Quasi-Monte Carlo methods and their applications

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Quasi-Monte Carlo methods

High-dimensional numerical integration

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

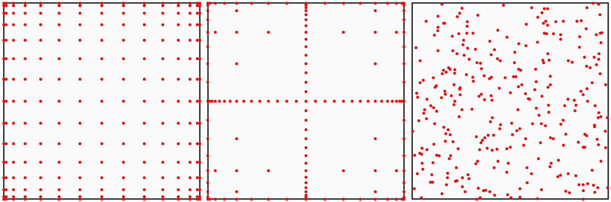


Figure 1: Tensor product grid, sparse grid, Monte Carlo nodes (not QMC rules)

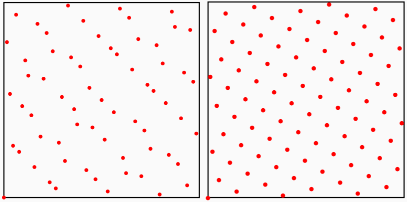


Figure 2: Sobol′ points, lattice rule (examples of QMC rules)

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

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

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

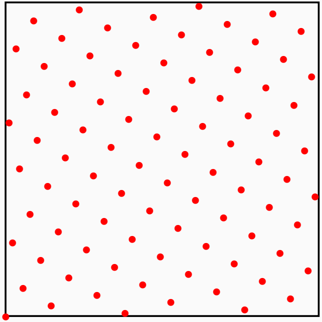
Rank-1 lattice rules

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

have the points

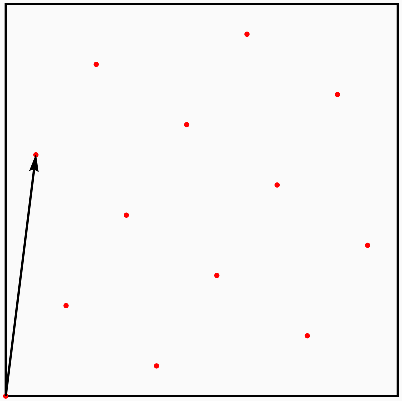
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{1, \ldots, n\},$$

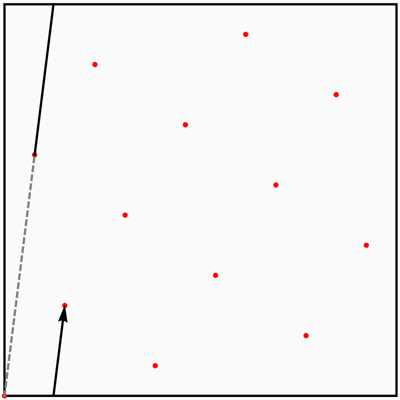
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

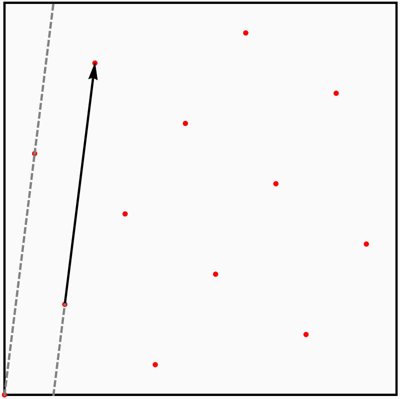


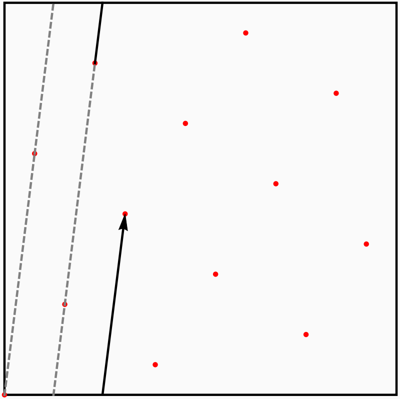
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

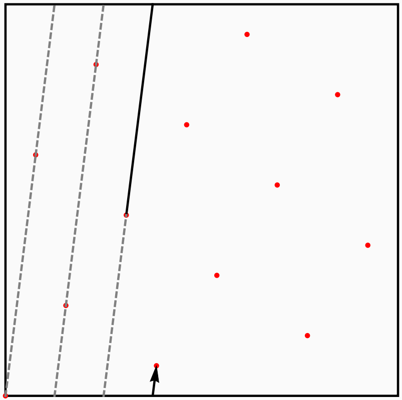
The quality of the lattice rule is determined by the choice of $\boldsymbol{z}$.

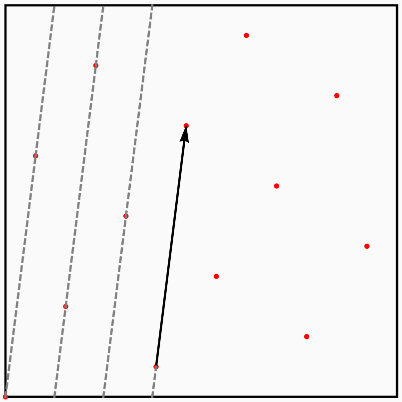


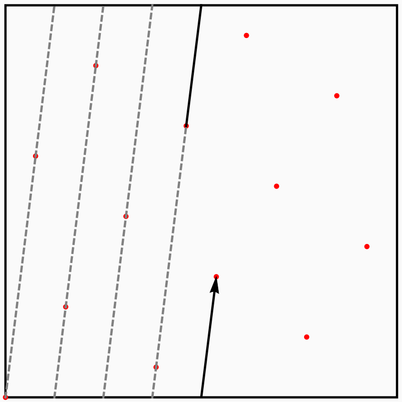


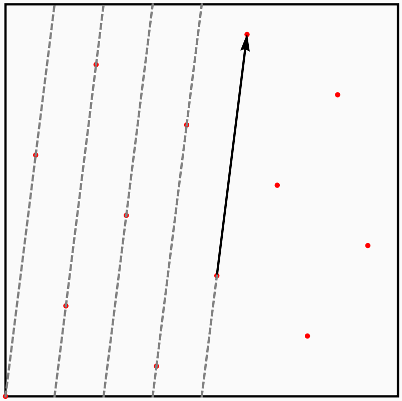


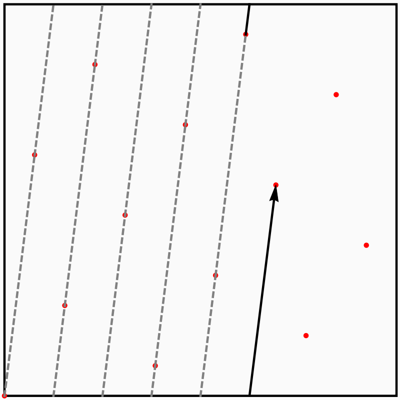


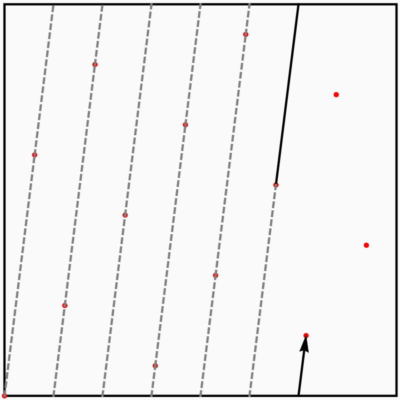


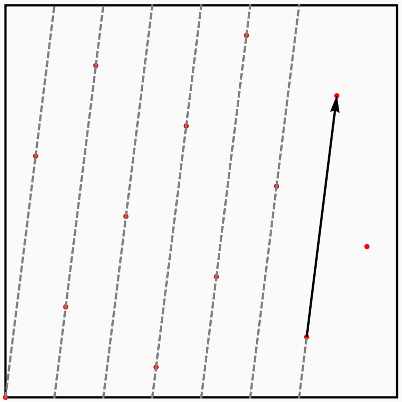


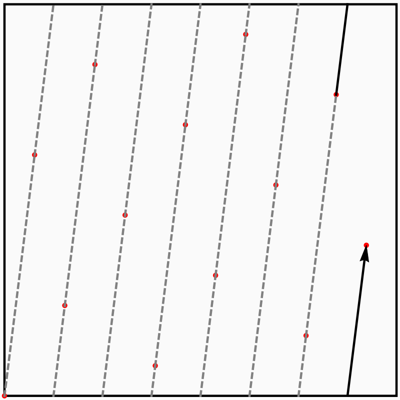












Dimension $s = 1$: the only lattice is the left-Riemann rule

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

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

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

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

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

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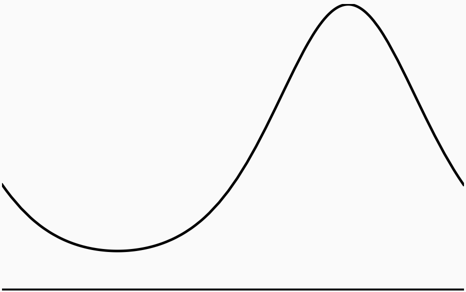
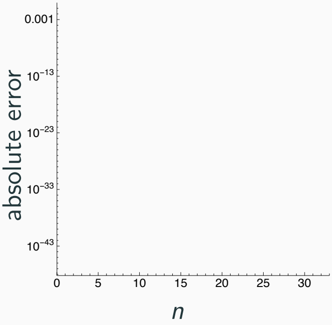
Exponential convergence for analytic, periodic functions

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





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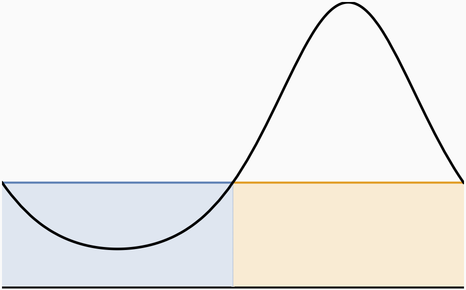

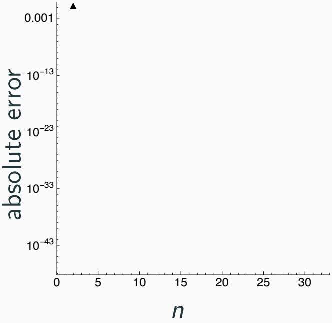

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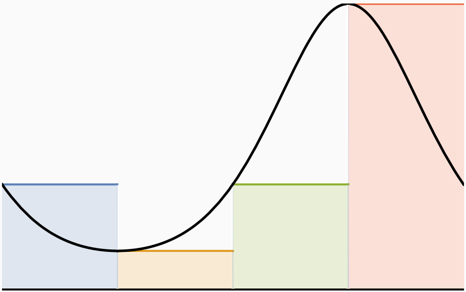

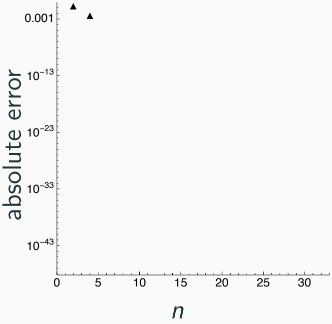

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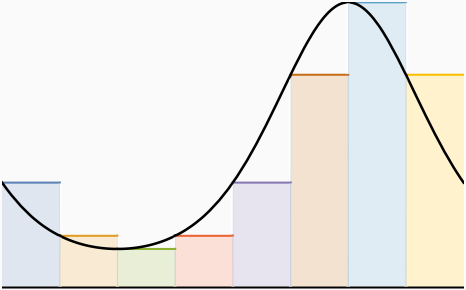

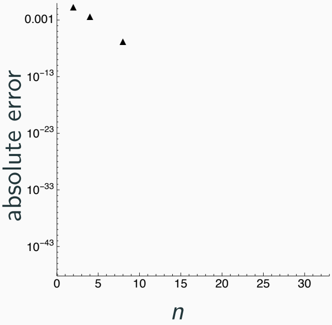

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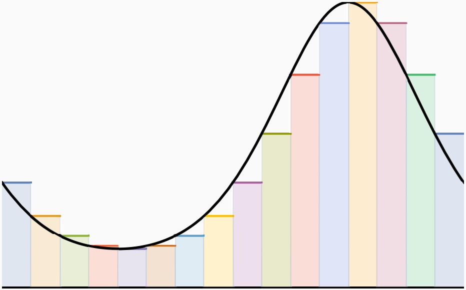

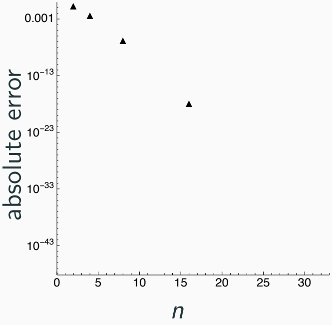

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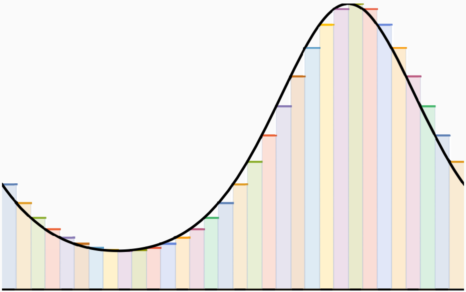

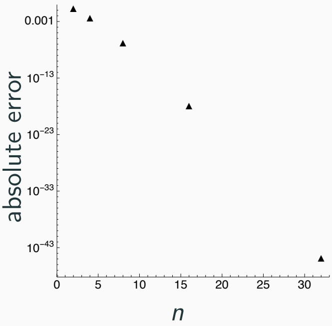

Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$?

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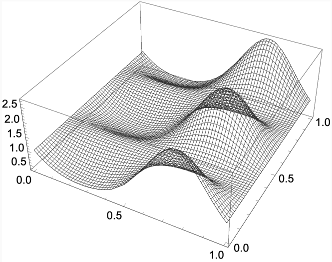

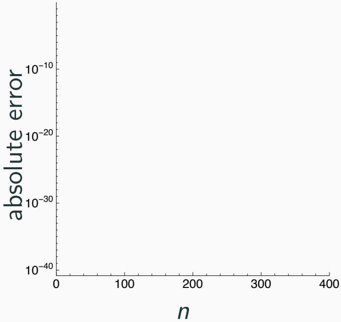

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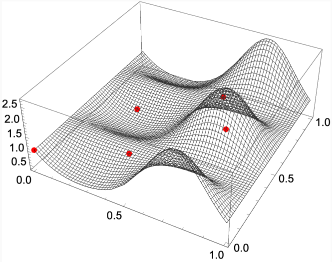

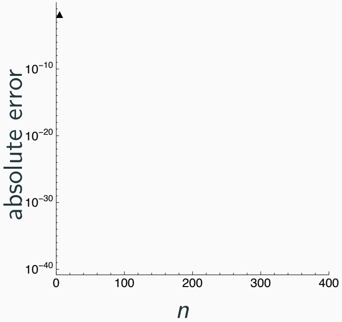

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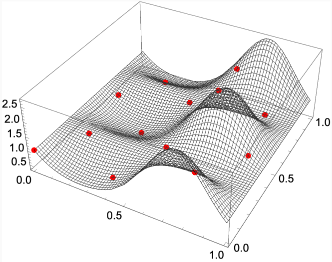

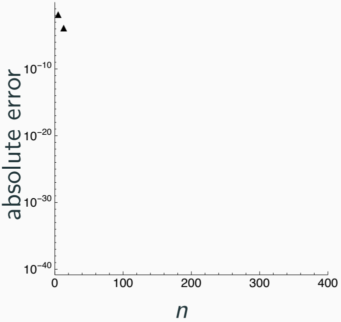

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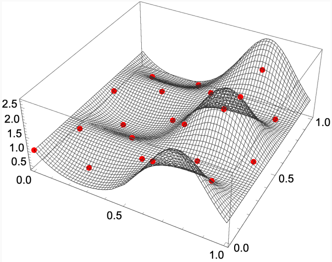

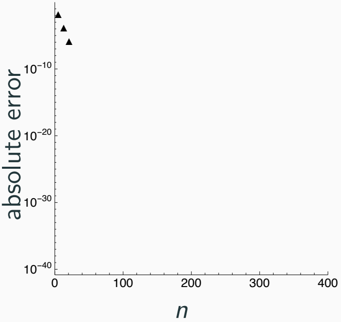

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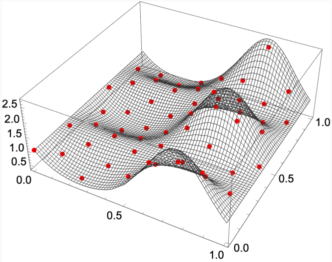

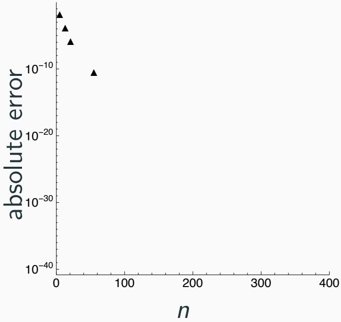

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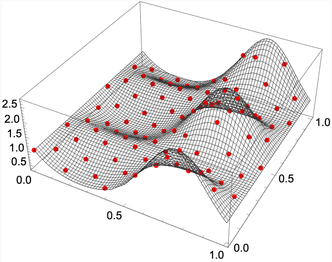

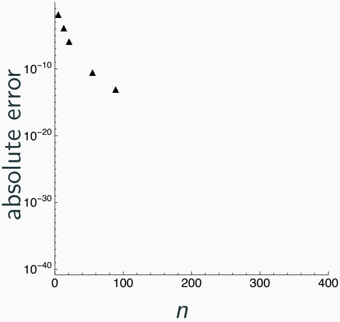

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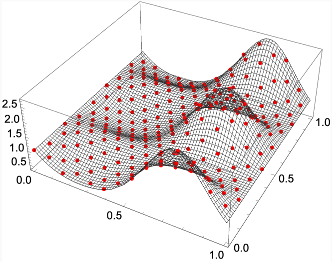

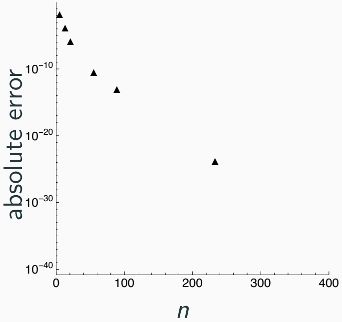

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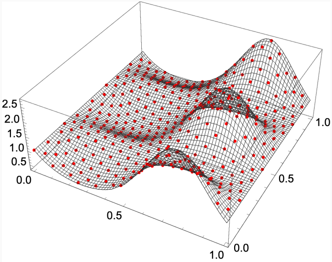
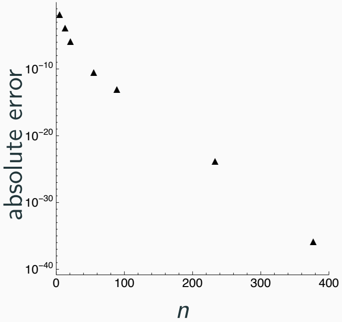




QMC error for (somewhat) smooth periodic functions

Theorem
A generating vector $\boldsymbol{z} \in \{1, \ldots, n-1\}^s$ *can be constructed by a component-by-component (CBC) algorithm such that*

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

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

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

where $\boldsymbol{\gamma} := (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1,\ldots,s\}}$ *is a sequence of positive weights, modeling the relative importance between difference subsets of variables (a small weight* $\gamma_{\mathfrak{u}}$ *means that* $\prod_{j \in \mathfrak{u}} \frac{\partial^{\alpha}}{\partial y_j^{\alpha}} f$ *must also be small in some sense).*

Application of QMC theory:

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

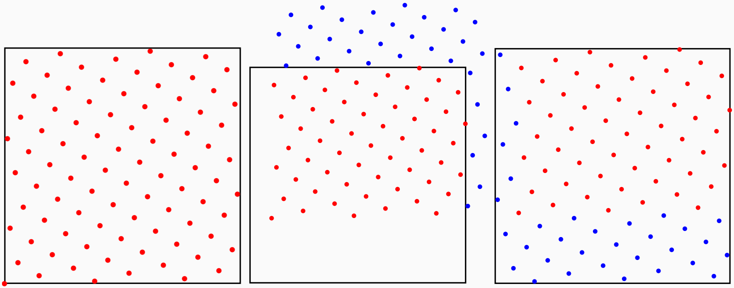
Non-periodic setting: randomly shifted lattice rules

Shifted rank-1 lattice rules have points

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

$\boldsymbol{\Delta} \in [0,1)^s$ 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

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

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 $I_s(f)$.

QMC error for (somewhat) smooth non-periodic functions

Theorem
A generating vector $\boldsymbol{z} \in \{1, \ldots, n-1\}^s$ *can be constructed by a component-by-component (CBC) algorithm such that*

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} |I_s(f) - \overline{Q}_{s,n}(f)|^2} \leq \left(\frac{2}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1, \ldots, s\}} \gamma_{\mathfrak{u}}^{\lambda} \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathfrak{u}|} \right)^{1/(2\lambda)} \|f\|_{\boldsymbol{\gamma}},$$

for $\lambda \in (1/2, 1]$*, n is any prime power,* $\zeta(x) := \sum_{k=1}^{\infty} k^{-x}$*,* $x > 1$*. Here,*

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

where $\boldsymbol{\gamma} := (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1, \ldots, s\}}$ *is a sequence of positive weights, modeling the relative importance between different subsets of variables.*

Application of QMC theory:

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

Some applications of QMC in PDE uncertainty quantification

Consider the elliptic PDE problem:

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

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

- PDE coefficient a may be uncertain;
- Source term f may be uncertain;
- Boundary conditions may be uncertain;
- The domain D itself may be uncertain.

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

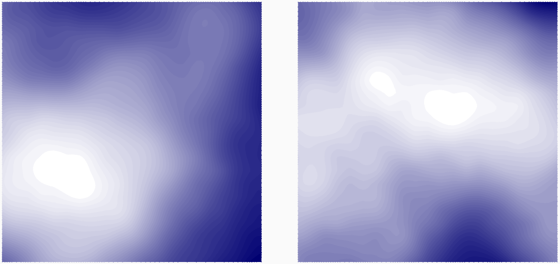
$\Rightarrow$ If the uncertain inputs are modeled as random fields, then the output of the PDE is also a random field. One may be interested in assessing the statistical response of the system, for example, the expectation or variance of the PDE solution (or some other quantity of interest thereof).

Uncertainty in groundwater flow

Risk analysis of radwaste disposal or CO_2 sequestration.

Darcy's law	$\boldsymbol{q}(\boldsymbol{x}) + \boldsymbol{a}(\boldsymbol{x})\nabla \boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x})$
mass conservation law	$\nabla \cdot \boldsymbol{q}(\boldsymbol{x}) = 0$

in $D \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$
together with boundary conditions

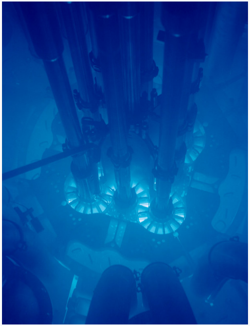


Uncertainty in $\boldsymbol{a}(\boldsymbol{x}, \boldsymbol{\omega})$ leads to uncertainty in $\boldsymbol{q}(\boldsymbol{x}, \boldsymbol{\omega})$ and $\boldsymbol{p}(\boldsymbol{x}, \boldsymbol{\omega})$

Criticality problem for nuclear reactors

$$-\nabla \cdot (\underbrace{a(\boldsymbol{x})}_{\text{diffusion}} \nabla u(\boldsymbol{x})) + \underbrace{b(\boldsymbol{x})}_{\text{absorption}} u(\boldsymbol{x}) = \lambda \underbrace{c(\boldsymbol{x})}_{\text{fission}} u(\boldsymbol{x})$$

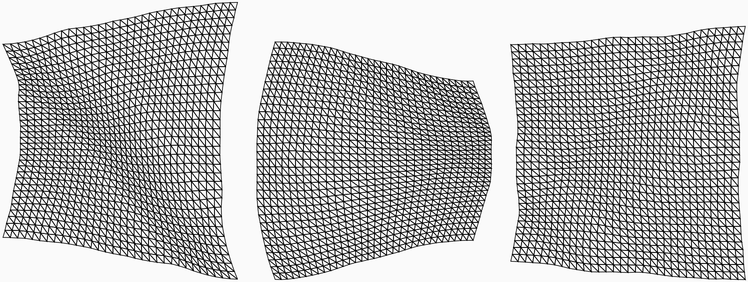
- The smallest eigenvalue $\lambda_1 \in \mathbb{R}$ measures *criticality* of a reactor.
- Eigenfunction $u_1(\boldsymbol{x})$ is the *neutron flux* at the point $\boldsymbol{x}$.



Source: Argonne National Laboratory on Flickr

- $\lambda_1 \approx 1 \Rightarrow$ operating efficiently
- $\lambda_1 > 1 \Rightarrow$ not self-sustaining
- $\lambda_1 < 1 \Rightarrow$ supercritical

Domain uncertainty quantification

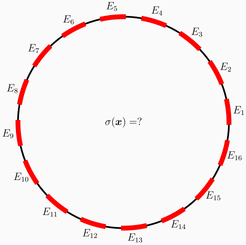


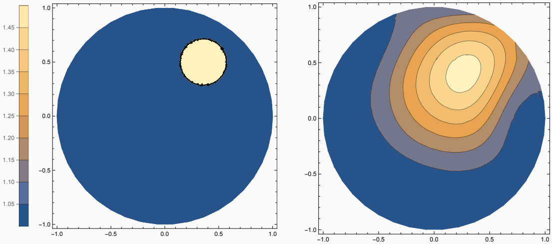
Three realizations of a random spatial domain

Electrical impedance tomography

Use measurements of current and voltage collected at electrodes covering part of the boundary to infer the interior conductivity of an object/body.

$$\begin{cases} \nabla \cdot (\sigma \nabla u) = 0 & \text{in } D, \\ \sigma \frac{\partial u}{\partial \boldsymbol{n}} = 0 & \text{on } \partial D \setminus \bigcup_{k=1}^{L} \overline{E_k}, \\ u + z_k \sigma \frac{\partial u}{\partial \boldsymbol{n}} = U_k & \text{on } E_k,\ k \in \{1, \ldots, L\}, \\ \int_{E_k} \sigma \frac{\partial u}{\partial \boldsymbol{n}} \, \mathrm{d}S = I_k, & k \in \{1, \ldots, L\}, \end{cases}$$





Introduction to QMC for PDE uncertainty quantification

`https://iki.fi/vesakaar/winterschool24/`

Quasi-Monte Carlo methods for

https://iki.fi/vesakaar/winterschool24/

General information

Description

High-dimensional numerical integration plays a central role in the contemporary study of uncertainty quantification. The analysis of how uncertainties associated with material parameters or the measurement configuration propagate within mathematical models leads to challenging high-dimensional integration problems.

Modern quasi-Monte Carlo (QMC) methods are based on tailoring specially designed cubature rules for high-dimensional integration problems. By leveraging the smoothness and anisotropy of an integrand, it is possible to achieve faster-than-Monte Carlo convergence rates. QMC methods have become a popular tool for solving partial differential equations (PDEs) involving random coefficients, a central topic within the field of uncertainty quantification.

This course provides a brief introduction to forward and inverse uncertainty quantification for elliptic PDE problems using QMC methods.

Lecture notes

- Lecture notes (updated 22.2.)
- Programs: fastcbc.m, generator.m, affine_example.m, lognormal_example.m

Last edited Thu Feb 22 2024

Conclusions

- We are always looking for new problems where we can apply QMC!
  - Do you have a problem where QMC might be useful? :)
- Recent trends: function approximation using QMC point sets, training neural networks over QMC point sets, superconvergence properties of smooth functions, extending QMC theory for nonsmooth functions, high-dimensional double integrals (design of experiments), . . .

V. Kaarnioja, F. Y. Kuo, and I. H. Sloan. Lattice-based kernel approximation and serendipitous weights for parametric PDEs in very high dimensions. To appear in: A. Hinrichs, P. Kritzer, F. Pillichshammer (eds.). *Monte Carlo and Quasi-Monte Carlo Methods 2022*. Springer Verlag. Preprint: arXiv:2303.17755 [math.NA]

I. H. Sloan and V. Kaarnioja. Doubling the rate – improved error bounds for orthogonal projection in Hilbert spaces. Preprint 2023, arXiv:2308.06052 [math.NA]

Thank you for your attention!