

# **On the Periodic Model of Uncertainty Quantification With Application to Inverse Problems**

---

Vesa Kaarnioja (FU Berlin)

Thanks to collaborators: Yoshihito Kazashi (Uni. Strathclyde), Frances Kuo (UNSW Sydney), Fabio Nobile (EPFL), and Ian Sloan (UNSW Sydney)

# Table of contents

- Part I: Quasi-Monte Carlo (QMC) cubature using lattice rules
- Part II: The periodic model of uncertainty quantification for PDEs
- Part III: Kernel interpolation over lattice point sets
- Part IV: Application to an inverse problem

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

---

# Lattice rules

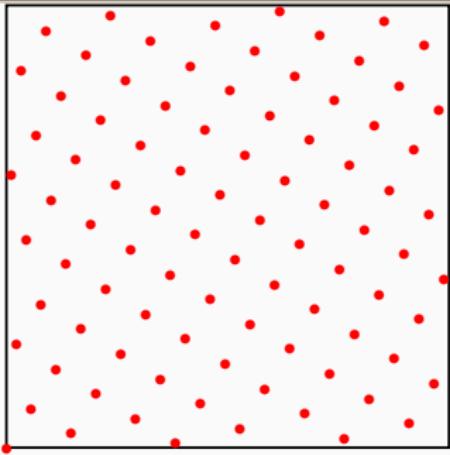
Rank-1 lattice rules

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

have the points

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

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



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

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

Periodic means

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

$$\int_0^1 f(x) dx \approx \left[ \int_0^1 f(x) dx + \sum_{k=1}^{\lfloor p/2 \rfloor} \frac{B_{2k}}{(2k)!} (f^{(2k-1)}(1) - f^{(2k-1)}(0)) \right] - (-1)^p h^p \int_0^1 \tilde{B}_p(x) f^{(p)}(x) dx$$

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

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

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

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

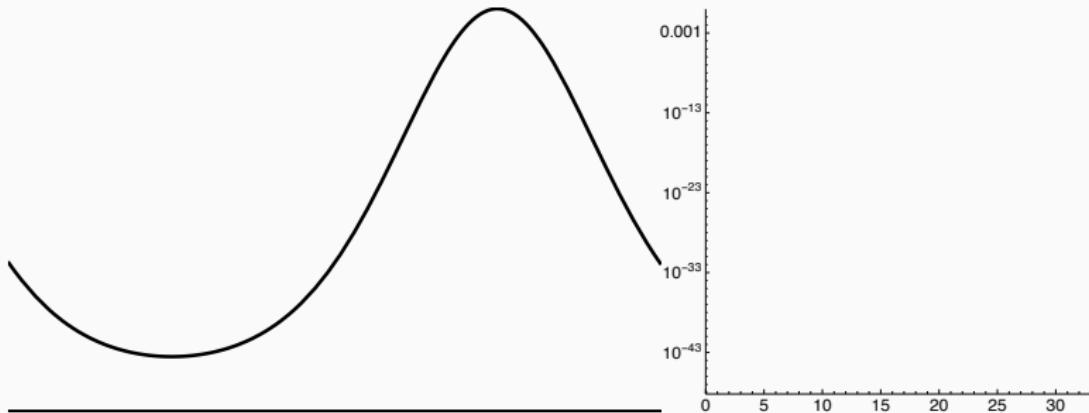
Let  $h = \frac{1}{n}$ . Then the Euler–Maclaurin summation formula gives

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

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

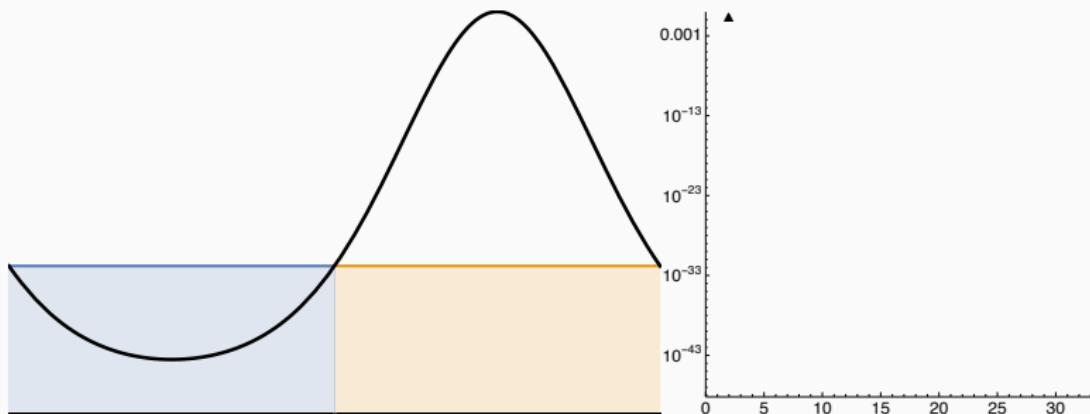
# Exponential convergence for analytic, periodic functions

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



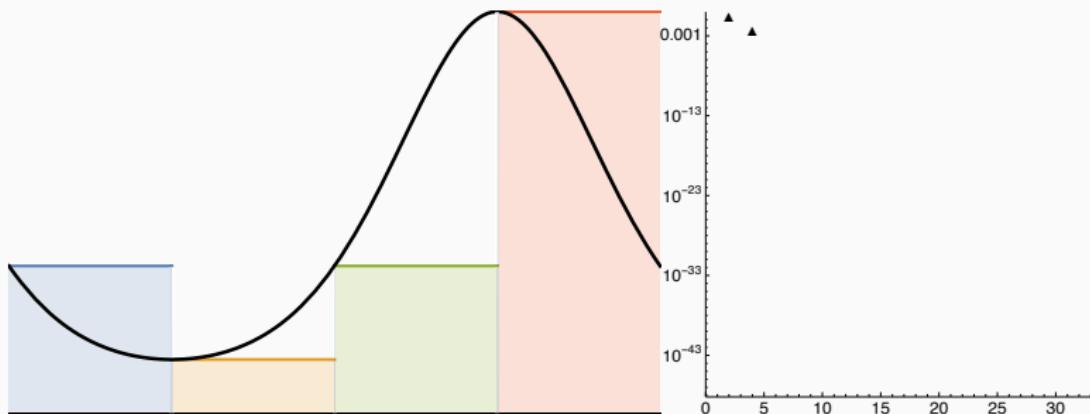
# Exponential convergence for analytic, periodic functions

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



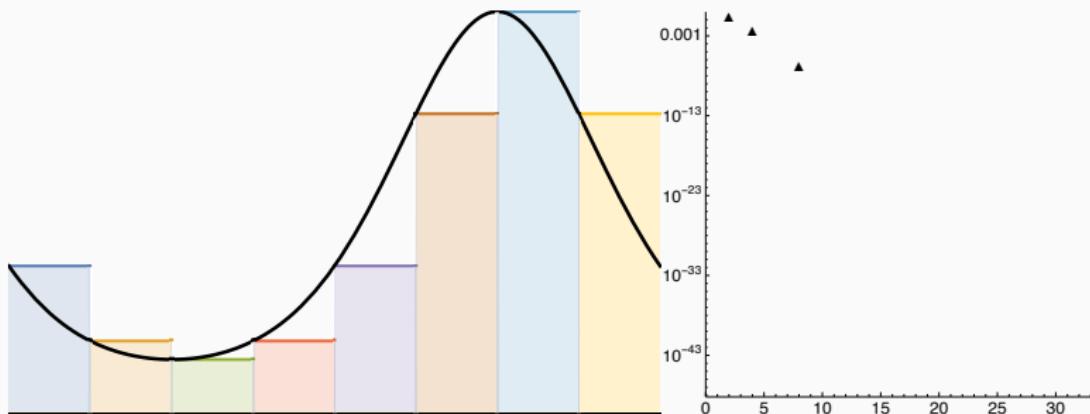
# Exponential convergence for analytic, periodic functions

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



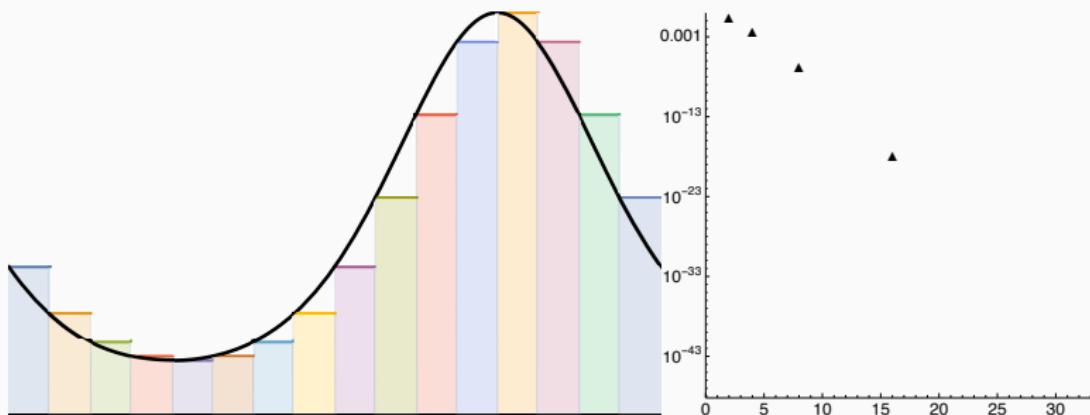
# Exponential convergence for analytic, periodic functions

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



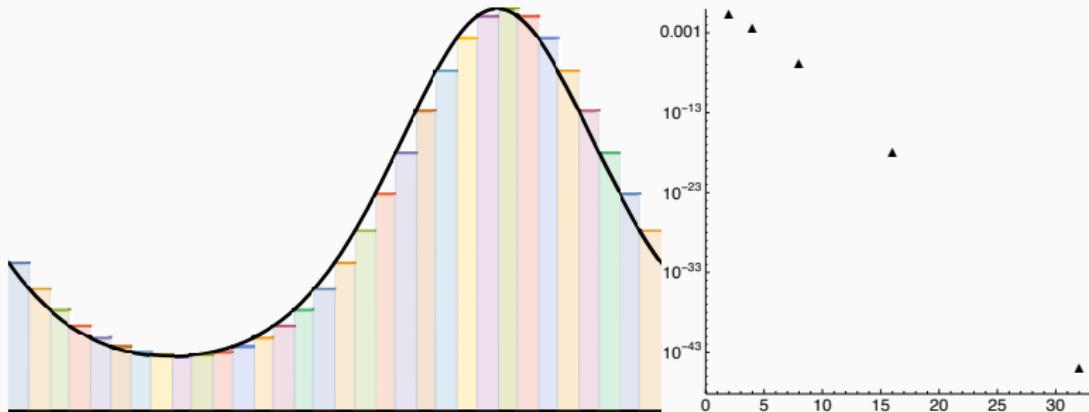
# Exponential convergence for analytic, periodic functions

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



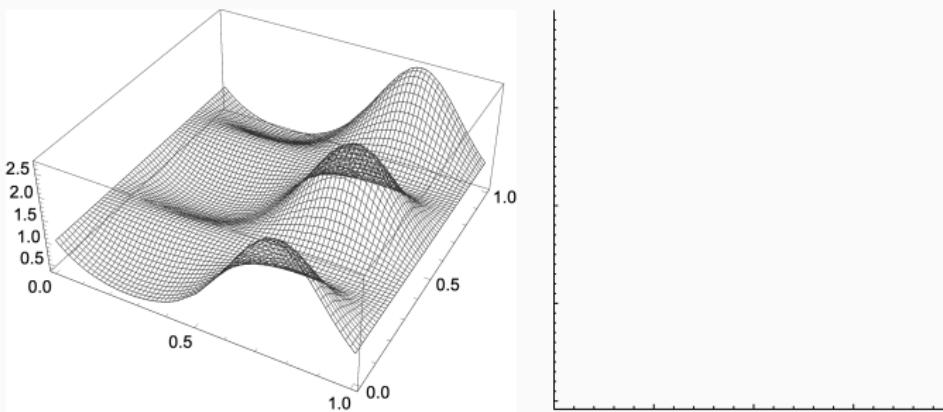
# Exponential convergence for analytic, periodic functions

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



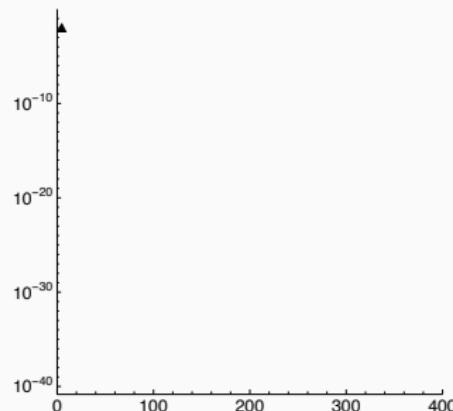
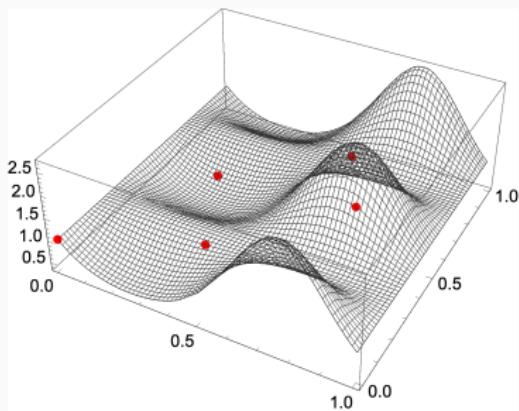
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



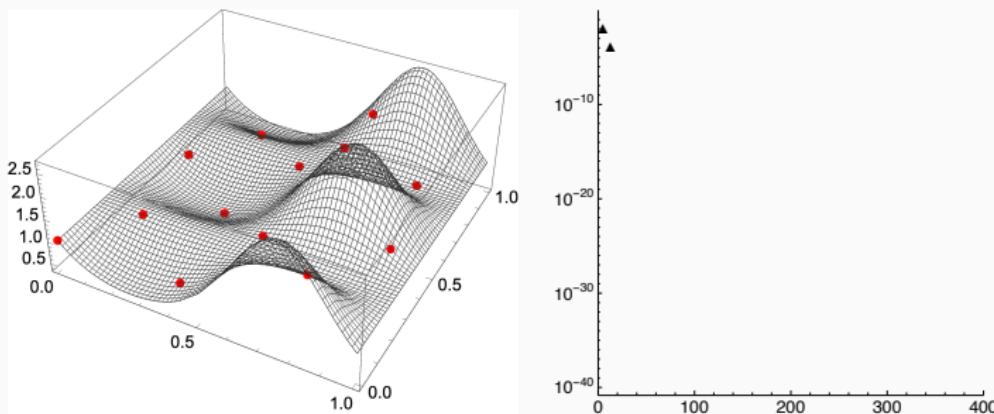
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



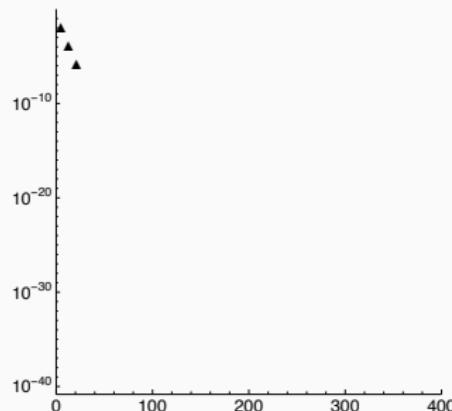
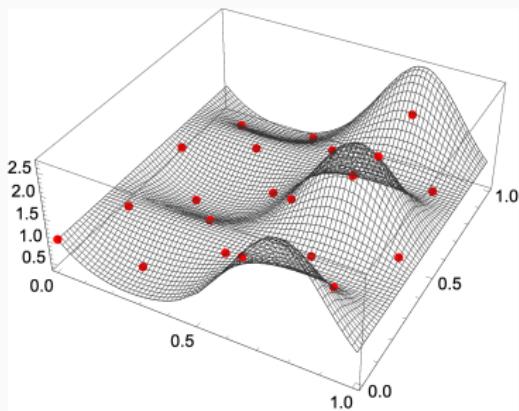
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



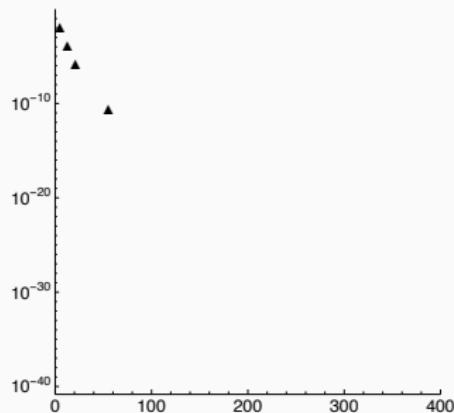
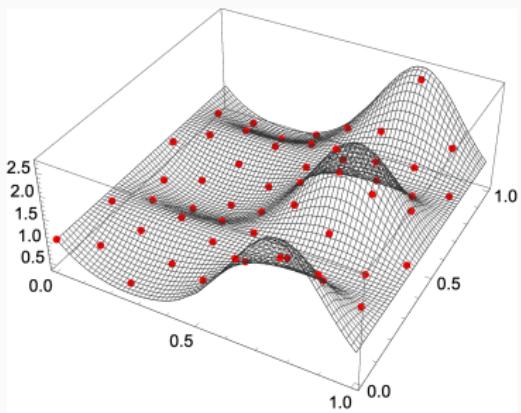
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



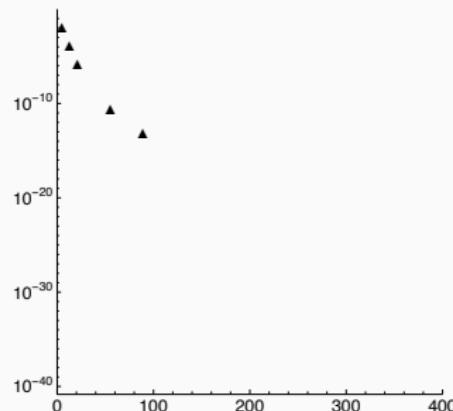
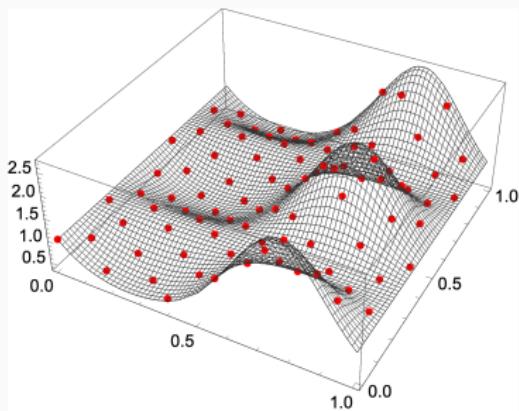
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



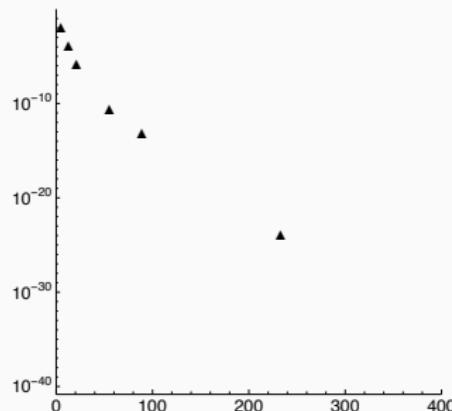
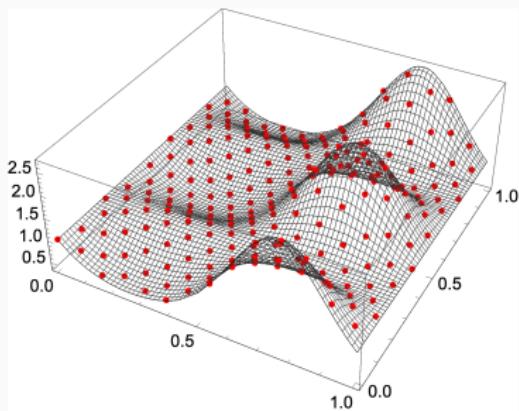
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

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



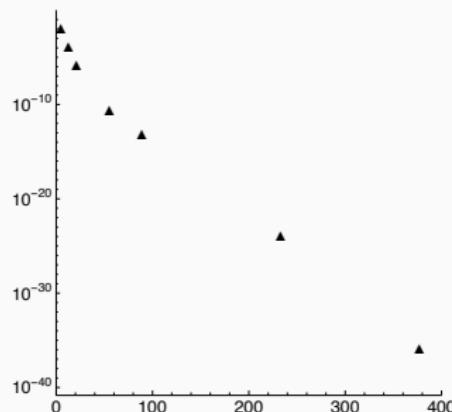
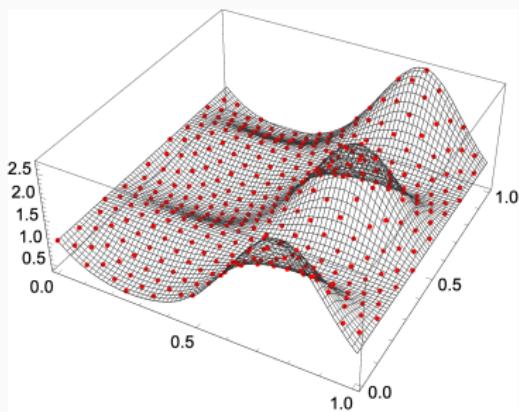
# Can we observe exponential convergence with lattice rules for analytic, periodic functions when dimension $s = 2$ ?

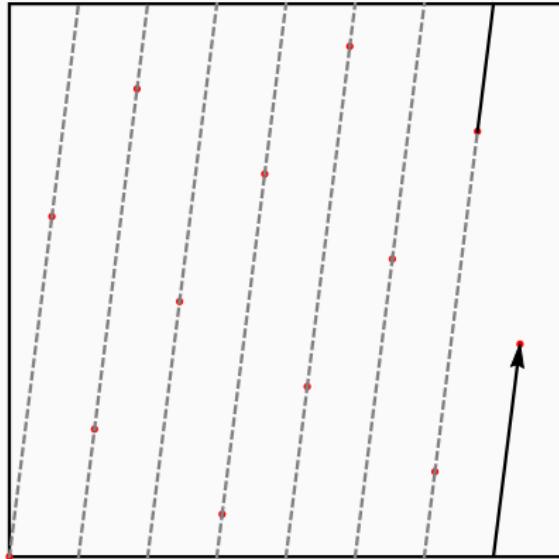
$$\int_0^1 \int_0^1 \exp(-\sin(2\pi x) \cos(2\pi y)^2) dx dy$$



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

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





A suitable generating vector for an integrand satisfying certain smoothness properties can be found using a *component-by-component* (CBC) algorithm (Nuyens and Cools 2006; Kuo, Nuyens, and Cools 2006).

- For integrands belonging to certain weighted Sobolev spaces of smooth functions, the CBC algorithm can be used to produce a generating vector satisfying a rigorous error bound. As input, the CBC algorithm takes the weights and smoothness parameter of the Sobolev space (and number of QMC nodes  $n$ ).
- Fast CBC: FFT can be used to reduce the computational complexity of the CBC algorithm.

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

---

Let  $(\Omega, \mathcal{F}, \mathbb{P})$  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  $u: D \times \Omega \rightarrow \mathbb{R}$  that satisfies

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

for almost all events  $\omega \in \Omega$ . Here, the diffusion coefficient  $a(\cdot, \omega) \in L_+^\infty(D)$  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  $\text{Var}[u]$  or  $\text{Var}[G(u)]$ , 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  $\mathbf{x} \in D$  and  $\omega \in \Omega$ ,

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

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

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

## Periodic model of UQ

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

For  $x \in D$  and  $\omega \in \Omega$ ,

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

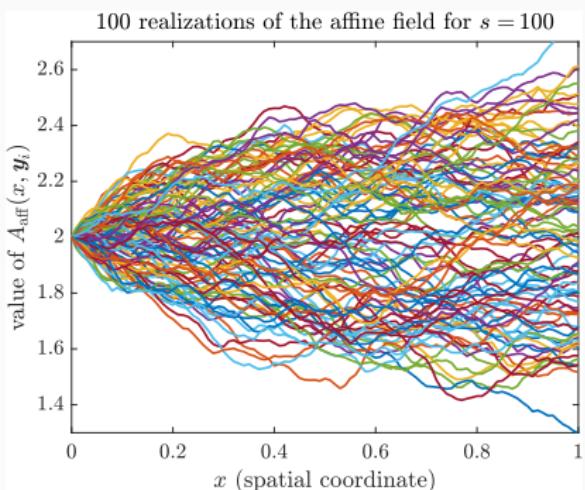
with the special choice  $\Theta(y) = \sin(2\pi y)$ .

- Note that  $Z(\omega) := \sin(2\pi Y(\omega))$  has the probability density  $\frac{1}{\pi} \frac{1}{\sqrt{1-z^2}}$  on  $[-1, 1]$ , i.e,  $Z \sim \text{Arcsine}(-1, 1)$ .
- We can match the mean and covariance of  $a$  with the “uniform model” by choosing  $\Theta(y) = \frac{1}{\sqrt{6}} \sin(2\pi y)$ .
- Note that the periodicity is only assumed for the *random/uncertain* variable!

# Affine vs. periodic

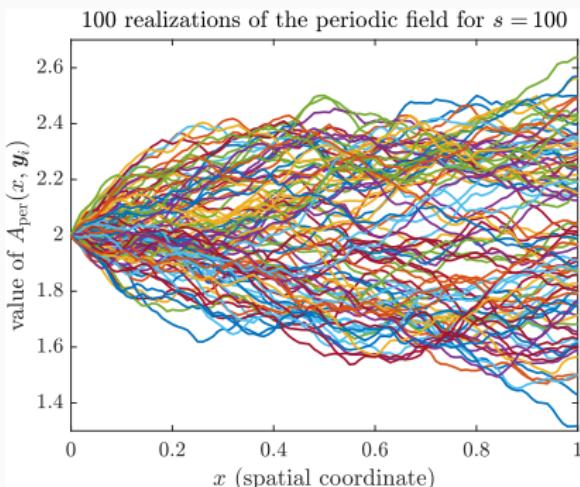
Affine

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



Periodic

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



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

Let  $U := [-1/2, 1/2]^{\mathbb{N}}$  and  $D \subset \mathbb{R}^d$ ,  $d \in \{1, 2, 3\}$ , a nonempty bounded Lipschitz domain. For the parametric PDE

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

with  $u(\cdot, \mathbf{y}) \in H_0^1(D)$ ,  $f \in H^{-1}(D)$ , and

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

with assumptions

- $0 < a_{\min} \leq a(\mathbf{x}, \mathbf{y}) \leq a_{\max} < \infty$  for all  $\mathbf{x} \in D, \mathbf{y} \in U$
- $\sum_{j=1}^{\infty} \|\psi_j\|_{L^\infty}^p < \infty$  for some  $p \in (0, 1)$
- $\|\psi_1\|_{L^\infty} \geq \|\psi_2\|_{L^\infty} \geq \dots$

[K–Kuo–Sloan 2020] showed that there exists a constructible lattice rule satisfying the QMC cubature error

$|I_s(G(u)) - Q_{n,s}(G(u))| \leq Cn^{-1/p}$  with constant  $C > 0$  independent of  $s$ ,  
for any linear quantity of interest  $G: H_0^1(D) \rightarrow \mathbb{R}$ .

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

Let us consider the PDE problem

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

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

$$a_{\text{per}}(\mathbf{x}, \mathbf{y}) = 2 + \sum_{j=1}^{100} \sin(2\pi y_j) \psi_j(x), \quad y_j \in [-\frac{1}{2}, \frac{1}{2}],$$

where  $\psi_j(\mathbf{x}) = \frac{c}{\sqrt{6}} j^{-\theta} \sin(j\pi x_1) \sin(j\pi x_2)$ . **Note that**  $\|\psi_j\|_{L^\infty} \propto j^{-\theta}$ .

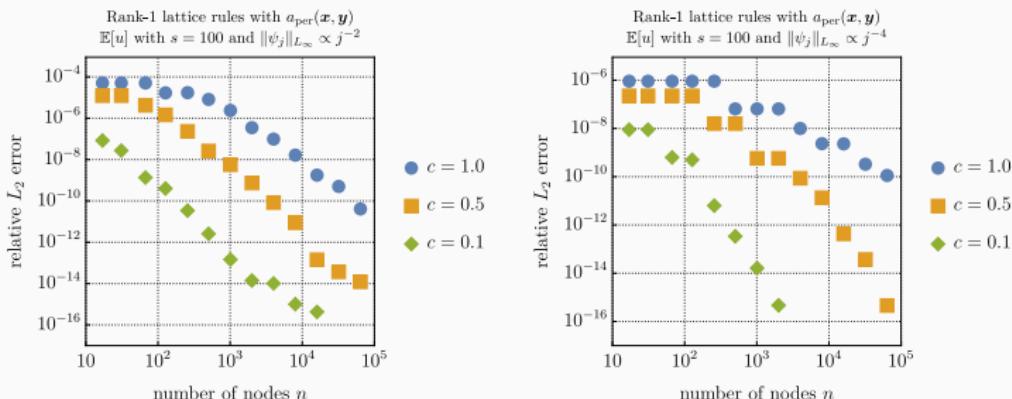


Figure 7: Left:  $\theta = 2$ . Right:  $\theta = 4$ .

## **Part III: Kernel interpolation over lattice point sets**

---

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

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

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

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

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

where

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

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*. In particular,

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

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

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

then

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

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

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

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

$$\mathbf{Kc} = \mathbf{f},$$

where  $\mathbf{c} := [c_1, \dots, c_n]^\top$  are the coefficients in (1) and

$$K_{k,\ell} = K(\mathbf{t}_k, \mathbf{t}_\ell) \quad \text{and} \quad \mathbf{f} := [f(\mathbf{t}_1), \dots, f(\mathbf{t}_n)]^\top.$$

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

$$\mathbf{c} = \text{ifft}(\text{fft}(\mathbf{f}) ./ \text{fft}(\mathbf{K}_{:,1}))$$

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

**The kernel interpolant is cheap to construct!**

In analogy to the cubature setting, the PDE problem

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

with  $u(\cdot, \mathbf{y}) \in H_0^1(D)$ ,  $f \in H^{-1}(D)$ , and

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

and assumptions

- $0 < a_{\min} \leq a(\mathbf{x}, \mathbf{y}) \leq a_{\max} < \infty$  for all  $\mathbf{x} \in D, \mathbf{y} \in U$
- $\sum_{j=1}^{\infty} \|\psi_j\|_{L^\infty}^p < \infty$  for some  $p \in (0, 1)$
- $\|\psi_1\|_{L^\infty} \geq \|\psi_2\|_{L^\infty} \geq \dots$

[K–Kazashi–Kuo–Nobile–Sloan 2022] showed that there exists a sequence of SPOD weights (entering both the expression of the kernel  $K$  in the interpolant and as inputs to a CBC algorithm) and a constructible lattice rule satisfying the kernel approximation error

$$\|u - u_n\|_{L^2(U \times D)} = \mathcal{O}(n^{-\frac{1}{2p} + \frac{1}{4}}) \quad \text{with constant } C > 0 \text{ independent of } s.$$

# Kernel approximation for PDE: $L^2$ error

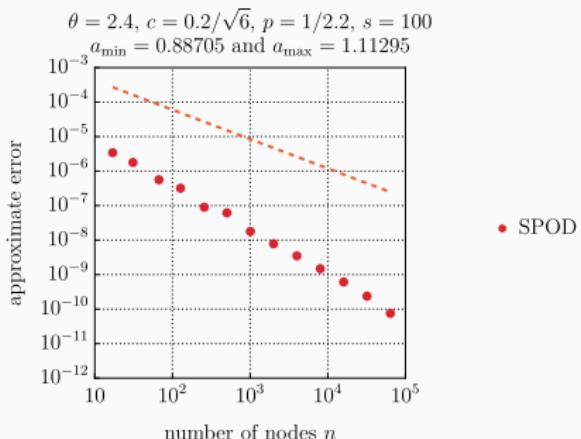
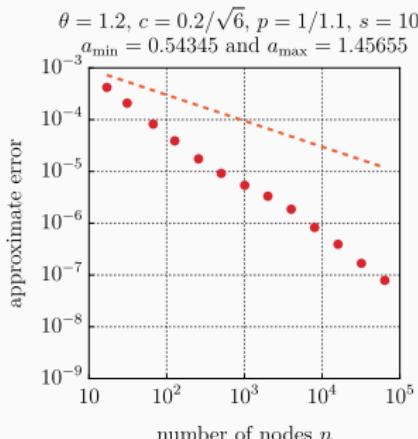
Let us consider the PDE problem

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

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

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

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



## Reducing the computational complexity

The SPOD weights used in the construction of the kernel interpolant were

$$\gamma_u := \sum_{m_u \in \{1:\alpha\}^{|u|}} (|m_u|!)^{\frac{2}{1+\lambda}} \prod_{j \in u} \left( \frac{b_j^{m_j} S(\alpha, m_j)}{\sqrt{2e^{1/e} \zeta(2\alpha\lambda)}} \right)^{\frac{2}{1+\lambda}}. \quad (2)$$

- the cost to obtain the generating vector  $\mathbf{z}$  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 (see Ian's talk on Friday):** leave out the order-dependent part  $(|m_u|!)^{\frac{2}{1+\lambda}}$  in (2), get

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

These are *product weights* ("serendipitous weights"), where

- the cost to obtain the generating vector  $\mathbf{z}$  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)

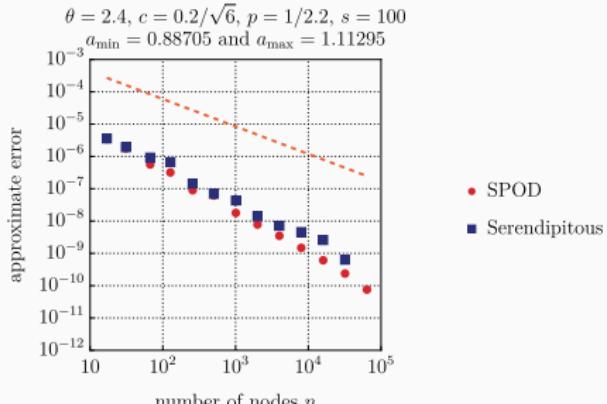
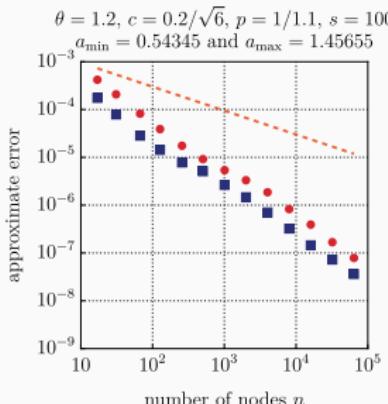
Let us consider the PDE problem

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

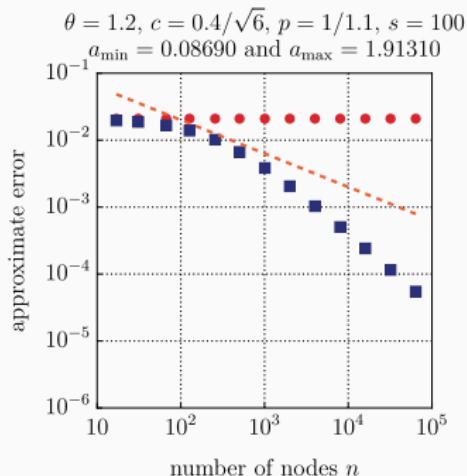
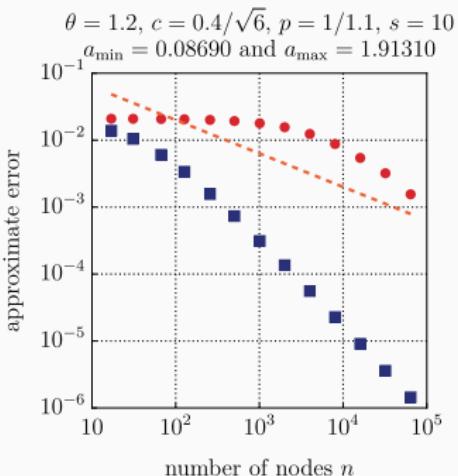
in the physical domain  $D = (0, 1)^2$  with the diffusion coefficient

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

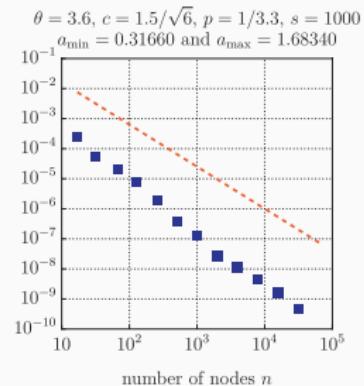
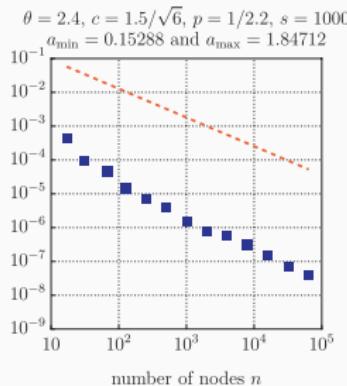
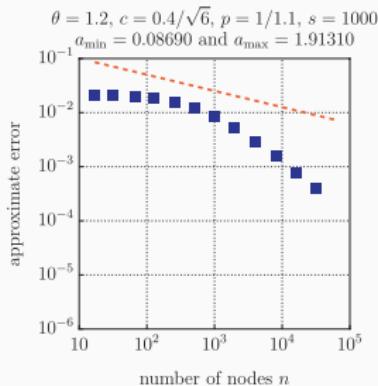
where  $\psi_j(\mathbf{x}) = c j^{-\theta} \sin(j\pi x_1) \sin(j\pi x_2)$ . **Note that**  $\|\psi_j\|_{L^\infty} \propto j^{-\theta}$ .



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



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



## **Part IV: Application to an inverse problem**

---

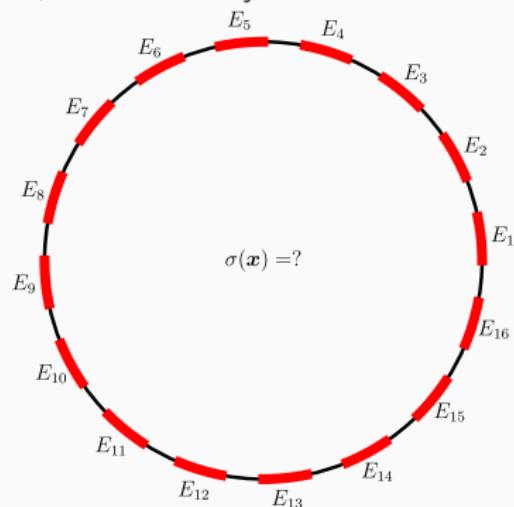
## The complete electrode model

Let  $D := \{\mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| \leq 1\}$ . Let  $\{E_k\}_{k=1}^L \subseteq \partial D$  be an array of  $L := 16$  equidistantly spaced non-overlapping electrodes of width 0.2 on the boundary  $\partial D$ . Fix the current feed  $\mathbf{I} \in \mathbb{R}_+^L$  and let  $\sigma \in L_+^\infty(D)$ . The *forward problem* is to find the electromagnetic potential  $u \in H^1(D)$  as well as  $\mathbf{U} \in \mathbb{R}^L$ , the potentials on the electrodes, which satisfy

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

with  $\mathbf{n}$  denoting the outer normal.

Moreover, we take  $z_k = 1 \ \forall k$ .



The forward problem is solved numerically using EIDORS software (FEM).

Fix the current pattern  $\mathbf{I}_k := \mathbf{e}_1 - \mathbf{e}_{k+1} \in \mathbb{R}_\diamond^L$ ,  $k \in \{1, \dots, L-1\}$ .

**Kernel-based surrogate for the forward problem:** Let us parameterize the conductivity as

$$\sigma(\mathbf{x}, \mathbf{y}) := 1 + \frac{1}{\sqrt{6}} \sum_{k=1}^s \sin(2\pi y_k) \psi_k(\mathbf{x}), \quad \mathbf{x} \in D, \quad \mathbf{y} \in [0, 1]^s,$$

where  $\psi_k(\mathbf{x}) := \frac{1}{(i_k^2 + j_k^2)^\vartheta} \sin(\pi i_k \frac{x_1+1}{2}) \sin(\pi j_k \frac{x_2+1}{2})$ ,  $\vartheta = 1.2$ , the sequence  $(i_k, j_k)_{k \geq 1}$  is an ordering of the elements of  $\mathbb{N} \times \mathbb{N}$  s.t.  $\|\psi_k\|_{L^\infty} = \mathcal{O}(k^{-\vartheta})$  by Weyl's asymptotics. We set  $s = 30$ .

Denote by  $\mathcal{U}(\mathbf{y}) := \text{vec}([\mathbf{U}_1, \dots, \mathbf{U}_{L-1}]) \in \mathbb{R}^{L(L-1)}$  the (flattened) voltage matrix, comprised of the electrode potential measurements corresponding to the current pattern  $\mathbf{I}_1, \dots, \mathbf{I}_{L-1}$  and  $\mathbf{y} \in [0, 1]^s$ .

We construct the (vector-valued) QMC–kernel interpolant

$\mathcal{U}_n(\mathbf{y}) := \sum_{k=1}^n \mathbf{c}_k K(\mathbf{t}_k, \mathbf{y}) \in \mathbb{R}^{L(L-1)}$  (using **serendipitous weights**) for the mapping  $G: \mathbf{y} \mapsto \mathcal{U}(\mathbf{y})$  based on  $n = 1\,024\,207$  QMC nodes satisfying  $G(\mathbf{t}_k) = \mathcal{U}_n(\mathbf{t}_k) \forall k$ .

## Experiment setup

We have constructed the QMC–kernel interpolant  $\mathcal{U}_n(\mathbf{y})$  offline based on the periodically parameterized model for  $\sigma(\mathbf{x}, \mathbf{y})$ . For the numerical experiments, we

- fix some target conductivity  $\sigma_{\text{target}}$  and numerically compute the “exact” electrode potential measurements  
 $\mathbf{U}_{\text{exact}} := \text{vec}([\mathbf{U}_{\text{exact}}^1, \dots, \mathbf{U}_{\text{exact}}^{L-1}]) \in \mathbb{R}^{L(L-1)}$ . To avoid the inverse crime, we do not use the same FE mesh that was used to build the surrogate; instead we use a finer FE mesh.
- we contaminate the electrode potential measurements with noise

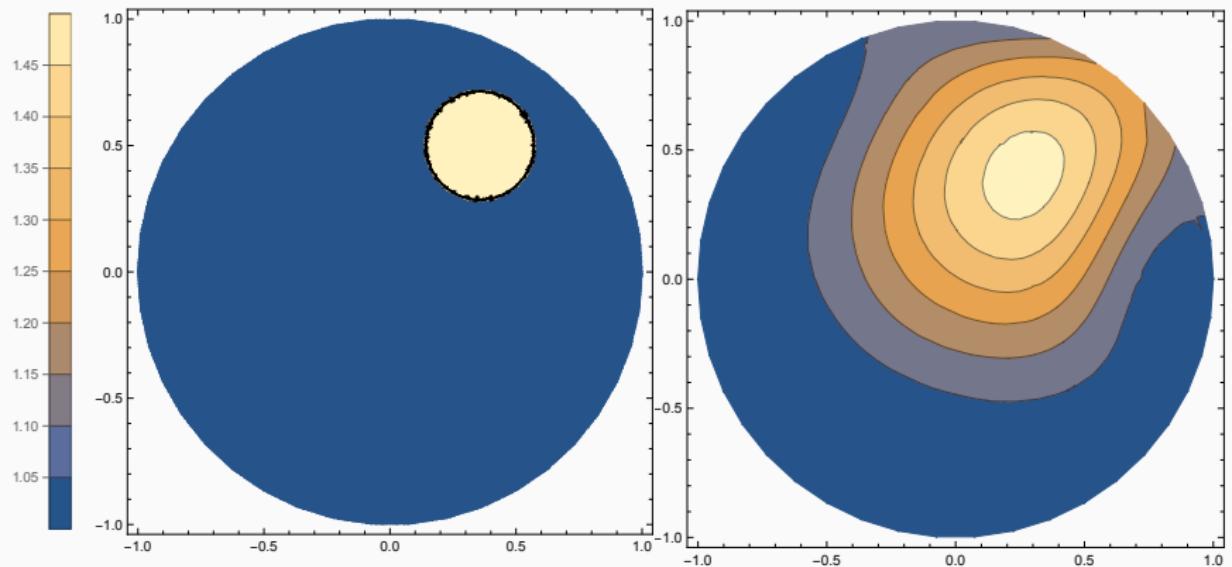
$$\mathbf{U}_{\text{noisy}} = \mathbf{U}_{\text{exact}} + \boldsymbol{\eta}, \quad \boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \tau^2 I),$$

where  $\tau := 10^{-3} \max_{j,k=1,\dots,L(L-1)} |(U_{\text{exact}})_j - (U_{\text{exact}})_k|$ .

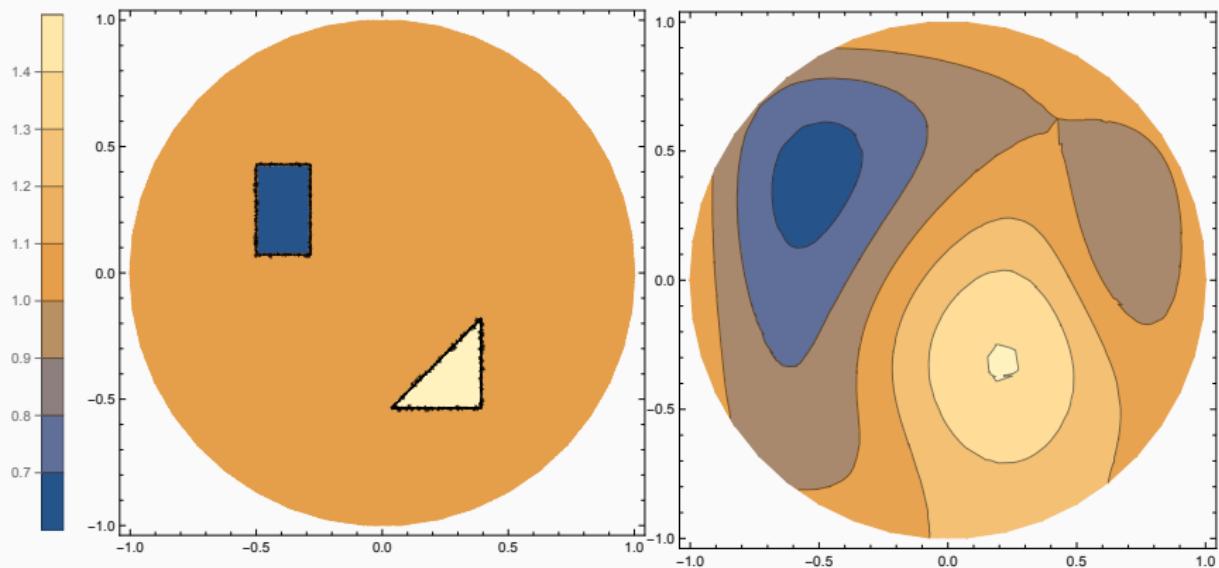
Our reconstruction is  $\sigma(\mathbf{x}, \mathbf{y}^*)$ , where

$$\mathbf{y}^* := \arg \min_{\mathbf{y} \in [0,1]^s} \{ \| \mathbf{U}_{\text{noisy}} - \mathcal{U}_n(\mathbf{y}) \|^2 \}.$$

The minimization is carried out using `lsqnonlin` in MATLAB with the levenberg–marquardt algorithm.



**Figure 10:** Left: target conductivity. Right: reconstructed conductivity.



**Figure 11:** Left: target conductivity. Right: reconstructed conductivity.

## 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.)
- Using product weights, practical for challenging high-dimensional problems (e.g., as surrogates for Bayesian inversion).
- For EIT, the kernel interpolation scheme could be useful for efficient recovery of other uncertainties (domain shape, electrode positions, contact resistances, etc.).

## References

-  K., F. Y. Kuo, and I. H. Sloan. Uncertainty quantification using periodic random variables. *SIAM J. Numer Anal.* **58**(2):1068–1091, 2020.
-  K., Y. Kazashi, F. Y. Kuo, F. Nobile, and I. H. Sloan. Fast approximation by periodic kernel-based lattice-point interpolation with application in uncertainty quantification. *Numer. Math.* **150**:33–77, 2022.
-  K., F. Y. Kuo, and I. H. Sloan. Lattice-based kernel approximation and serendipitous weights for parametric PDEs in very high dimensions. Preprint arXiv:2303.17755, 2023.