Quasi-Monte Carlo methods for domain uncertainty quantification using periodic random variables

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Part I: Quasi-Monte Carlo cubature

High-dimensional numerical integration

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

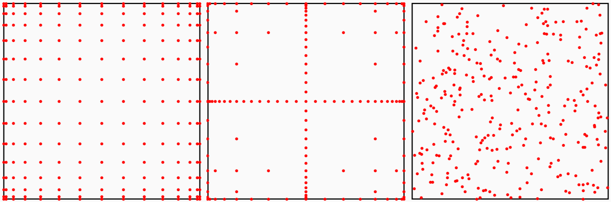


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

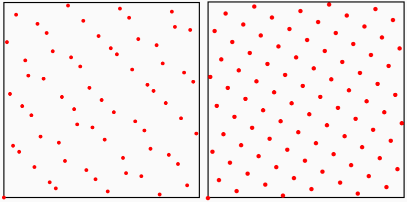


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

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

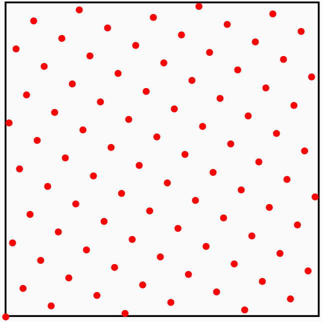
Rank-1 lattice rules

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

have the points

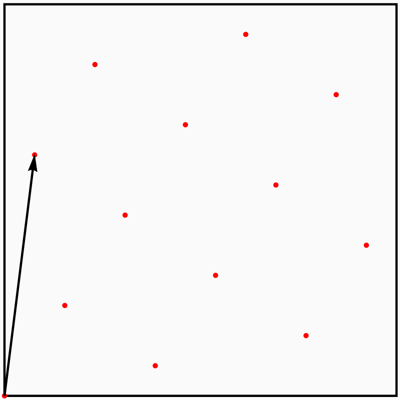
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

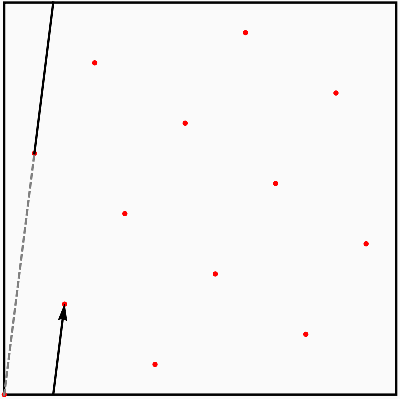
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

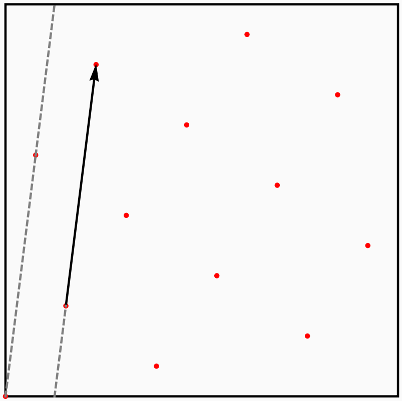


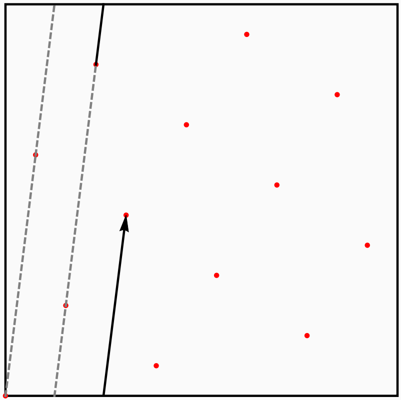
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

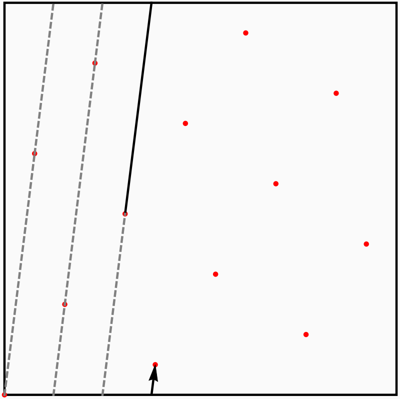
Lattice rules and periodic functions are a match made in heaven!

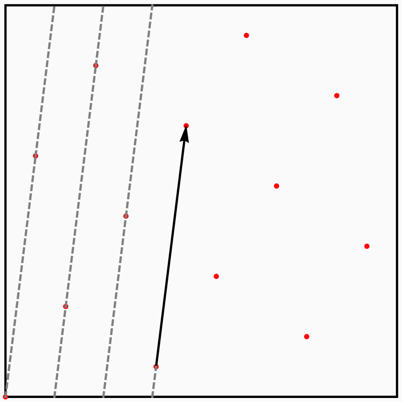


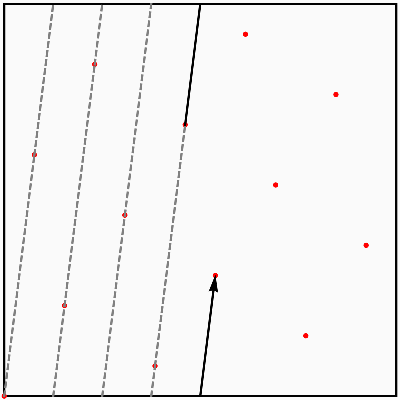


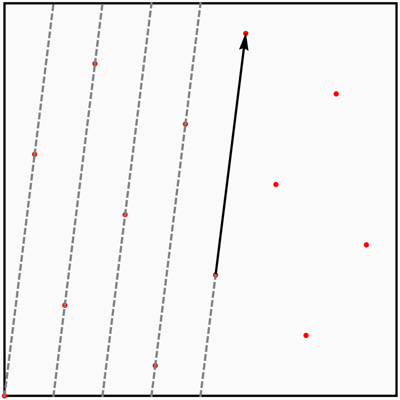


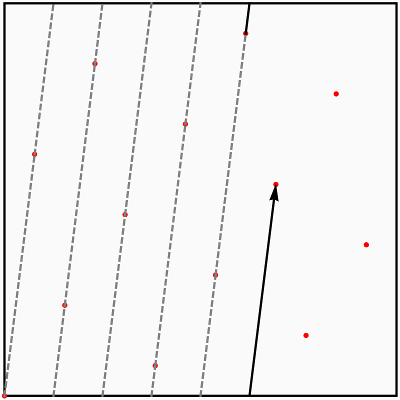


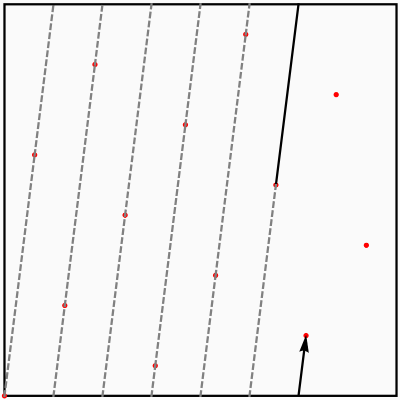


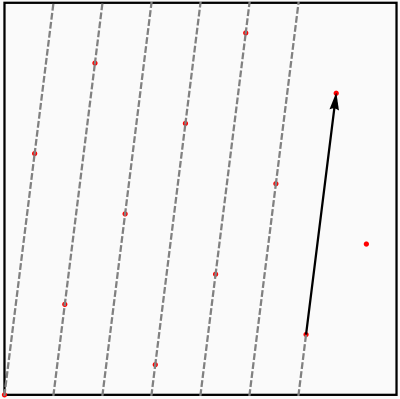


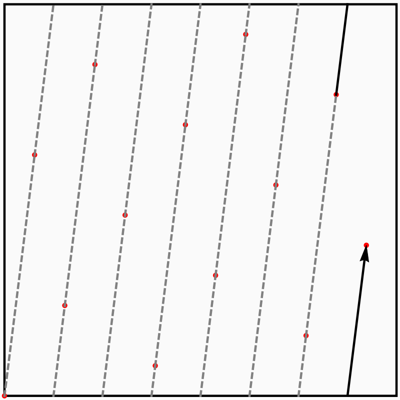












Dimension $s = 1$: the only lattice is the left-Riemann rule

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

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

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

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

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

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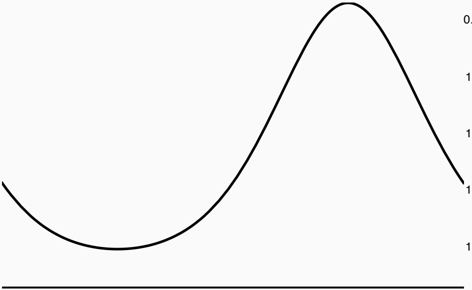
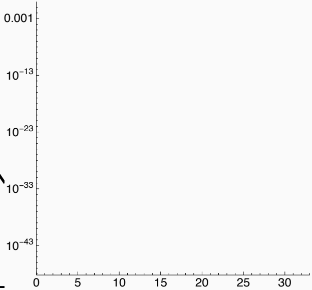
Exponential convergence for analytic, periodic functions

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





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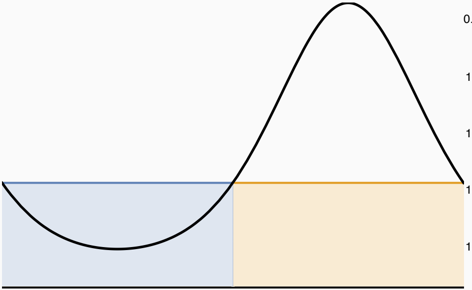

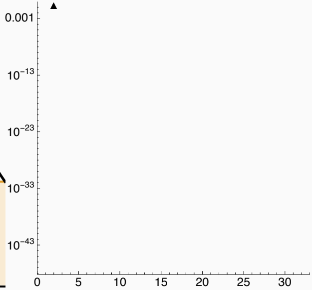

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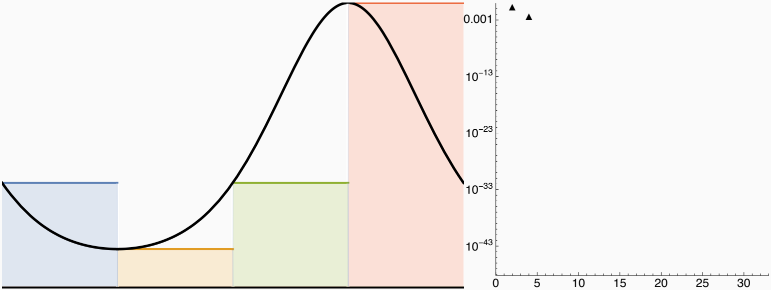

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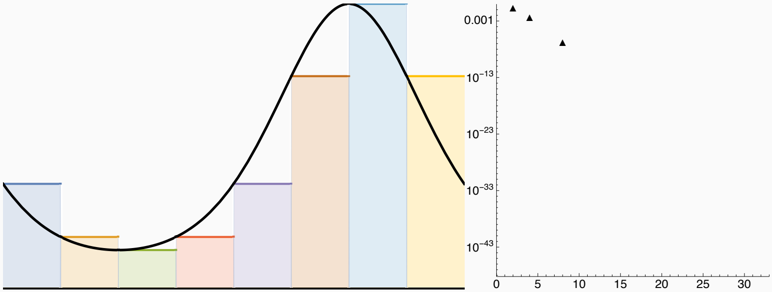

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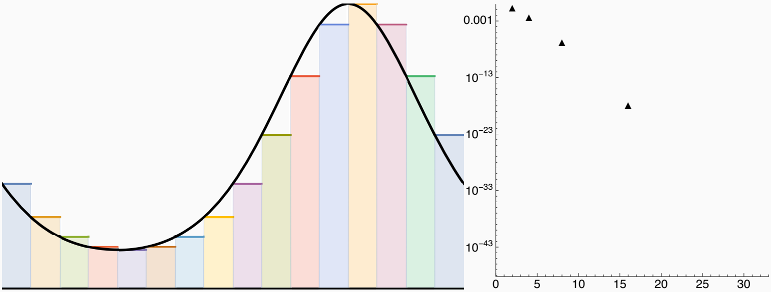

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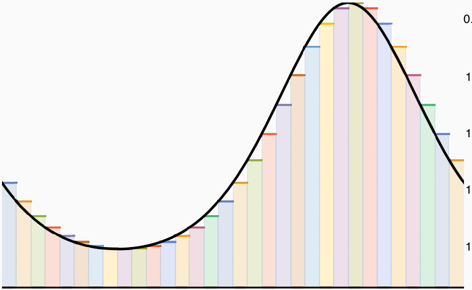

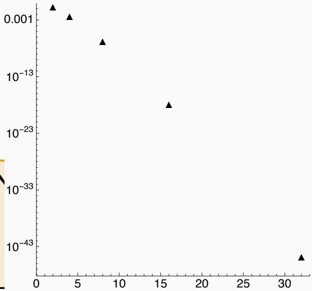

Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$?

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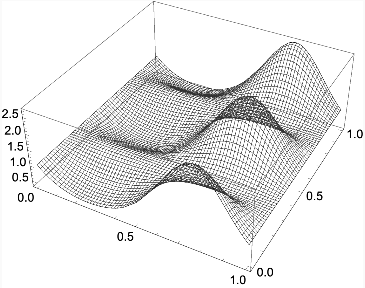

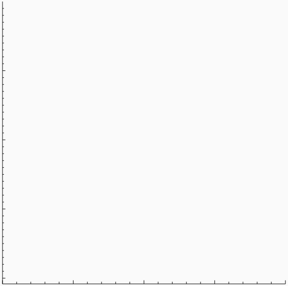

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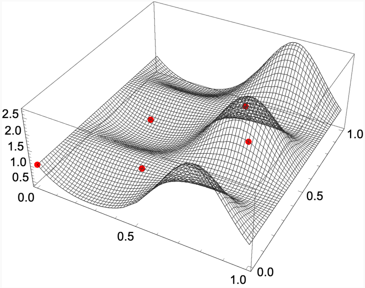

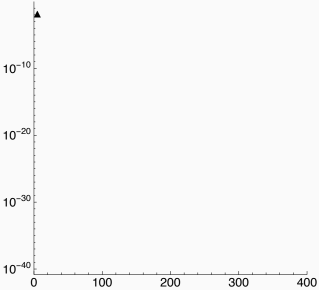

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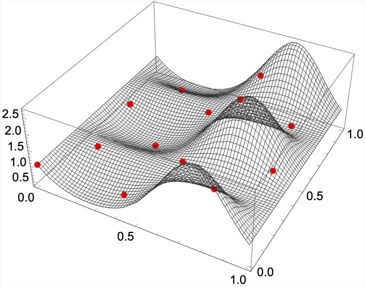

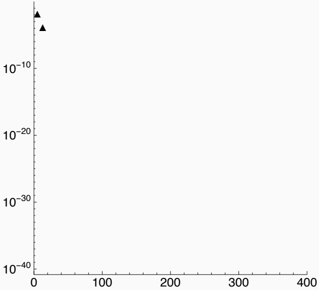

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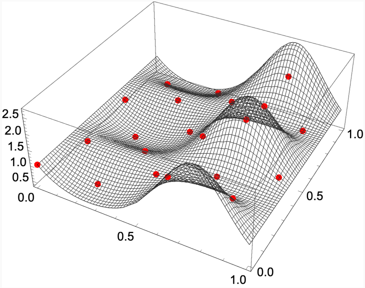

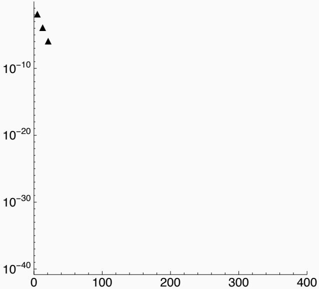

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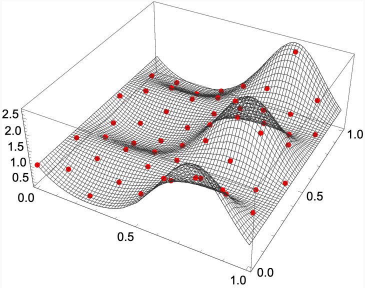

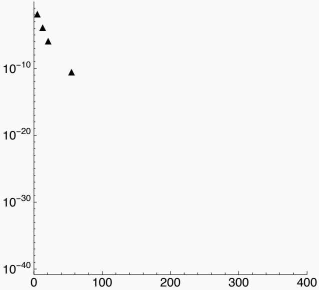

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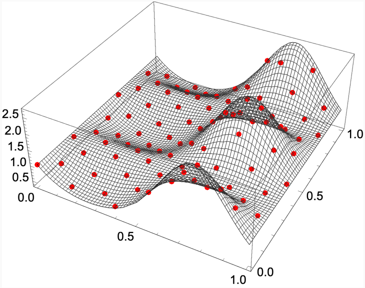

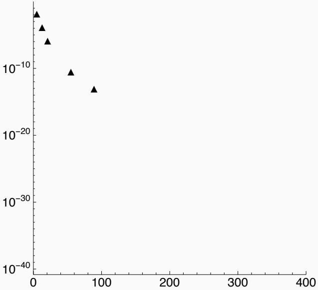

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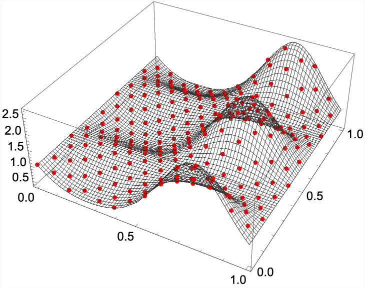

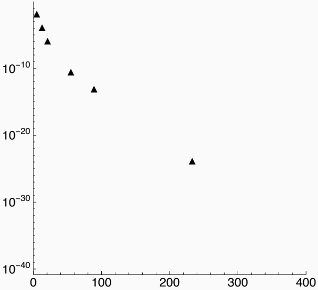

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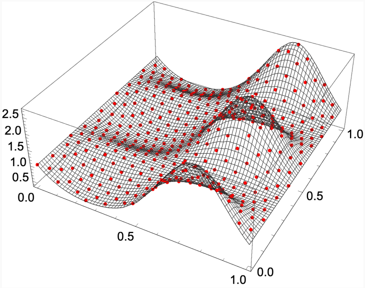
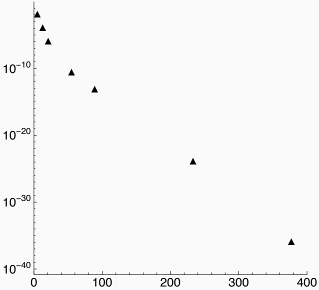




For continuous 1-periodic functions with absolutely convergent Fourier series, the lattice rule error is precisely (Sloan and Kachoyan 1987):

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

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

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

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.

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

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

   $\boldsymbol{p}_{0,\ell} = 1_n$ 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

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

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

   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 $\to$ the matrix-vector product can be implemented in $\mathcal{O}(n \log n)$ operations using FFT.

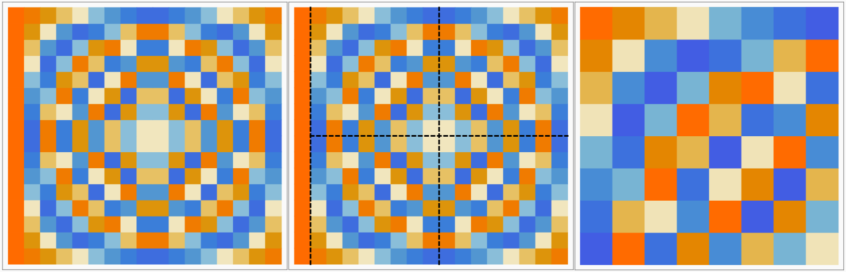


Figure 3: Example with Ω_{17}. Note that the first column is a constant and can be left out (the components of $\Omega_n \boldsymbol{x}$ are shifted by a constant $\to$ the smallest component stays invariant). Noting the obvious symmetries in the remaining four blocks, we can focus on the top left block.

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.)

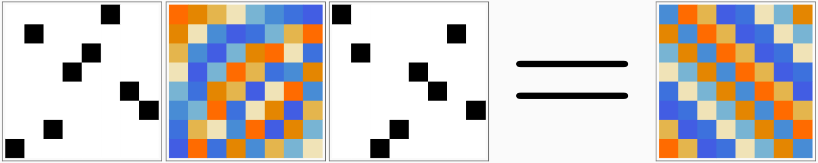


Figure 4: The original block matrix is multiplied from both sides by Rader permutation matrices (the black elements indicate the value 1 and white elements indicate the value 0) to obtain a circulant matrix.

Example with $n = 1009$

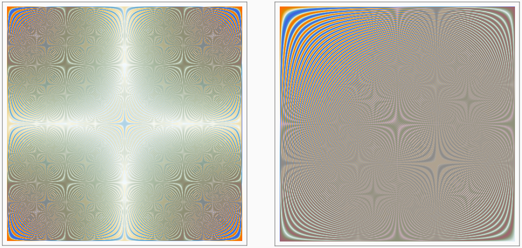


Figure 5: LHS: Original Ω_{1009}. RHS: top left block of Ω_{1009} (sans first column).

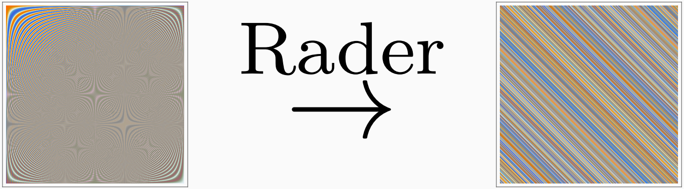


Figure 6: Rader transformation turns the top left block matrix circulant.

- 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

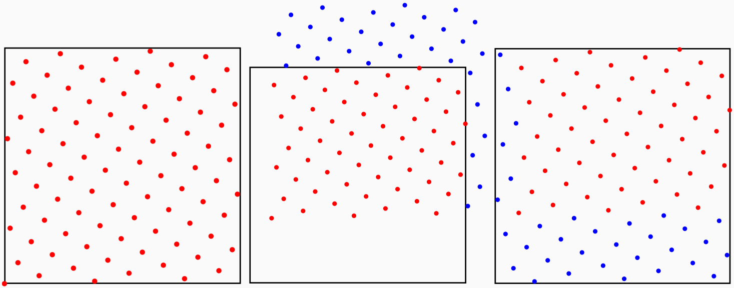
Non-periodic setting: randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

$\Delta \in [0,1)^s$ 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

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

Then

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

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

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

Error bound (one random shift):

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

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

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

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

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

and (squared) worst case error

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

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

Part II: 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 $\boldsymbol{\omega} \in \Omega$,

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

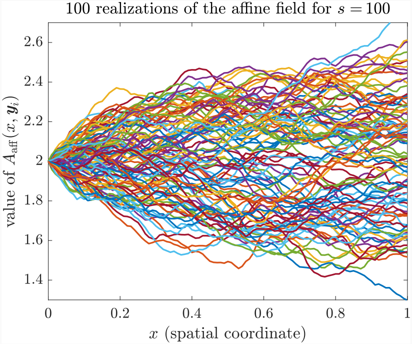
with the special choice $\Theta(y) = \frac{1}{\sqrt{6}} \sin(2\pi y)$.

- 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

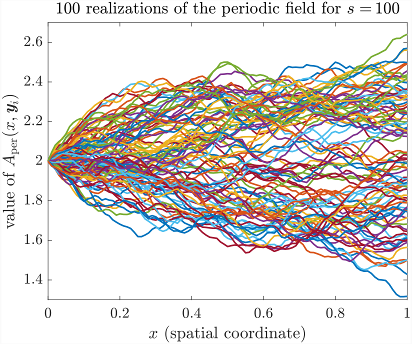
Affine

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



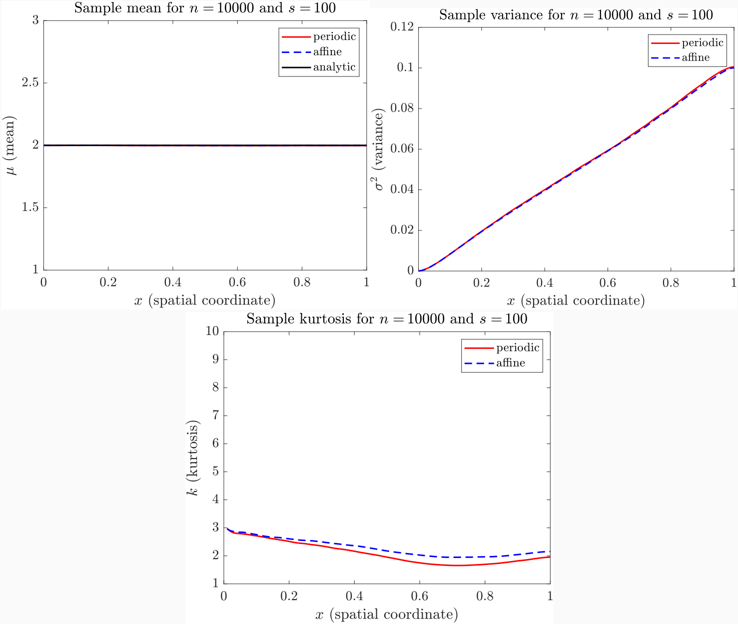
Periodic

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



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

Affine vs. periodic



Part III: Domain uncertainty quantification for elliptic PDEs

Consider the Poisson problem

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

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

Domain mapping method: Let $D_{\mathrm{ref}} \subset \mathbb{R}^d$, $d \in \{2,3\}$, be a fixed reference domain. Define perturbation field $\boldsymbol{V}(\omega)\colon \overline{D_{\mathrm{ref}}} \to \mathbb{R}^d$, 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 $U := [-\frac{1}{2}, \frac{1}{2}]^{\mathbb{N}}$ and let $\boldsymbol{V} \colon \overline{D_{\mathrm{ref}}} \times U \to \mathbb{R}^d$ be a vector field such that

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

with *stochastic fluctuations* $\boldsymbol{\psi}_i \colon D_{\mathrm{ref}} \to \mathbb{R}^d$. Denoting the Jacobian matrix of $\boldsymbol{\psi}_i$ by $\boldsymbol{\psi}_i'$, the Jacobian matrix $J(\cdot, \boldsymbol{y}) \colon D_{\mathrm{ref}} \to \mathbb{R}^{d \times d}$ of vector field $\boldsymbol{V}$ is

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

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

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

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

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

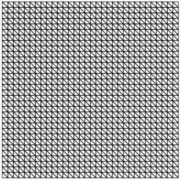


Figure 7: Reference domain

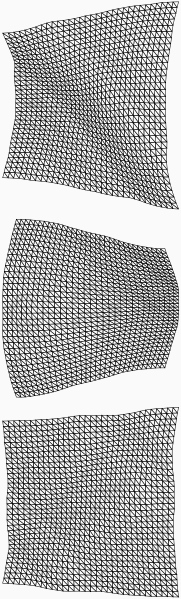


Figure 8: Three realizations of the random domain

Notations and assumptions

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

(A1) For each $\boldsymbol{y} \in U$, $\boldsymbol{V}(\cdot, \boldsymbol{y})\colon \overline{D_{\mathrm{ref}}} \to \mathbb{R}^d$ is an invertible, twice continuously differentiable vector field.

(A2) For some $C > 0$, it holds that

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

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

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

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

(A4) It holds that $\|\boldsymbol{\psi}_i\|_{W^{1,\infty}(D_{\mathrm{ref}};\mathbb{R}^d)} < \infty$ for all $i \in \mathbb{N}$ and $\sum_{i=1}^{\infty} \|\boldsymbol{\psi}_i\|_{W^{1,\infty}(D_{\mathrm{ref}};\mathbb{R}^d)} < \infty$.

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

$$\sum_{i=1}^{\infty} \|\boldsymbol{\psi}_i\|^p_{W^{1,\infty}(D_{\mathrm{ref}};\mathbb{R}^d)} < \infty.$$

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

$$\int_{D(\boldsymbol{y})} \nabla u(\boldsymbol{x}, \boldsymbol{y}) \cdot \nabla v(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} = \int_{D(\boldsymbol{y})} f(\boldsymbol{x})\, v(\boldsymbol{x}, \boldsymbol{y}) \,\mathrm{d}\boldsymbol{x} \quad \forall v \in H_0^1(D(\boldsymbol{y})), \tag{2}$$

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

We can transport the variational formulation (2) to the reference domain by a change of variable. Let us define

$$\begin{aligned} A(\boldsymbol{x}, \boldsymbol{y}) &:= (J(\boldsymbol{x}, \boldsymbol{y})^{\mathrm{T}} J(\boldsymbol{x}, \boldsymbol{y}))^{-1} \det J(\boldsymbol{x}, \boldsymbol{y}) \\ f_{\mathrm{ref}}(\boldsymbol{x}, \boldsymbol{y}) &:= f(V(\boldsymbol{x}, \boldsymbol{y})) \det J(\boldsymbol{x}, \boldsymbol{y}), \end{aligned}$$

for $\boldsymbol{x} \in D_{\mathrm{ref}}$, $\boldsymbol{y} \in U$. Then we can recast the problem (2) on the reference domain as follows: for $\boldsymbol{y} \in U$, find $\widehat{u}(\cdot, \boldsymbol{y}) \in H_0^1(D_{\mathrm{ref}})$ such that

$$\int_{D_{\mathrm{ref}}} \big(A(\boldsymbol{x}, \boldsymbol{y}) \nabla \widehat{u}(\boldsymbol{x}, \boldsymbol{y})\big) \cdot \nabla \widehat{v}(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} = \int_{D_{\mathrm{ref}}} f_{\mathrm{ref}}(\boldsymbol{x}, \boldsymbol{y})\, \widehat{v}(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x} \quad \forall \widehat{v} \in H_0^1(D_{\mathrm{ref}}). \tag{3}$$

The solutions to problems (2) and (3) are connected to one another by

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

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

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

where $\rho \geq 1$ satisfies $\|\partial_{\boldsymbol{x}}^{\boldsymbol{\nu}} f\|_{L^\infty(\mathcal{D})} \leq C_f \boldsymbol{\nu}! \rho^{|\boldsymbol{\nu}|}$, $\widetilde{C} := \frac{2\, d!\, (1+\sigma_{\max})^d\, \sigma_{\max}^3}{\sigma_{\min}^{d+4}}$, $\beta_j := \frac{2+\sqrt{2}}{\sqrt{6}} \max(1 + \sqrt{3}, \rho)\, \|\psi_j\|_{W^{1,\infty}(D_{\mathrm{ref}})}$, 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

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

and by setting $\lambda := p$ and $\alpha := \lfloor \frac{1}{p} \rfloor + 1$, we obtain QMC convergence rate $\|I_s(\widehat{u}_s) - Q_{s,n}(\widehat{u}_s)\|_{L^1(D_{\mathrm{ref}})} = \mathcal{O}(n^{-1/p})$ 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

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

where

$$a(x, \boldsymbol{y}) := 1 + \frac{c}{\sqrt{6}} \sum_{j=1}^{s} \sin(2\pi y_j)\psi_j(x), \quad x \in [0,1] \text{ and } \boldsymbol{y} \in [0,1]^s \quad (4)$$

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. It is possible to write $D(\boldsymbol{y}) = V(D(0), \boldsymbol{y})$ with the vector-valued expansion

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

Straightforward calculations show that $\|\boldsymbol{\psi}_j\|_{W^{1,\infty}} = c\pi j^{1-\theta}$ and $\sigma_{\max} = 1 + \frac{c\pi}{\sqrt{6}}\zeta(\theta - 1)$. The expected rate of QMC convergence is $\mathcal{O}(n^{-\theta+1})$. (The $W^{1,\infty}$-norm "penalizes" the convergence rate by an order of magnitude!)

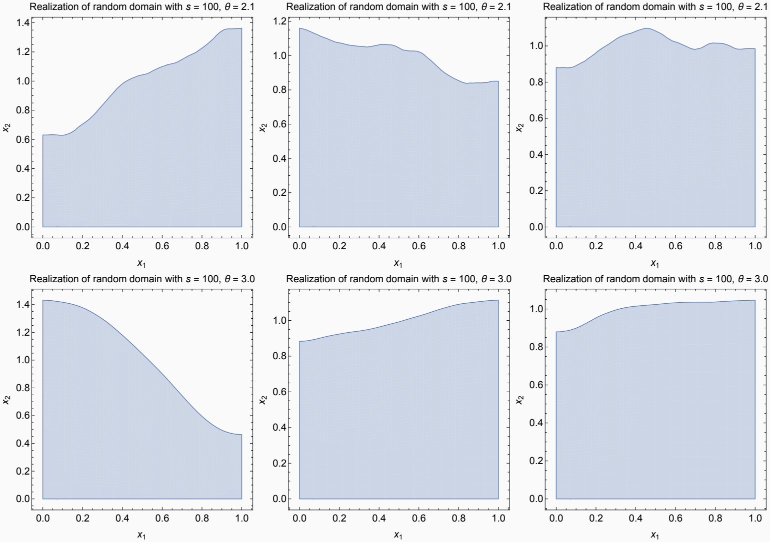


Figure 9: Realizations of the random domains in the numerical experiments. Here, we set $s = 100$ and $\theta \in \{2.1, 3.0\}$. Recall that the reference domain is $D_{\mathrm{ref}} = (0,1)^2$.

We will consider the Dirichlet–Neumann problem

$$\begin{cases} -\Delta u(\boldsymbol{x}, \boldsymbol{y}) = 0 \quad \text{for } \boldsymbol{x} \in D(\boldsymbol{y}),\ \boldsymbol{y} \in [0,1]^s, \\ \partial_{\mathrm{n}} u|_{x_1=0} = \partial_{\mathrm{n}} u|_{x_1=1} = 0, \\ u|_{x_2=0} = 0,\ u|_{x_2=a(x_1,\boldsymbol{y})} = 1. \end{cases} \tag{5}$$

As the quantity of interest, we consider the capacity

$$\mathrm{cap}(D(\boldsymbol{y})) := \int_{D(\boldsymbol{y})} |\nabla u(\boldsymbol{x}, \boldsymbol{y})|^2 \, \mathrm{d}\boldsymbol{x}, \quad \boldsymbol{y} \in [0,1]^s,$$

where u is the solution to (5).

The solutions to (5) are calculated numerically using *hp*-FEM. For each realization of $\boldsymbol{y} \in [0,1]^s$, the finite element solution is computed in $D(\boldsymbol{y})$

QMC error

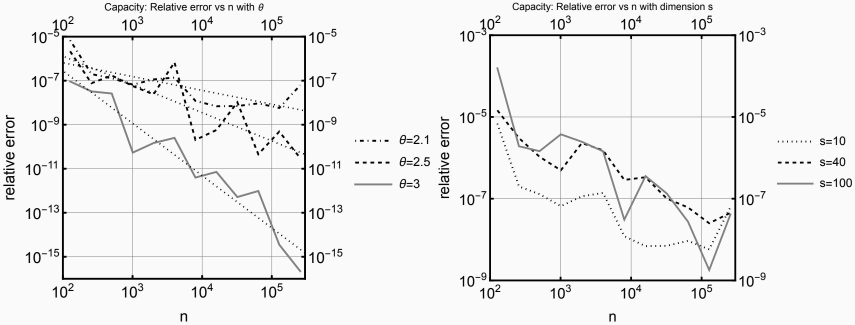


Figure 10: Left: Relative errors with increasing n, varying decay rate $\theta \in \{2.1, 2.5, 3.0\}$, and fixed dimension $s = 10$. Right: Relative errors with increasing n, varying dimension $s \in \{10, 40, 100\}$, and fixed decay rate $\theta = 2.1$. As the reference solution, we use a QMC approximation 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 applications 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.
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