High-dimensional kernel approximation of parametric PDEs over lattice point sets

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Part I: Quasi-Monte Carlo cubature

High-dimensional numerical integration

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

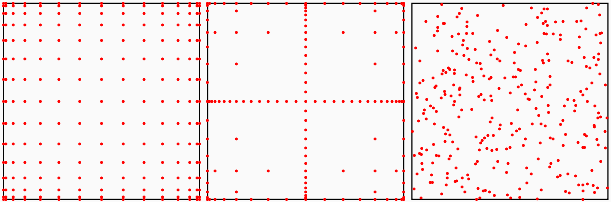


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

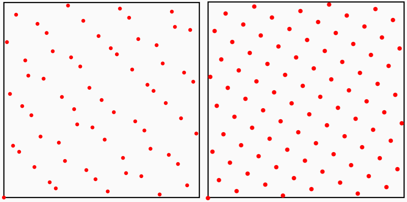


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

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.

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

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

Periodic means

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

Lattice rules

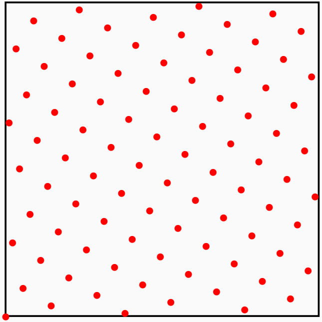
Rank-1 lattice rules

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

have the points

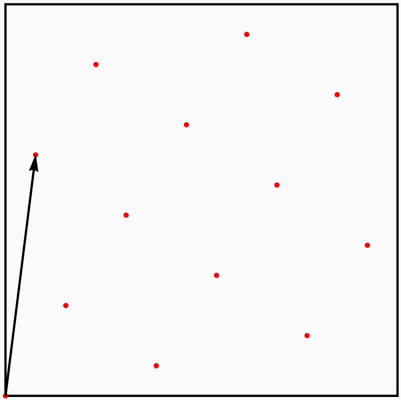
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

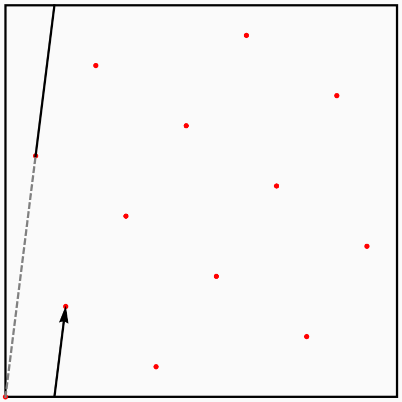
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

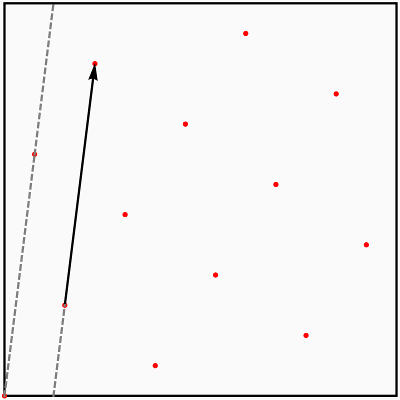


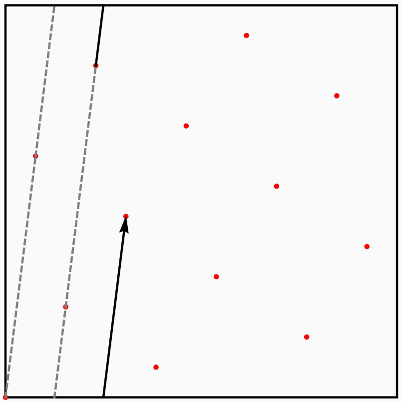
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

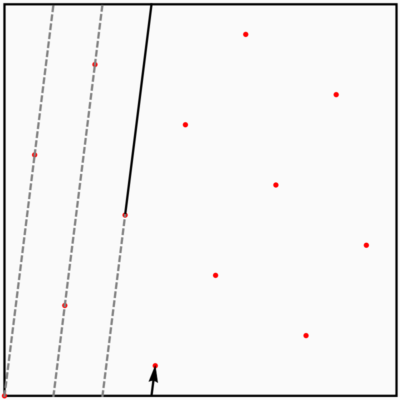
Lattice rules and periodic functions are a match made in heaven!

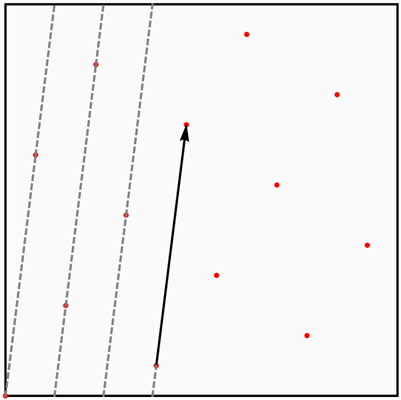


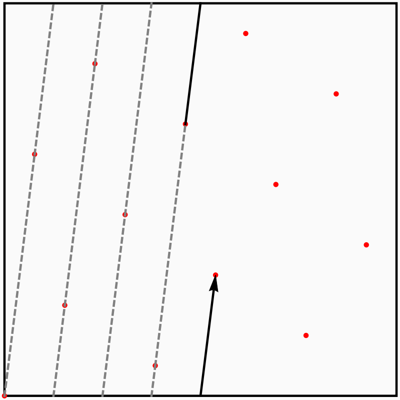


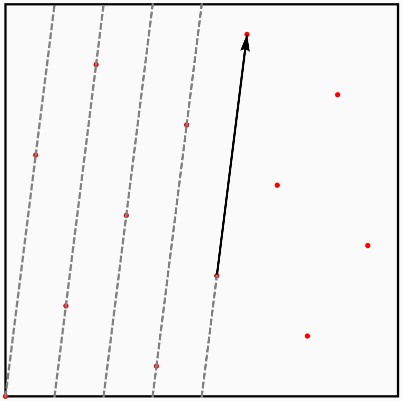


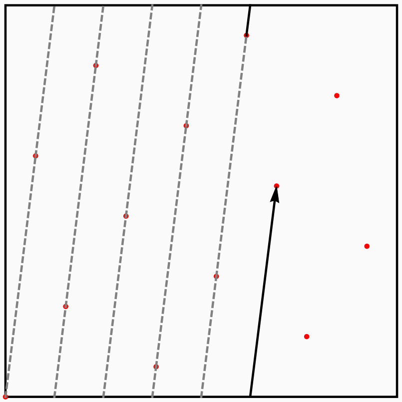


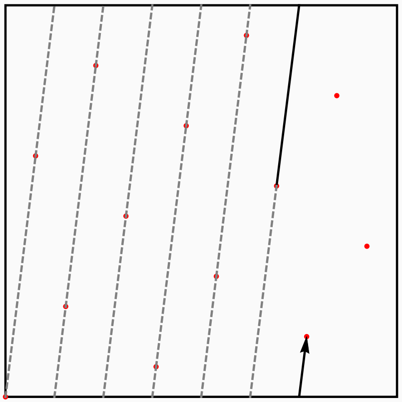


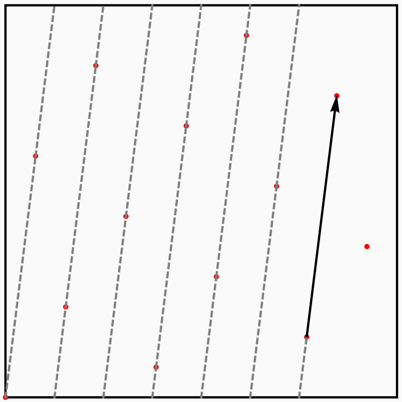


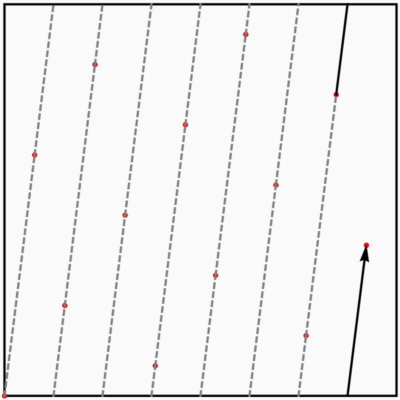












Dimension $s = 1$: the only lattice is the left-Riemann rule

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

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

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

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

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

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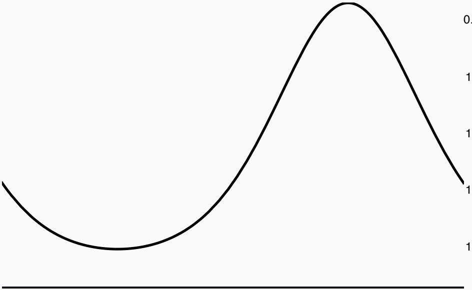
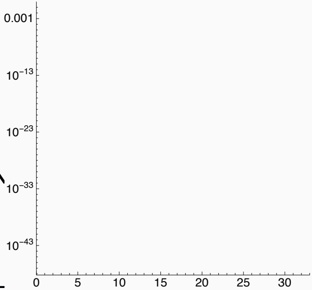
Exponential convergence for analytic, periodic functions

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





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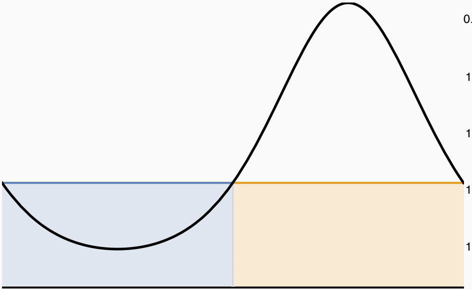

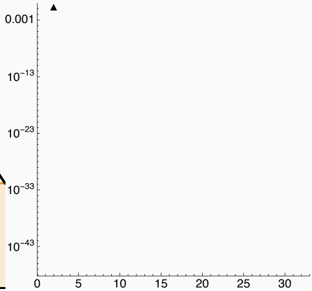

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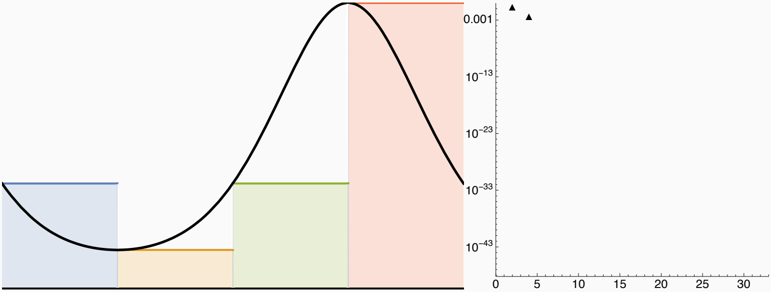

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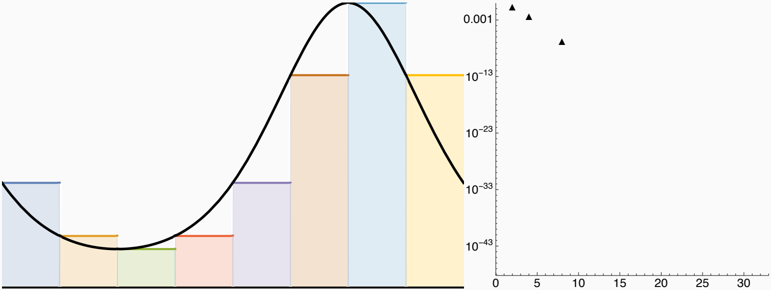

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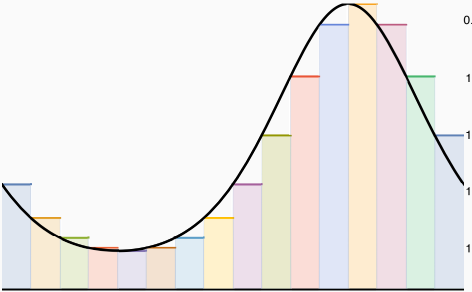

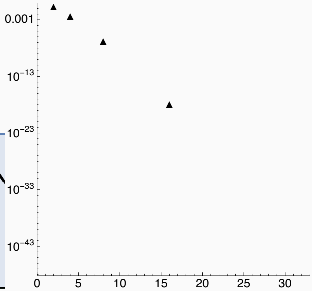

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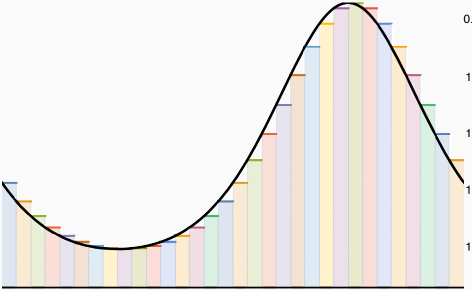

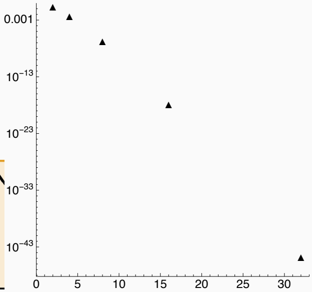

Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$?

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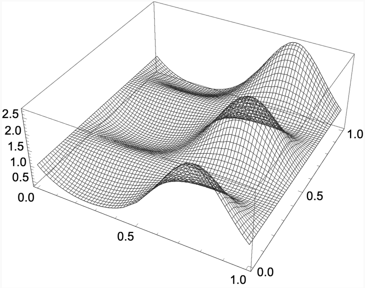

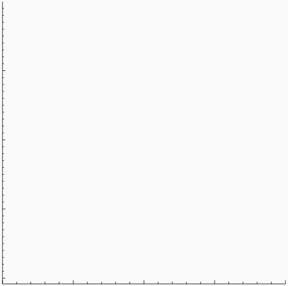

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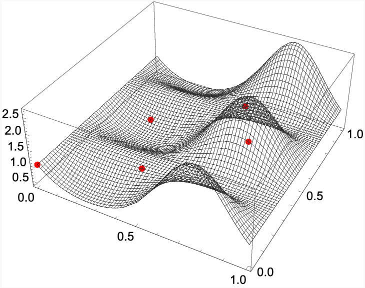

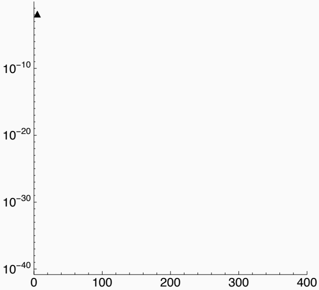

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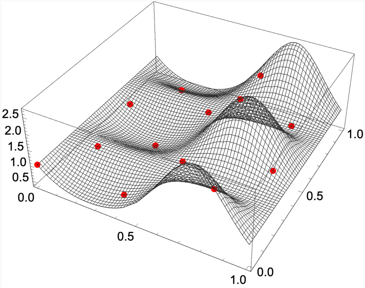

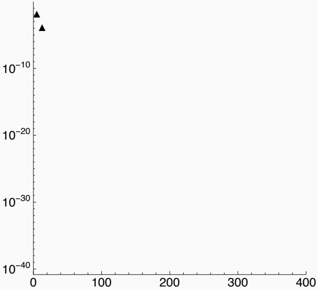

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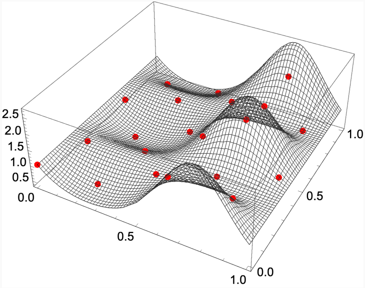

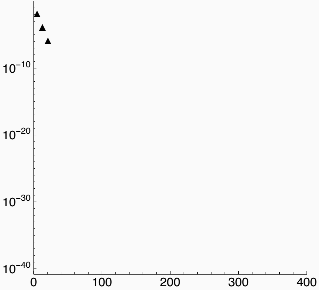

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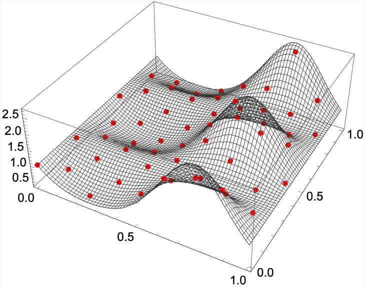

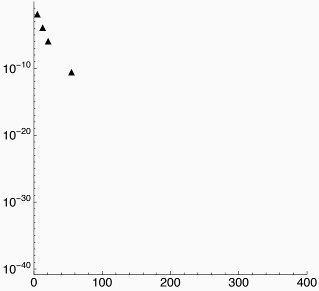

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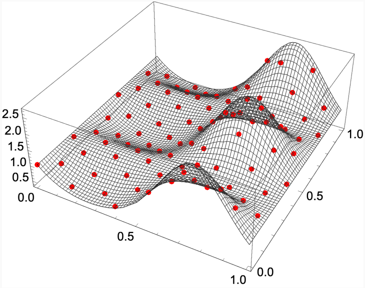

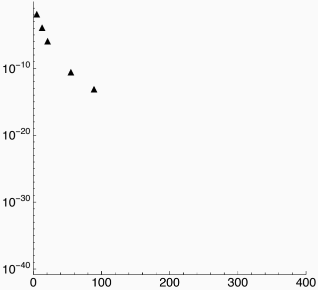

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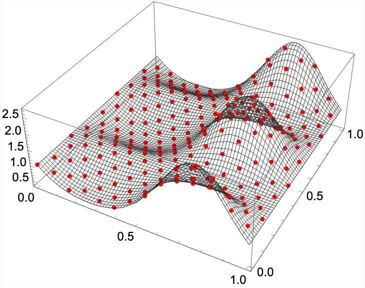

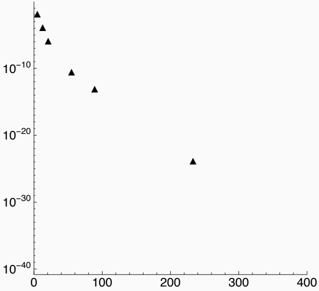

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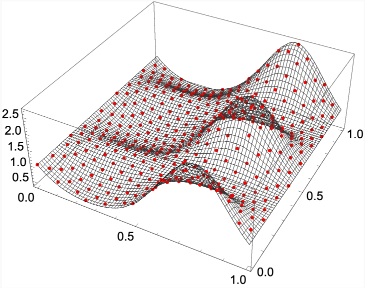
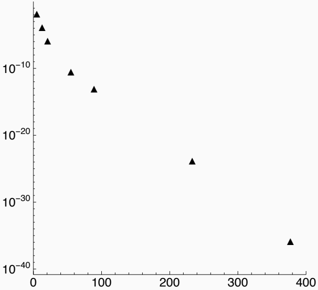




For continuous 1-periodic functions with absolutely convergent Fourier series, the lattice rule error is precisely (Sloan and Kachoyan 1987):

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

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

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

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

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

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.

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 a CBC algorithm such that*

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

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

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 $\boldsymbol{\omega} \in \Omega$,

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

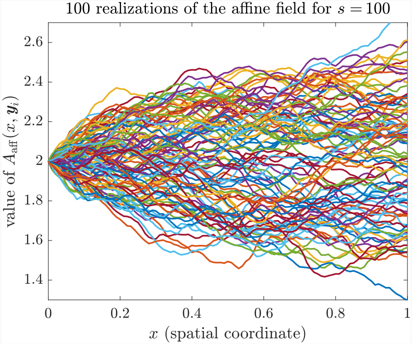
with the special choice $\Theta(y) = \frac{1}{\sqrt{6}} \sin(2\pi y)$.

- 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

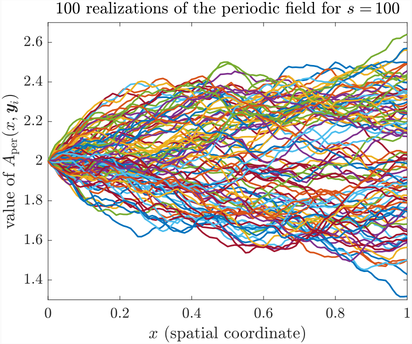
Affine

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



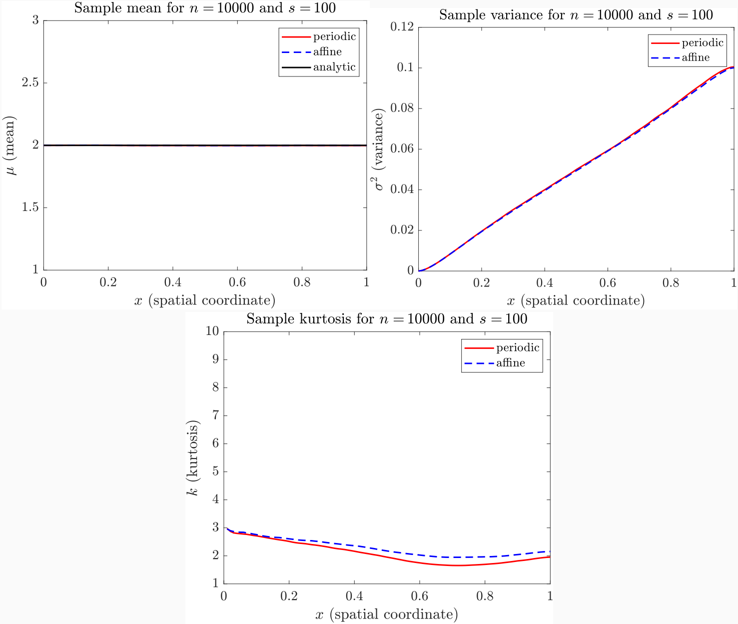
Periodic

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



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

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

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

where we impose the following assumptions:

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

(A2) There exist positive constants $a_{\max}$ and $a_{\min}$ 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 $\boldsymbol{z} \in \{1, \ldots, n-1\}^s$ can be constructed by a CBC algorithm such that

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

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

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

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

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

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

Here,

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

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

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

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

$$\|F\|_{\alpha} \leq \|G\|_{H^{-1}} \max_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}} (2\pi)^{\alpha|\mathfrak{u}|}} \left\| \left(\prod_{j \in \mathfrak{u}} \frac{\partial^{\alpha}}{\partial y_j^{\alpha}} \right) u(\cdot,\boldsymbol{y}) \right\|_{H_0^1}$$

$$\leq \frac{\|G\|_{H^{-1}} \|f\|_{H^{-1}}}{a_{\min}} \max_{\mathfrak{u} \subseteq \{1:s\}} \frac{1}{\gamma_{\mathfrak{u}}} \sum_{\boldsymbol{m}_{\mathfrak{u}} \in \{1:\alpha\}^{|\mathfrak{u}|}} |\boldsymbol{m}_{\mathfrak{u}}|! \prod_{j \in \mathfrak{u}} b_j^{m_j} S(\alpha, m_j).$$

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

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

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

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

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

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

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

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

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

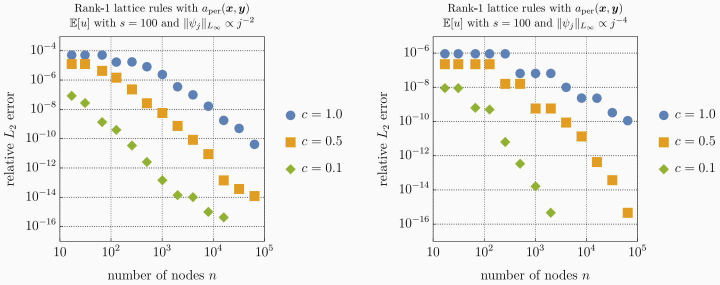


Figure 7: Left: $\beta = 2$. Right: $\beta = 4$.

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 $H := H_{s,\alpha,\gamma}$ be the Hilbert space containing absolutely continuous, somewhat smooth periodic functions $f\colon [0,1)^s \to \mathbb{R}$ endowed with the norm

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

  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*

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

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

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

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

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

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:

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

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

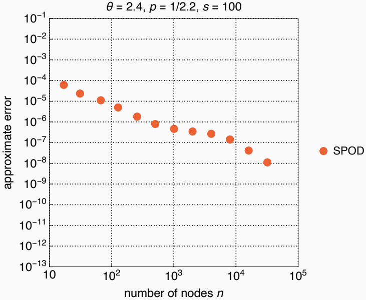
Let us consider the PDE problem

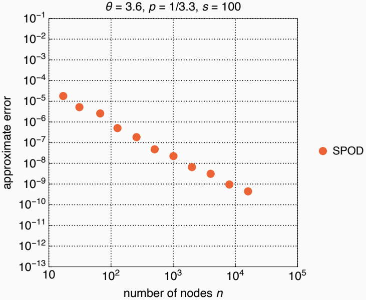
$$-\nabla \cdot (a_{\mathrm{per}}(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = x_2, \quad u(\cdot, \boldsymbol{y})|_{\partial D} = 0,$$

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)

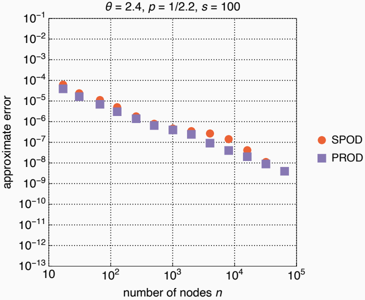
Let us consider the PDE problem

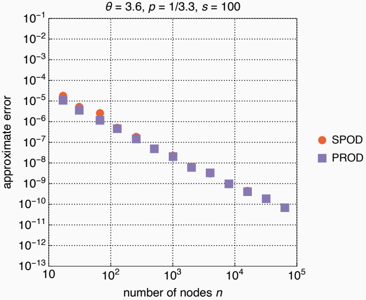
$$-\nabla \cdot (a_{\rm per}(\boldsymbol{x}, \boldsymbol{y}) \nabla u(\boldsymbol{x}, \boldsymbol{y})) = x_2, \quad u(\cdot, \boldsymbol{y})|_{\partial D} = 0,$$

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

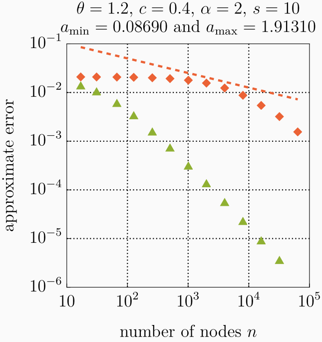
$$a_{\rm per}(\boldsymbol{x}, \boldsymbol{y}) = 1 + \frac{1}{\sqrt{6}} \sum_{j=1}^{100} \sin(2\pi y_j) \psi_j(x), \quad y_j \in [0,1],$$

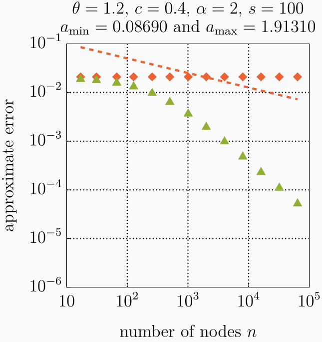
where $\psi_j(\boldsymbol{x}) = j^{-\theta} \sin(j\pi x_1) \sin(j\pi x_2)$. **Note that $\|\psi_j\|_{L^\infty} \propto j^{-\theta}$.**



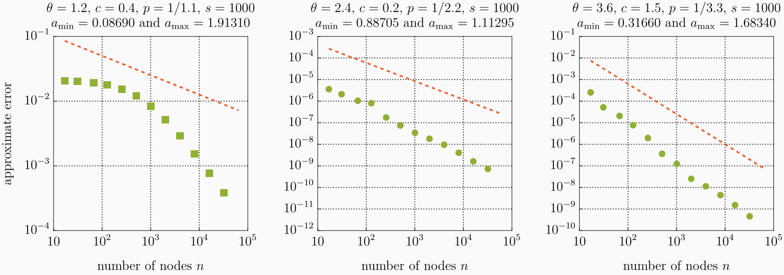


In certain situations, the product weights can outperform SPOD weights.





The product weights can be used to perform computations for higher dimensional problems (here, $s = 1000$).



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 high-dimensional problems (e.g., as surrogates for Bayesian inversion).

References

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