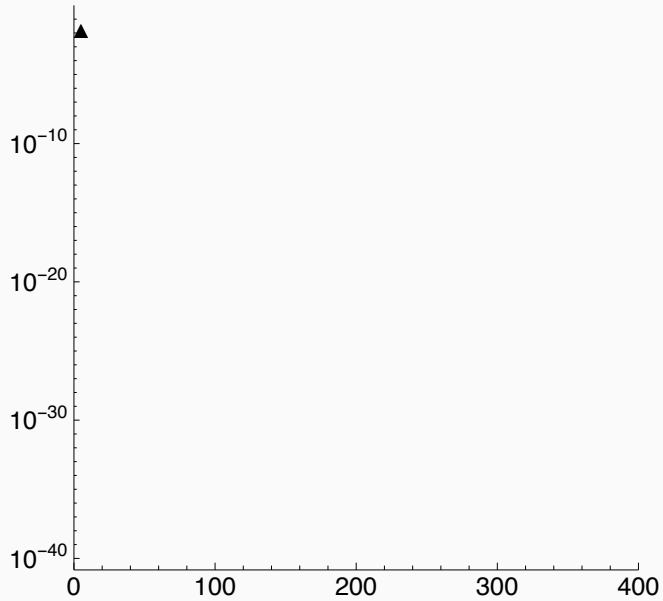

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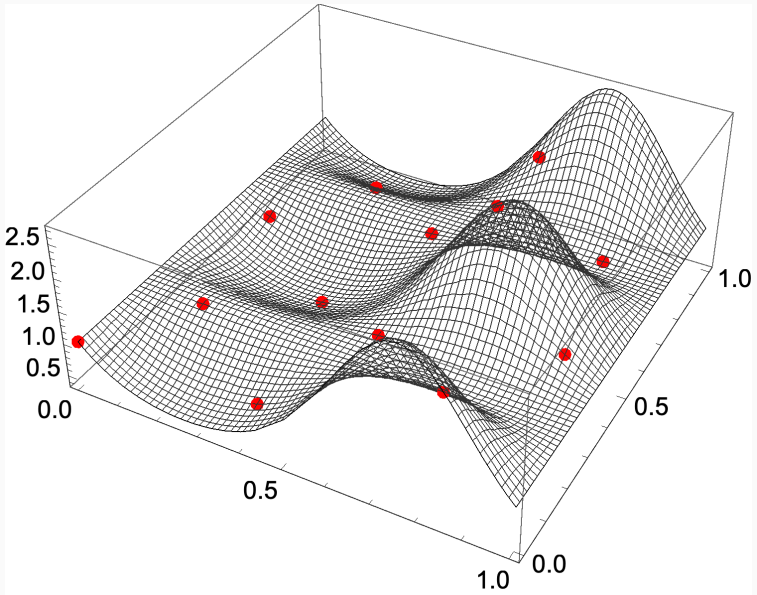

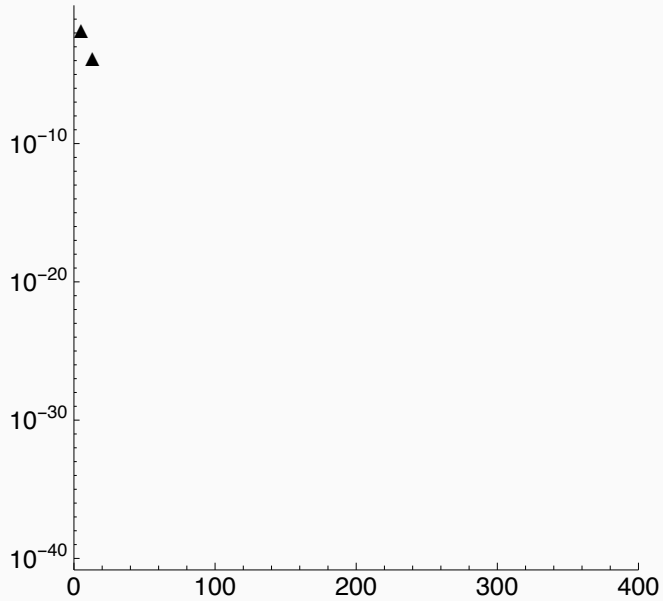

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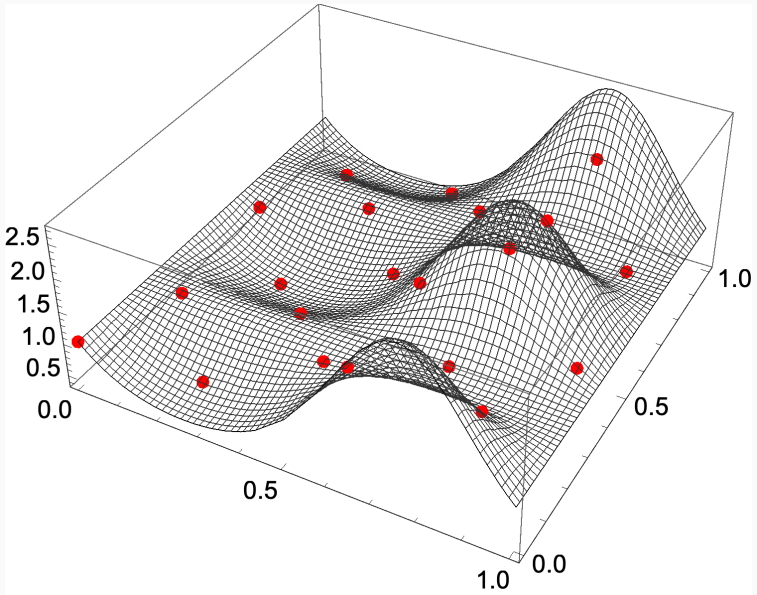

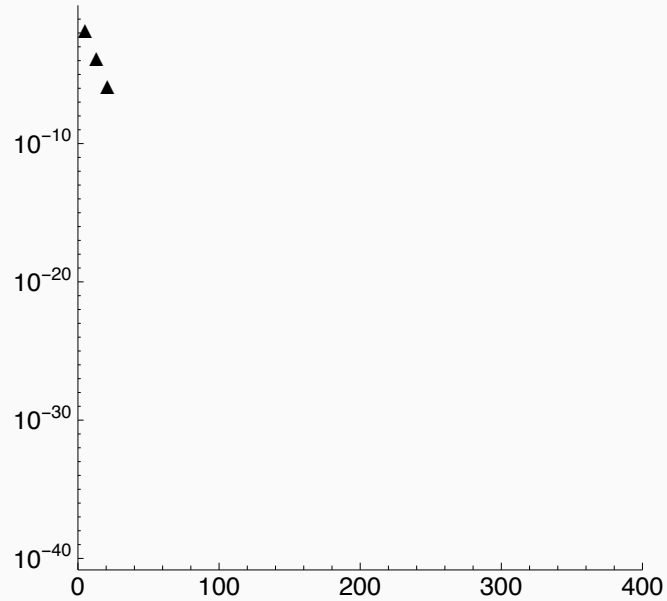

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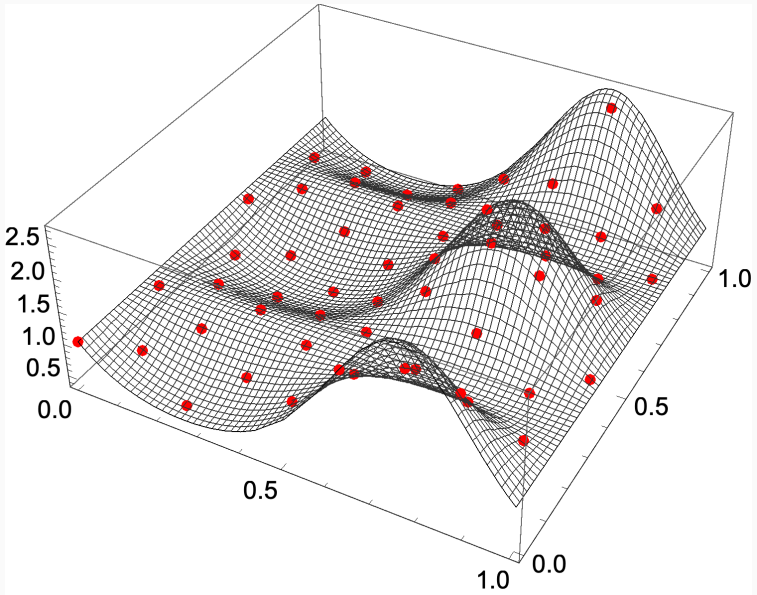

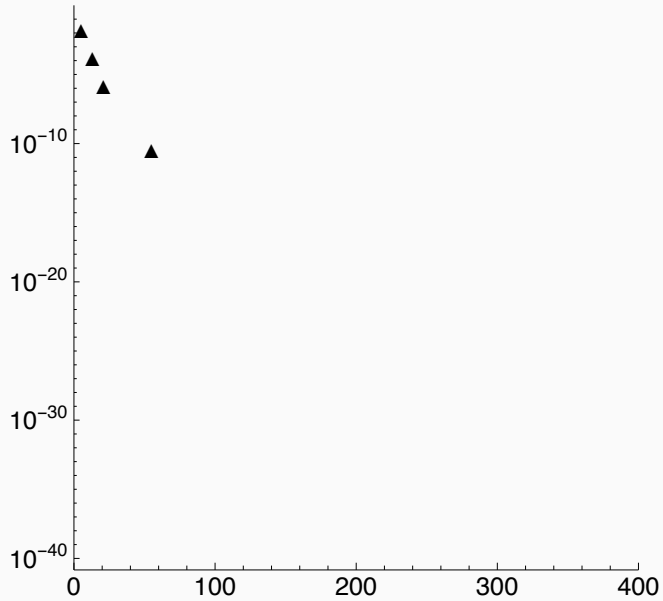

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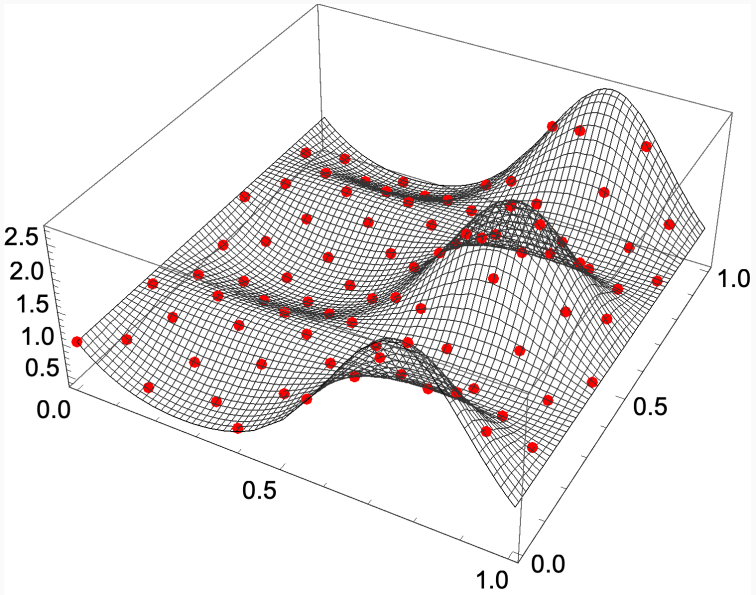

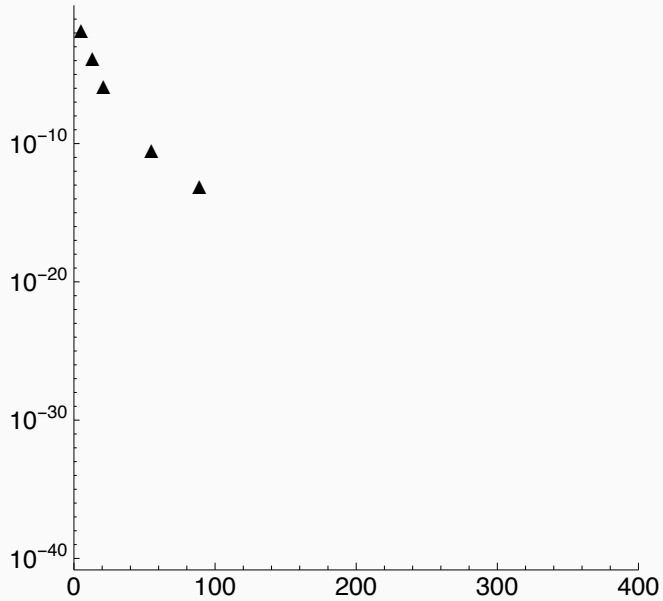

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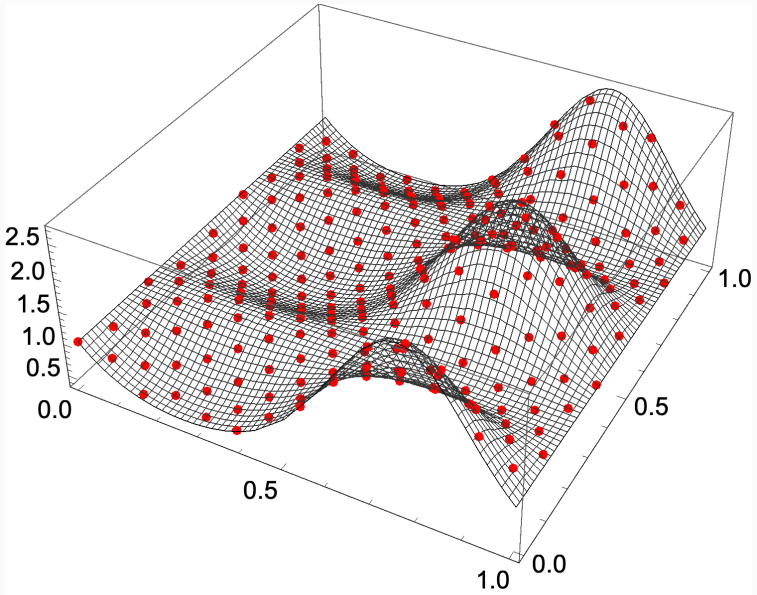

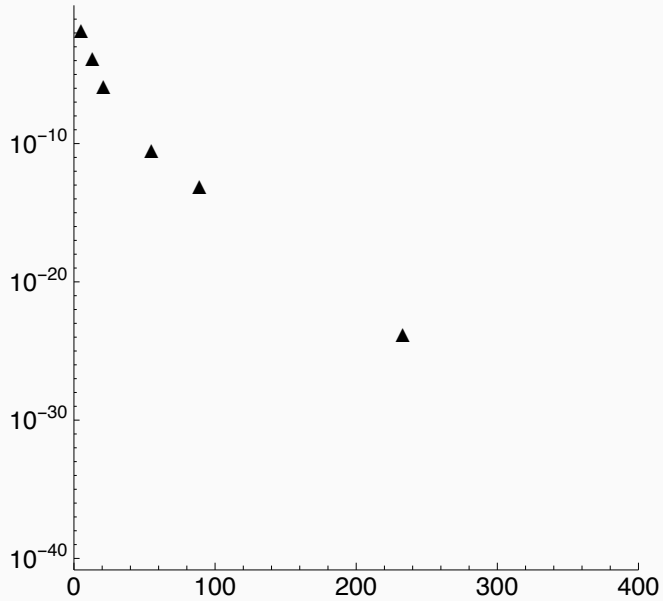

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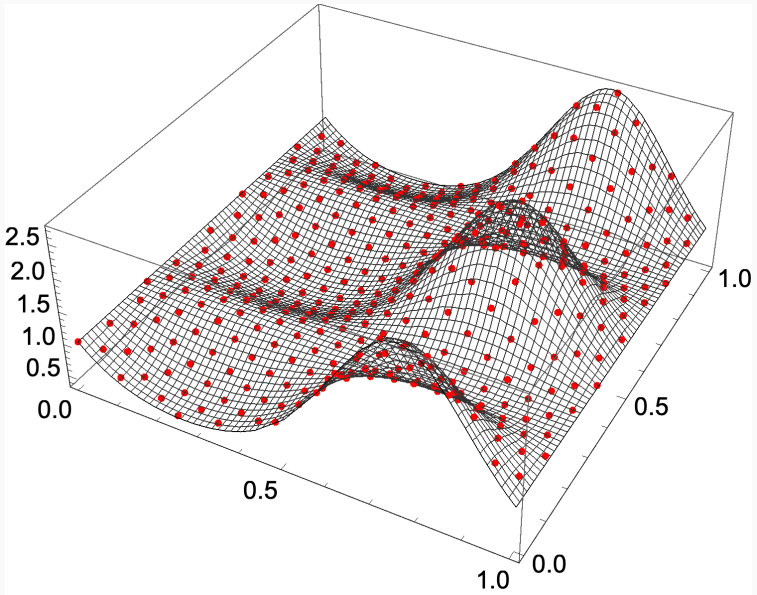
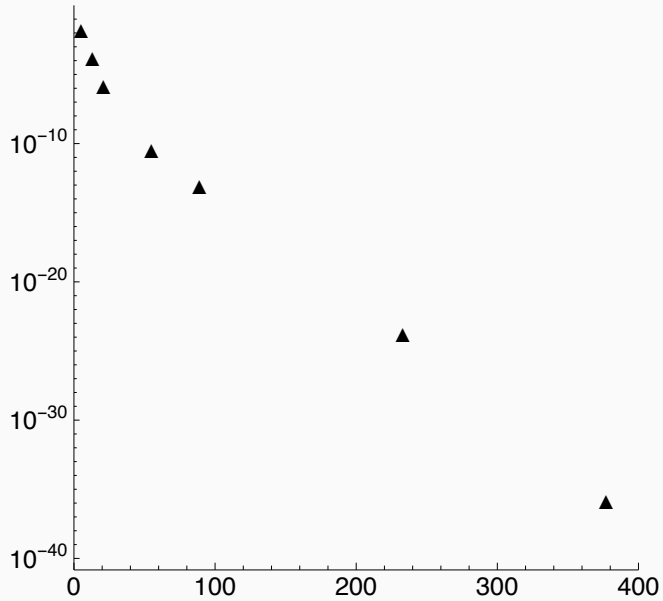




For continuous 1-periodic functions with absolutely convergent Fourier series, the lattice rule error is precisely (Sloan and Kachoyan 1987):

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

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

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

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

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

$$P_\alpha(\boldsymbol{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \omega\left(\left\{ \frac{k z_j}{n} \right\} \right), \quad \omega(x) := (2\pi)^\alpha \frac{B_\alpha(x)}{(-1)^{\alpha/2+1} \alpha!}.$$

CBC algorithm (Sloan, Kuo, Joe 2002)

The idea of the *component-by-component* (CBC) algorithm is to find a good generating vector $\boldsymbol{z} = (z_1, \ldots, z_s)$ 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 $P(z_1, z_2, z_3)$

   $\vdots$

Notes:

- The CBC algorithm is a *greedy algorithm*: in general, it will not find the generating vector $\boldsymbol{z}$ that minimizes $P(\boldsymbol{z})$. However, it can be shown that the generating vector obtained by the CBC algorithm satisfies an error bound (more on this later).
- For generic $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$, evaluating $P(\boldsymbol{z}) = P(\boldsymbol{\gamma}, \boldsymbol{z})$ 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

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

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

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

can be written in the dimensionally recursive form

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

where $p_{s,\ell}(k) = p_{s-1,\ell}(k) + \frac{\Gamma_\ell}{\Gamma_{\ell-1}} \gamma_s \omega\left(\left\{\frac{k z_s}{n}\right\}\right) p_{s-1,\ell-1}(k)$ 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.,

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

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

1. Define the matrix $\boldsymbol{\Omega}_n = \left[\omega\left(\left\{\frac{kz}{n}\right\}\right)\right]_{\substack{z \in \{1,\ldots,n-1\} \\ k \in \{0,\ldots,n-1\}}}$ and initialize vectors $\boldsymbol{p}_{0,\ell} = \mathbf{1}_n$ for $\ell = 1, \ldots, s$.
   for $d = 1, \ldots, s$**, do**
   2. Pick the value of $z_d \in \{1, \ldots, n-1\}$ corresponding to the smallest entry in the matrix-vector product

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

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

   end for

What makes fast CBC fast?

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

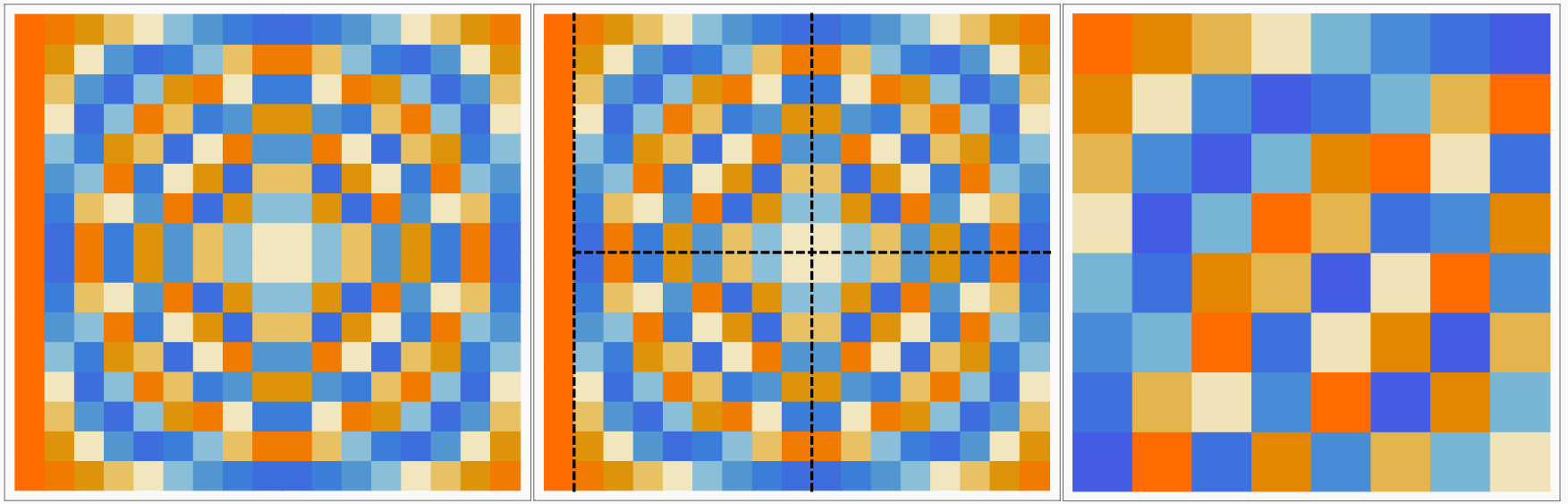


Figure 3: Example with Ω_{17}. Note that the first column is a constant and can be left out (the components of $\boldsymbol{\Omega}_n \boldsymbol{x}$ are shifted by a constant $\rightarrow$ the smallest component stays invariant). Noting the obvious symmetries in the remaining four blocks, we can focus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

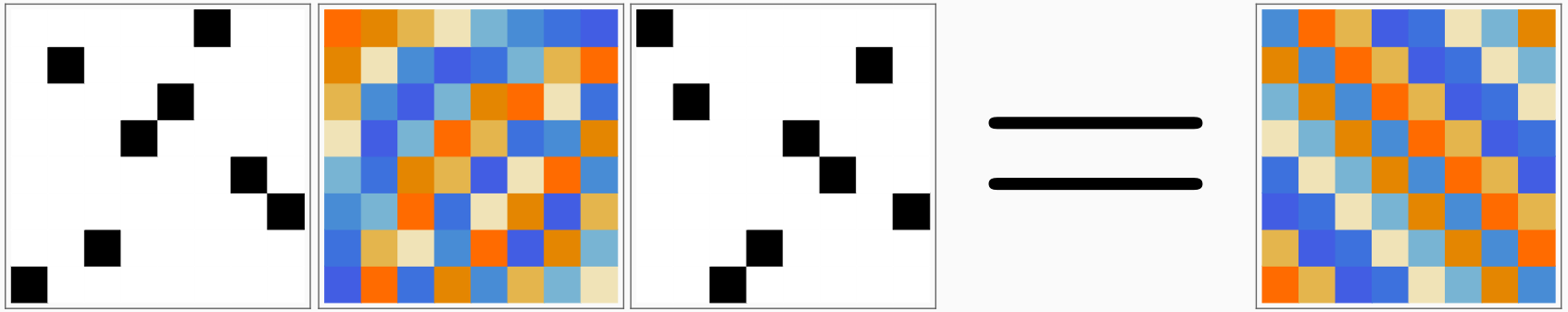


Figure 4: The original block matrix is multiplied from both sides by Rader permutation matrices (the black elements indicate the value 1 and white elements indicate the value 0) to obtain a circulant matrix.

Example with $n = 1009$

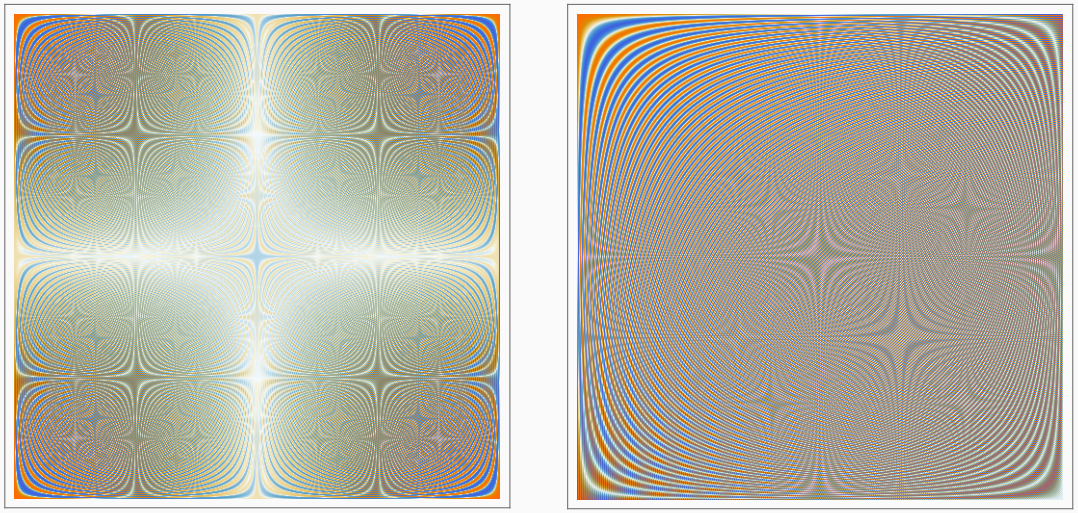


Figure 5: LHS: Original Ω_{1009}. RHS: top left block of Ω_{1009} (sans first column).

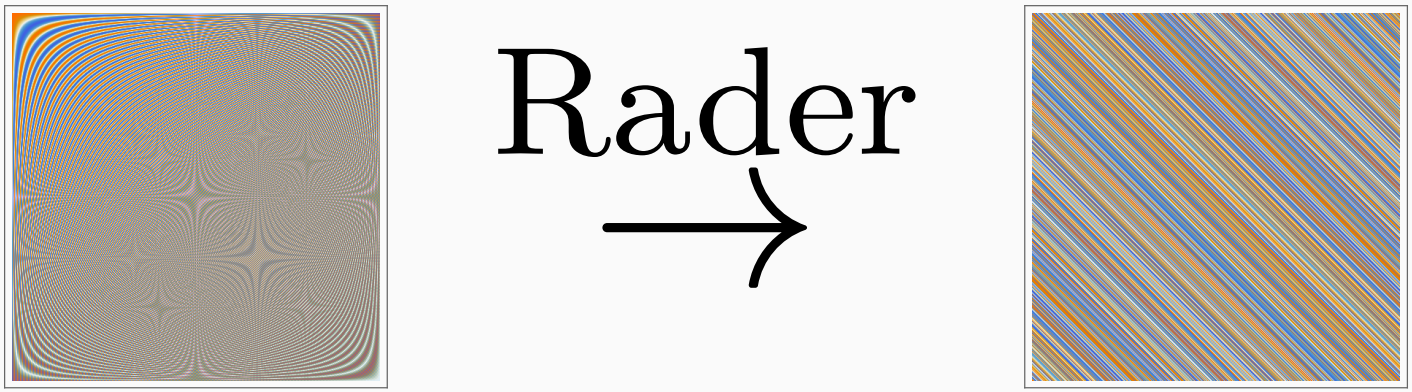


Figure 6: Rader transformation turns the top left block matrix circulant.

- 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 $\boldsymbol{z} \in \{1,\ldots,n-1\}^s$ *can be constructed by the CBC algorithm such that*

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

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

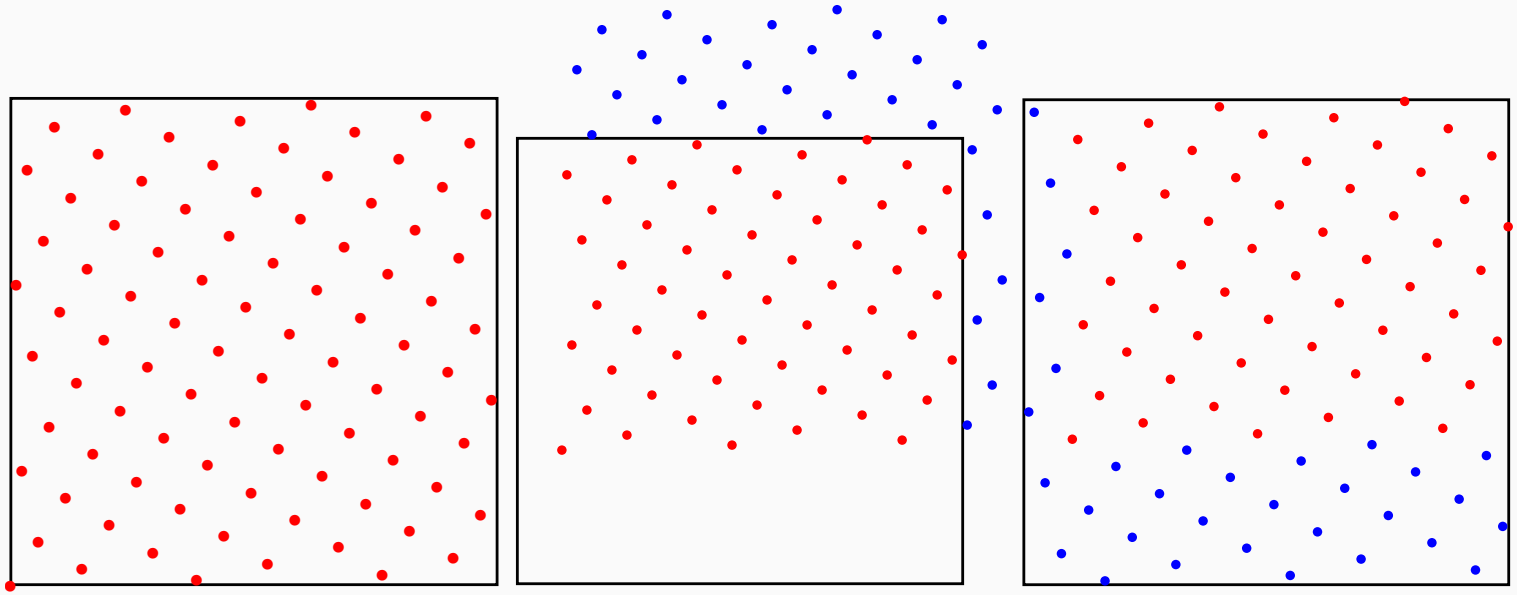
Non-periodic setting: randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

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

Use a number of random shifts for error estimation.



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

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

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

Then

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

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

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

Error bound (one random shift):

$$|I_s(f) - Q^{\boldsymbol{\Delta}}_{s,n}(f)| \le e^{\boldsymbol{\Delta}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z}) \|f\|_{\boldsymbol{\gamma}}.$$

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

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}}[|I_s(f) - \overline{Q}_{s,n}(f)|^2]} \le e^{\mathrm{sh}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z}) \|f\|_{\boldsymbol{\gamma}}.$$

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

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

and (squared) worst case error

$$P(\boldsymbol{z}) := e^{\mathrm{sh}}_{s,n,\boldsymbol{\gamma}}(\boldsymbol{z})^2 = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \omega\left(\left\{ \frac{k z_j}{n} \right\} \right), \quad \omega(x) = x^2 - x + \frac{1}{6}.$$

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 $P(\boldsymbol{z})$. For details, cf. [Dick, Kuo, Sloan, **Acta Numer.** 2013].

The periodic model of uncertainty quantification for PDEs

Let $(\Omega, \mathscr{F}, \mathbb{P})$ be a probability space and $D \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$, a bounded physical domain with Lipschitz boundary.

Elliptic PDE with uncertain/random coefficient

Find $u\colon D \times \Omega \to \mathbb{R}$ that satisfies

$$\begin{aligned} -\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{\omega}) \nabla u(\boldsymbol{x}, \boldsymbol{\omega})) &= f(\boldsymbol{x}) && \text{for } \boldsymbol{x} \in D, \\ + \text{boundary conditions} && && \text{on } \partial D \end{aligned}$$

for almost all events $\boldsymbol{\omega} \in \Omega$. Here, the diffusion coefficient $a(\cdot, \boldsymbol{\omega}) \in L^\infty_+(D)$ is *uncertain*.

In forward uncertainty quantification, one is interested in computing certain response statistics of the solution, usually $\mathbb{E}[u]$ *or* $\mathbb{E}[G(u)]$ *and* $\mathrm{Var}[u]$ *or* $\mathrm{Var}[G(u)]$*, where* G *is a (linear) functional representing some quantity of interest derived from the solution.*

Depending on the application, two common models for the random field A that appear in the literature are

- uniform and affine;
- lognormal.

Background

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

For $\boldsymbol{x} \in D$ and $\boldsymbol{\omega} \in \Omega$,

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

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

- Rank-1 lattice cubature rules with random shifts
  $\Rightarrow$ cubature error $\mathcal{O}(n^{-1+\varepsilon})$ at best. (Kuo, Schwab, Sloan 2012)
- Interlaced polynomial lattice rules
  $\Rightarrow$ 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.

For $\boldsymbol{x} \in D$ and $\boldsymbol{\omega} \in \Omega$,

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

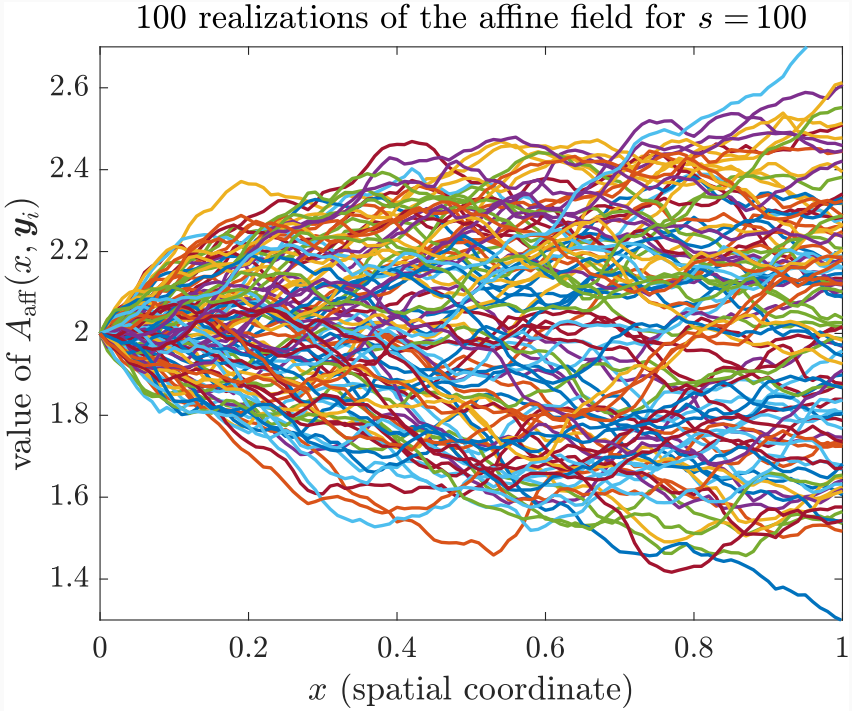
with the special choice $\Theta(y) = \frac{1}{\sqrt{6}} \sin(2\pi y)$.

- 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, $Z \sim \mathrm{Arcsine}(-1, 1)$.
- 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

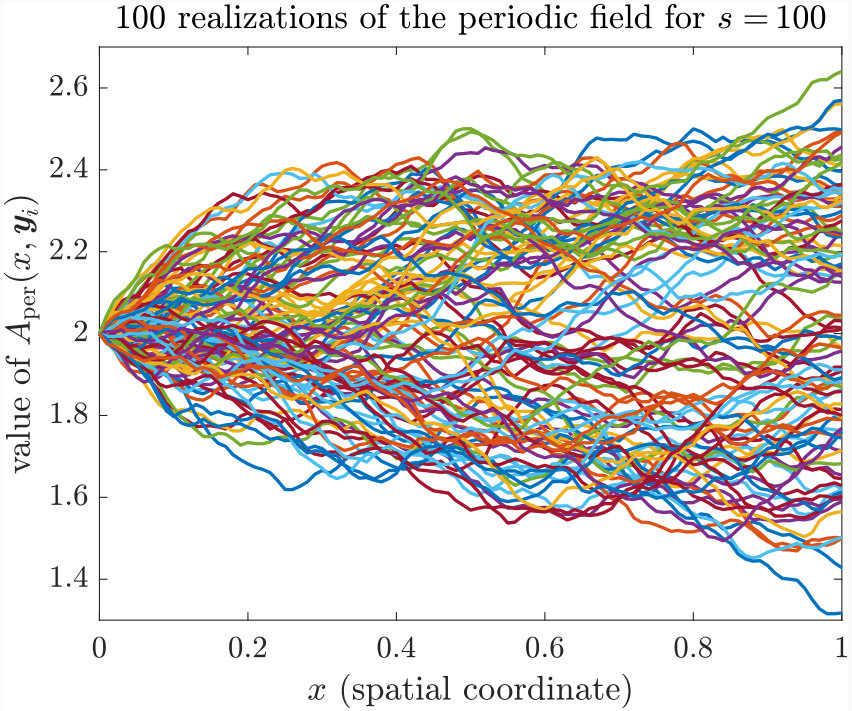
Affine

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



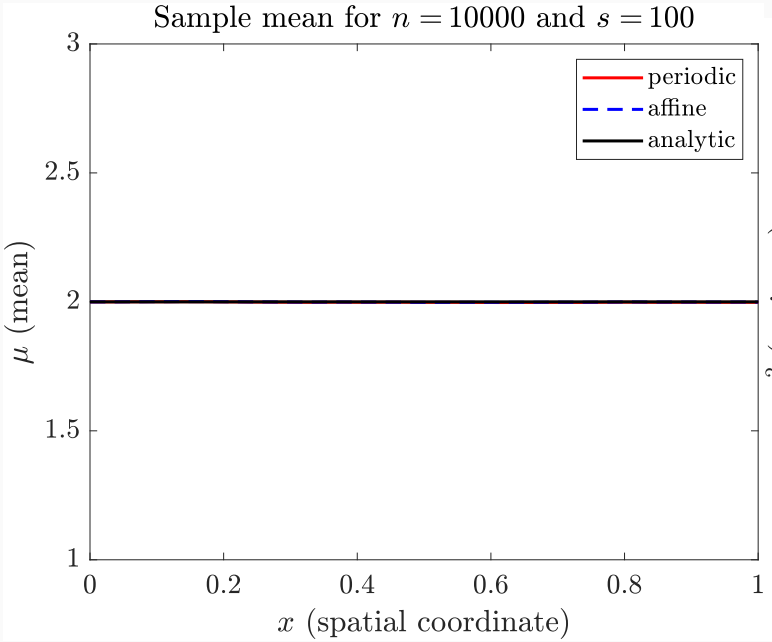
Periodic

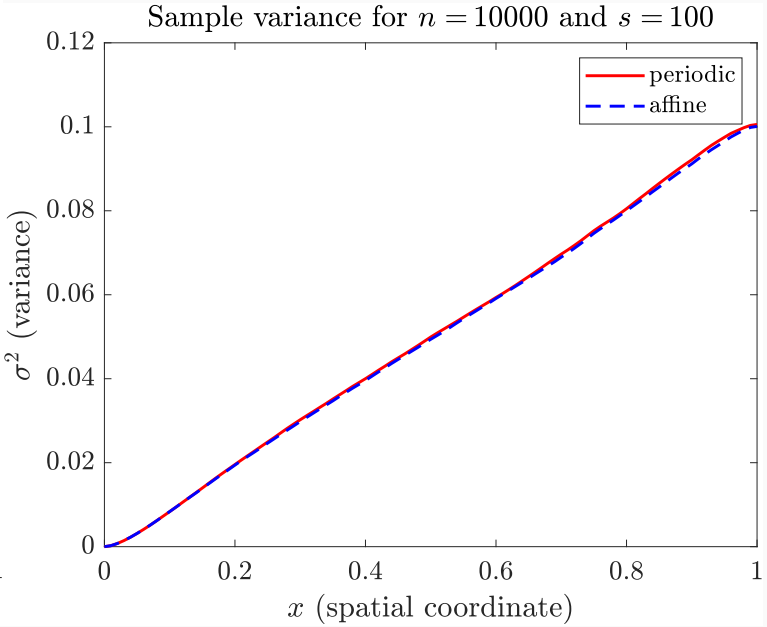
$$a(x, \boldsymbol{y}) = \bar{a}(x) + \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j)\psi_j(x)$$

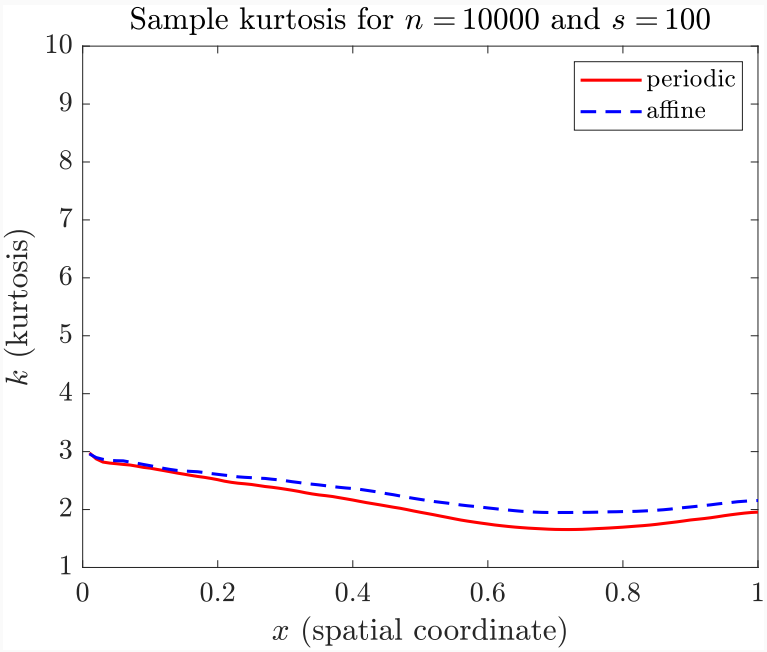


$$\bar{a}(x) = 2, \quad \psi_j(x) = j^{-3/2} \sin((j - \tfrac{1}{2})\pi x), \quad x \in [0, 1]$$

Affine vs. periodic







Parametric PDE model problem

The physical domain $D \subset \mathbb{R}^d$ is assumed to be a bounded domain with Lipschitz boundary. Let $U := [0,1]^s$ denote a set of parameters.

The diffusion coefficient is defined as

$$a(\boldsymbol{x}, \boldsymbol{y}) = \bar{a}(\boldsymbol{x}) + \frac{1}{\sqrt{6}} \sum_{j=1}^{s} \sin(2\pi y_j)\psi_j(\boldsymbol{x}), \quad \boldsymbol{x} \in D, \ \boldsymbol{y} \in U,$$

where we impose the following assumptions:

(A1) $\bar{a} \in L^\infty(D)$ and $\sum_{j\geq 1} \|\psi_j\|_{L^\infty} < \infty$.

(A2) There exist positive constants $a_{\min}$ and $a_{\max}$ such that $0 < a_{\min} \leq a(\boldsymbol{x}, \boldsymbol{y}) \leq a_{\max} < \infty$ for all $\boldsymbol{x} \in D$ and $\boldsymbol{y} \in U$.

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

N.B. Assuming that we have a conforming FE method, all regularity and QMC convergence results can be transported to the discretized problem.

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

$$|I_s(f) - Q_{s,n}(f)| \le \left(\frac{2}{n} \sum_{\varnothing \ne \mathfrak{u} \subseteq \{1,\dots,s\}} \gamma_{\mathfrak{u}}^{\lambda} (2\zeta(\alpha\lambda))^{|\mathfrak{u}|} \right)^{1/\lambda} \|f\|_{\alpha} \qquad (1)$$

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

When $\alpha \ge 2$ *is an integer, the norm* $\|\cdot\|_{\alpha}$ *in* (1), *corresponding to a weighted Korobov space with dominating mixed smoothness* α, *can be replaced by*

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

provided that f *is periodic and has mixed partial derivatives of order* α.

Given our PDE problem, our goal is to

- Establish derivative bounds for $\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} u(\boldsymbol{x}, \boldsymbol{y})$ to estimate $\|u(\boldsymbol{x}, \cdot)\|_{\alpha}$.
- Find weights $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$ and choose α, λ in (1) to obtain a higher order cubature convergence rate independently of s.

For the parametric PDE

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

with $u(\cdot, \boldsymbol{y}) \in H_0^1(D)$ and $f \in H^{-1}(D)$ and $a(\boldsymbol{x}, \boldsymbol{y}) = \bar{a}(\boldsymbol{x}) + \frac{1}{\sqrt{6}} \sum_{j=1}^{s} \sin(2\pi y_j) \psi_j(\boldsymbol{x})$, we obtained the following bound:

Theorem (K–Kuo–Sloan 2020)
For all multi-indices $\boldsymbol{\nu} \in \mathbb{N}_0^s$ and $\boldsymbol{y} \in U$, we have that

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} u(\cdot, \boldsymbol{y})\|_{H_0^1(D)} \lesssim (2\pi)^{|\boldsymbol{\nu}|} \sum_{\boldsymbol{m} \le \boldsymbol{\nu}} |\boldsymbol{m}|! \prod_{j \ge 1} (b_j^{m_j} S(\nu_j, m_j)), \quad b_j := \frac{\|\psi_j\|_{L^\infty}}{\sqrt{6} a_{\min}}.$$

Here,

$$S(n, k) = \frac{1}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} j^n, \quad n \ge k \ge 0,$$

are *Stirling numbers of the second kind*, with the convention that $S(0, 0) = 1$.

Higher-order convergence

Let $F(\boldsymbol{y}) := G(u(\cdot, \boldsymbol{y}))$, $\boldsymbol{y} \in U$, $G \in H^{-1}(D)$. We're interested in minimizing the QMC quadrature error

$$|I_s(F) - Q_{s,n}(F)| \leq \left(\frac{2}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} (2\zeta(\alpha\lambda))^{|\mathfrak{u}|} \right)^{1/\lambda} \|F\|_{\alpha}.$$

We have for any integer $\alpha \geq 2$ that

$$\begin{aligned} \|F\|_{\alpha} &\leq \|G\|_{H^{-1}} \max_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}} (2\pi)^{\alpha|\mathfrak{u}|}} \left\| \left(\prod_{j \in \mathfrak{u}} \frac{\partial^{\alpha}}{\partial y_j^{\alpha}} \right) u(\cdot, \boldsymbol{y}) \right\|_{H_0^1} \\ &\leq \frac{\|G\|_{H^{-1}} \|f\|_{H^{-1}}}{a_{\min}} \max_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha\}^{|\mathfrak{u}|}} |\boldsymbol{m}_{\mathfrak{u}}|! \prod_{j \in \mathfrak{u}} b_j^{m_j} S(\alpha, m_j). \end{aligned}$$

We choose the weights to be

$$\gamma_{\mathfrak{u}} = \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha\}^{|\mathfrak{u}|}} |\boldsymbol{m}_{\mathfrak{u}}|! \prod_{j \in \mathfrak{u}} b_j^{m_j} S(\alpha, m_j), \quad \mathfrak{u} \subseteq \{1:s\},$$

which ensures that $\|F\|_{\alpha}$ is bounded. These are *smoothness-driven product and order dependent weights* (*SPOD weights*), first seen in [J. Dick, F. Y. Kuo, Q. T. Le Gia, D. Nuyens, Ch. Schwab. Higher order QMC Petrov–Galerkin discretization for affine parametric operator equations with random field inputs, 2014].

The QMC quadrature error is

$$|I_s(F) - Q_{s,n}(F)| \lesssim \left(\frac{2}{n}\right)^{1/\lambda} C(s,\alpha,\lambda),$$

where

$$C(s,\alpha,\lambda) := \left(\sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:s\}} \left(\sum_{\boldsymbol{m}_\mathfrak{u} \in \{1:\alpha\}^{|\mathfrak{u}|}} |\boldsymbol{m}_\mathfrak{u}|! \prod_{j \in \mathfrak{u}} b_j^{m_j} S(\alpha, m_j) \right)^{\lambda} (2\zeta(\alpha\lambda))^{|\mathfrak{u}|} \right)^{1/\lambda}$$

for $\lambda \in (1/\alpha, 1]$.

Finally, we need to choose λ in such a way that $C(s,\alpha,\lambda)$ is bounded *independently of* s. It is possible to estimate

$$C(s,\alpha,\lambda)^\lambda \leq \cdots \leq \sum_{\ell=0}^{\infty} (\ell!)^{\lambda-1} \left(c(\alpha,\lambda) \sum_{j=1}^{\infty} b_j^\lambda \right)^\ell$$

where $c(\alpha,\lambda) := \alpha \max\{1, \alpha!(2\zeta(\alpha\lambda))^{1/\lambda}\}^\lambda$. The d'Alembert ratio test ensures that the upper bound converges if we choose $\lambda = p$ and $\alpha = \lfloor 1/p \rfloor + 1 \Rightarrow$ we obtain $\mathcal{O}(n^{-1/p})$ convergence with an implied constant independent of s.

Numerical example: QMC for PDE [K–Kuo–Sloan (2020)]

Let us consider the PDE problem

$$-\nabla \cdot (a_{\rm per}(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = x_2, \quad u(\cdot, \boldsymbol{y})|_{\partial D} = 0,$$

in the physical domain $D = (0,1)^2$ with the diffusion coefficient

$$a_{\rm per}(\boldsymbol{x}, \boldsymbol{y}) = 2 + c \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j) \psi_j(x), \quad y_j \in [-\tfrac{1}{2}, \tfrac{1}{2}],$$

where $\psi_j(\boldsymbol{x}) = j^{-\beta} \sin(j\pi x_1) \sin(j\pi x_2)$. **Note that** $\|\psi_j\|_{L^\infty} \propto j^{-\beta}$.

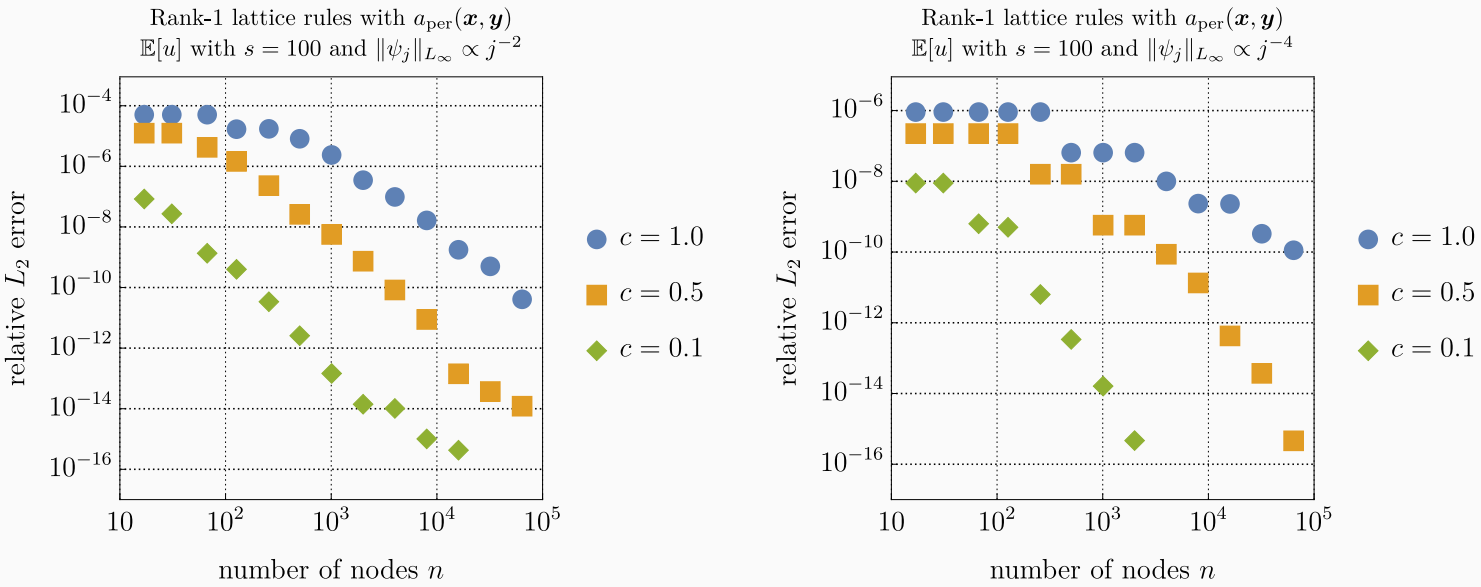


Figure 7: Left: $\beta = 2$. Right: $\beta = 4$.

QMC–kernel approximation for UQ

Let us continue the study of our elliptic model PDE problem.

In [K–Kazashi–Kuo–Nobile–Sloan (2022)], we studied *kernel interpolation of smooth, periodic functions based on lattice point sets*. We considered the following setting:

- Let $\alpha \geq 2$ be an even integer and let $H := H_{s,\alpha,\boldsymbol{\gamma}}$ be the Hilbert space containing absolutely continuous, somewhat smooth periodic functions $f : [0,1)^s \to \mathbb{R}$ endowed with the norm

$$\|f\|_H^2 := \sum_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{(2\pi)^{\alpha|\mathfrak{u}|}\gamma_{\mathfrak{u}}} \int_{[0,1]^{|\mathfrak{u}|}} \left| \int_{[0,1]^{s-|\mathfrak{u}|}} \left(\prod_{j \in \mathfrak{u}} \frac{\partial^{\alpha/2}}{\partial y_j^{\alpha/2}} \right) f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}_{-\mathfrak{u}} \right|^2 \mathrm{d}\boldsymbol{y}_{\mathfrak{u}},$$

  provided that f has mixed partial derivatives of order $\alpha/2$.

The space H is actually a *reproducing kernel Hilbert space* (RKHS), with an explicitly known and analytically simple reproducing kernel:

$$K(\boldsymbol{y}, \boldsymbol{y}') := \sum_{\mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \eta_\alpha(y_j, y_j'),$$

where

$$\eta_\alpha(y, y') = \frac{(2\pi)^\alpha}{(-1)^{\alpha/2+1}\alpha!} B_\alpha(\mathrm{frac}(y - y')), \quad y, y' \in [0, 1],$$

where $B_2(y) = y^2 - y + \frac{1}{6}$, $B_4(y) = y^4 - 2y^3 + y^2 - \frac{1}{30}$, and so on, are the *Bernoulli polynomials* provided that $\alpha \geq 2$ is an even integer. In particular,

$$\langle f, K(\cdot, \boldsymbol{y}) \rangle_H = f(\boldsymbol{y}) \quad \text{for all } f \in H \text{ and } \boldsymbol{y} \in [0, 1]^s.$$

Example: If $(\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\ldots,s\}}$ are *product weights*, i.e.,

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

then

$$K(\boldsymbol{y}, \boldsymbol{y}') = \prod_{j=1}^{s} (1 + \gamma_j \eta_\alpha(y_j, y_j')).$$

Suppose that one is interested in finding an approximation for the function $f \in H$ based on the point evaluations $f(\boldsymbol{t}_1), \ldots, f(\boldsymbol{t}_n)$, $\boldsymbol{t}_j \in [0,1]^s$. We introduce the *kernel interpolant*

$$f_n(\boldsymbol{y}) := \sum_{k=1}^{n} c_k K(\boldsymbol{t}_k, \boldsymbol{y}), \quad \boldsymbol{t}_k := \operatorname{frac}\left(\frac{k\boldsymbol{z}}{n}\right), \tag{2}$$

and require the interpolation property $f_n(\boldsymbol{t}_k) = f(\boldsymbol{t}_k)$ for hold for all $k = 1, \ldots, n$. Then the coefficients can be solved from the linear system

$$\boldsymbol{K}\boldsymbol{c} = \boldsymbol{f},$$

where $\boldsymbol{c} := [c_1, \ldots, c_n]^{\mathrm{T}}$ are the coefficients in (2) and

$$K_{k,\ell} = K(\boldsymbol{t}_k, \boldsymbol{t}_\ell) \quad \text{and} \quad \boldsymbol{f} := [f(\boldsymbol{t}_1), \ldots, f(\boldsymbol{t}_n)]^{\mathrm{T}}.$$

Note that $K_{k,\ell} = K(\frac{(k-\ell)\boldsymbol{z}}{n}, \boldsymbol{0})$, i.e., $\boldsymbol{K}$ is a *circulant matrix* $\Rightarrow$

$$\boldsymbol{c} = \texttt{ifft}\big(\texttt{fft}(\boldsymbol{f})./\texttt{fft}(\boldsymbol{K}_{:,1})\big)$$

This can be computed in $\mathcal{O}(n \log n)$ time!

The kernel interpolant is cheap to construct!

In analogy to the cubature case, we have the following result.

Proposition (K–Kazashi–Kuo–Nobile–Sloan (2022))
A generating vector $\boldsymbol{z} \in \{1, \dots, n-1\}^s$ *can be constructed by the CBC algorithm such that*

$$\|f - f_n\|_{L^2(U)} \le \frac{\kappa}{n^{1/(4\lambda)}} \left(\sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \max\{1, |\mathfrak{u}|\} \gamma_{\mathfrak{u}}^{\lambda} (2\zeta(\alpha\lambda))^{|\mathfrak{u}|} \right)^{1/\lambda} \|f\|_H$$

for $\lambda \in (1/\alpha, 1]$, $\alpha > 1$, *prime* n, *and* $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$, $x > 1$. *Here,* $\gamma_{\varnothing} := 1$ *and* $\kappa = \sqrt{2}(2.5 + 2^{2\alpha\lambda+1})^{1/(2\lambda)}$.

Remark. This result follows from the analysis performed for trigonometric function approximation by Cools, Kuo, Nuyens, Sloan (2021, Math. Comp.).

As we saw in the cubature setting, our PDE problem

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

equipped with $a(\boldsymbol{x}, \boldsymbol{y}) = \bar{a}(\boldsymbol{x}) + \frac{1}{\sqrt{6}} \sum_{j=1}^{s} \sin(2\pi y_j) \psi_j(\boldsymbol{x})$, satisfies

$$\|\partial_{\boldsymbol{y}}^{\boldsymbol{\nu}} u(\cdot, \boldsymbol{y})\|_{H_0^1(D)} \lesssim (2\pi)^{|\boldsymbol{\nu}|} \sum_{\boldsymbol{m} \le \boldsymbol{\nu}} |\boldsymbol{m}|! \prod_{j \ge 1} (b_j^{m_j} S(\nu_j, m_j)), \quad b_j := \frac{\|\psi_j\|_{L^\infty}}{\sqrt{6} a_{\min}}.$$

We derived **SPOD weights** for the kernel approximations of $\boldsymbol{y} \mapsto u_h(\cdot, \boldsymbol{y})$ and $\boldsymbol{y} \mapsto G(u_h(\cdot, \boldsymbol{y}))$, where $G \colon H_0^1(D) \to \mathbb{R}$ is some linear bounded QoI:

$$\gamma_{\mathfrak{u}} := \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha/2\}^{|\mathfrak{u}|}} (|\boldsymbol{m}_{\mathfrak{u}}|!)^{\frac{2}{1+\lambda}} \prod_{j \in \mathfrak{u}} \left(\frac{b_j^{m_j} S(\alpha/2, m_j)}{\sqrt{2 \mathrm{e}^{1/\mathrm{e}} \zeta(\alpha\lambda)}} \right)^{\frac{2}{1+\lambda}}, \ \varnothing \ne \mathfrak{u} \subseteq \{1, \dots, s\},$$

where $\alpha := 2\lfloor \frac{1}{p} + \frac{1}{2} \rfloor$, $\lambda := \frac{p}{2-p}$, and $\gamma_\varnothing := 1$. This yields $\|u - u_n\|_{L^2(U \times D)} = \mathcal{O}(n^{-\frac{1}{2p} + \frac{1}{4}})$ and $\|G(u) - G(u_n)\|_{L^2(U)} = \mathcal{O}(n^{-\frac{1}{2p} + \frac{1}{4}})$ where the implied constant is *independent* of the dimension s.

Kernel approximation for PDE: L^2 error

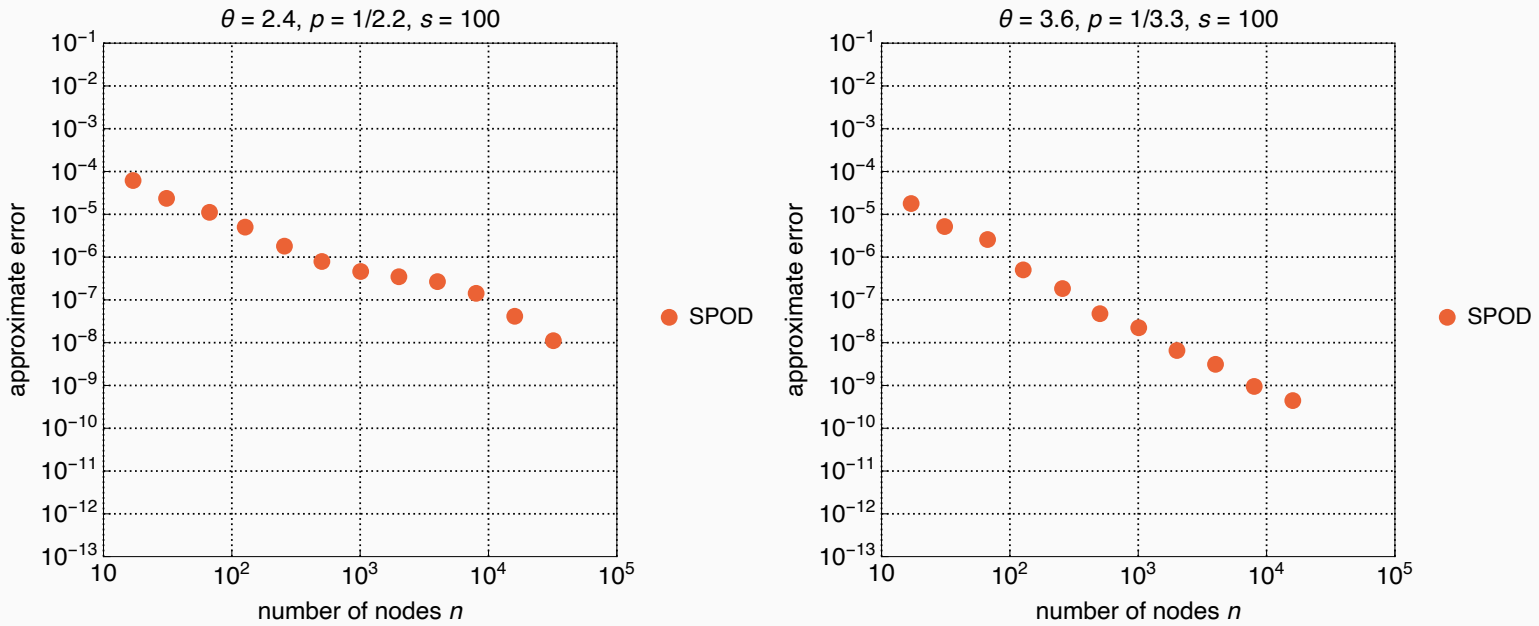
Let us consider the PDE problem

$$-\nabla \cdot (a_{\mathrm{per}}(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = x_2, \quad u(\cdot, \boldsymbol{y})|_{\partial D} = 0,$$

in the physical domain $D = (0,1)^2$ with the diffusion coefficient

$$a_{\mathrm{per}}(\boldsymbol{x}, \boldsymbol{y}) = 1 + \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j)\psi_j(x), \quad y_j \in [0,1],$$

where $\psi_j(\boldsymbol{x}) = j^{-\theta} \sin(j\pi x_1) \sin(j\pi x_2)$. **Note that** $\|\psi_j\|_{L^\infty} \propto j^{-\theta}$.



Reducing the computational complexity

Before, we used the SPOD weights

$$\gamma_{\mathfrak{u}} := \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha/2\}^{|\mathfrak{u}|}} (|\boldsymbol{m}_{\mathfrak{u}}|!)^{\frac{2}{1+\lambda}} \prod_{j \in \mathfrak{u}} \left(\frac{b_j^{m_j} S(\alpha/2, m_j)}{\sqrt{2\mathrm{e}^{1/\mathrm{e}} \zeta(\alpha\lambda)}} \right)^{\frac{2}{1+\lambda}}. \tag{3}$$

- the cost to obtain the generating vector $\boldsymbol{z}$ is $\mathcal{O}(s\, n \log n + s^3\, \alpha^2\, n)$;
- the cost of evaluating the kernel interpolant is $\mathcal{O}(s^2\, \alpha^2\, n)$.

New idea: leave out the order-dependent part $(|\boldsymbol{m}_{\mathfrak{u}}|!)^{\frac{2}{1+\lambda}}$ in (3), get

$$\tilde{\gamma}_{\mathfrak{u}} := \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha/2\}^{|\mathfrak{u}|}} \prod_{j \in \mathfrak{u}} \left(\frac{b_j^{m_j} S(\alpha/2, m_j)}{\sqrt{2\mathrm{e}^{1/\mathrm{e}} \zeta(\alpha\lambda)}} \right)^{\frac{2}{1+\lambda}} = \prod_{j \in \mathfrak{u}} \left(\sum_{m=1}^{\alpha/2} \left(\frac{b_j^{m} S(\alpha/2, m)}{\sqrt{2\mathrm{e}^{1/\mathrm{e}} \zeta(\alpha\lambda)}} \right)^{\frac{2}{1+\lambda}} \right).$$

These are *product weights*, where

- the cost to obtain the generating vector $\boldsymbol{z}$ is $\mathcal{O}(s\, n \log n)$;
- the cost of evaluating the kernel interpolant is $\mathcal{O}(s\, n)$.

Kernel approximation for PDE: L^2 error (redux)

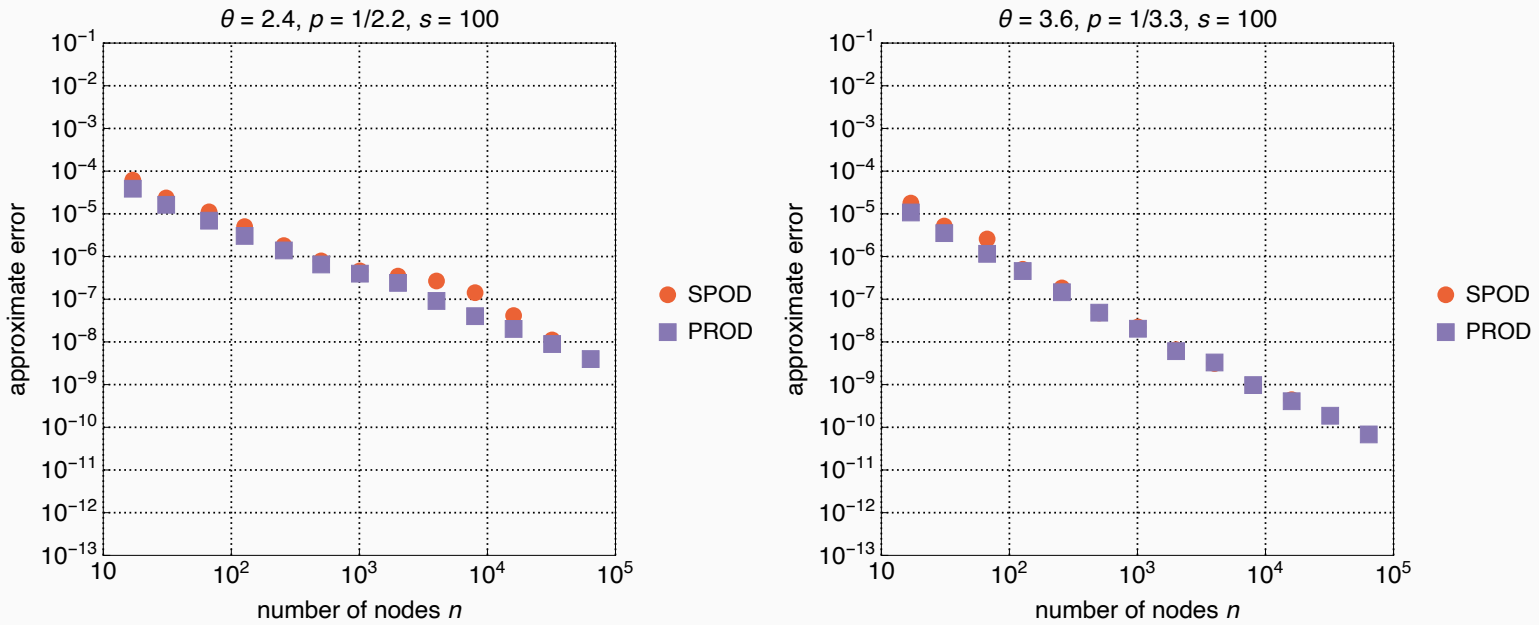
Let us consider the PDE problem

$$-\nabla \cdot (a_{\mathrm{per}}(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = x_2, \quad u(\cdot, \boldsymbol{y})|_{\partial D} = 0,$$

in the physical domain $D = (0,1)^2$ with the diffusion coefficient

$$a_{\mathrm{per}}(\boldsymbol{x}, \boldsymbol{y}) = 1 + \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j)\psi_j(x), \quad y_j \in [0,1],$$

where $\psi_j(\boldsymbol{x}) = j^{-\theta} \sin(j\pi x_1) \sin(j\pi x_2)$. **Note that** $\|\psi_j\|_{L^\infty} \propto j^{-\theta}$.



Conclusions

- Kernel interpolation method that can be used to approximate the output high-dimensional parametric PDEs. Kernel interpolant can be constructed efficiently at cost $\mathcal{O}(n \log n)$. No multi-index sets! (Compare with sparse grids or trigonometric approximation.)
- Rigorous error bounds independently of the dimension s.
- Using product weights, practical for challenging problems (e.g., as surrogates for Bayesian inversion).

References


K., F. Y. Kuo, and I. H. Sloan. Uncertainty quantification using periodic random variables. SIAM J. Numer Anal. **58**(2):1068–1091, 2020.


K., Y. Kazashi, F. Y. Kuo, F. Nobile, and I. H. Sloan. Fast approximation by periodic kernel-based lattice-point interpolation with application in uncertainty quantification. Numer. Math. **150**:33–77, 2022.

Fast CBC algorithm for function approximation


R. Cools, F. Y. Kuo, D. Nuyens, and I. H. Sloan. Fast component-by-component construction of lattice algorithms for multivariate approximation with POD and SPOD weights. Math. Comp. **90**:787–812, 2021.

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/`

F. J. Hickernell et al. QMCPy. `https://arxiv.org/abs/2102.07833`