

Doubling the rate in high-dimensional function approximation with application to numerical integration

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Part I: Kernel interpolation over lattice point sets



K–Kazashi–Kuo–Nobile–Sloan (2022): Fast approximation by periodic kernel-based lattice-point interpolation with application in uncertainty quantification. *Numer. Math.* **150**:33–77.



K–Kuo–Sloan (2024): Lattice-based kernel approximation and serendipitous weights for parametric PDEs in very high dimensions. To appear in *Monte Carlo and Quasi-Monte Carlo Methods 2022*. Preprint arXiv:2303.17755 [math.NA].

Part II: Doubling the rate for high-dimensional function approximation



Sloan–K (2023+): Doubling the rate – improved error bounds for orthogonal projection in Hilbert spaces. Preprint 2023, arXiv:2308.06052 [math.NA].

Part III: Application to numerical integration?

- K–Klebanov–Schillings (ongoing work)

Kernel interpolation over lattice point sets

Lattice rules

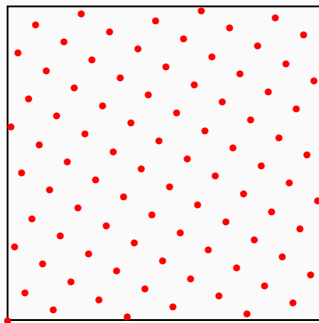
Rank-1 lattice rules

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

have the nodes

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

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 $[0, 1]^2$

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

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

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

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

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

The space $H_{s,\alpha,\gamma}$ is actually a *reproducing kernel Hilbert space* (RKHS), with an explicitly known and analytically simple reproducing kernel:

$$K(\mathbf{y}, \mathbf{y}') = \sum_{\mathbf{u} \subseteq \{1, \dots, s\}} \gamma_{\mathbf{u}} \prod_{j \in \mathbf{u}} \eta_{\alpha}(y_j, y'_j), \quad \mathbf{y}, \mathbf{y}' \in [0, 1]^s,$$

where

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

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

$$\langle f, K(\cdot, \mathbf{y}) \rangle_{H_{s,\alpha,\gamma}} = f(\mathbf{y}) \quad \text{for all } f \in H_{s,\alpha,\gamma}, \quad \mathbf{y} \in [0, 1]^s.$$

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

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

then the kernel has a computationally attractive form

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

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

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

where the coefficients are determined by requiring the interpolation condition $f_n(\mathbf{t}_k) = f(\mathbf{t}_k)$ to hold for all $k = 1, \dots, n$. Equivalently, the coefficients can be solved from the linear system

$$\mathcal{K}\mathbf{c} = \mathbf{f},$$

where $\mathbf{c} := [c_1, \dots, c_n]^T$,

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

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

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

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

The kernel interpolant is cheap to construct!

Proposition (K–Kazashi–Kuo–Nobile–Sloan (2022))

A generating vector $\mathbf{z} \in \{1, \dots, n-1\}^s$ can be constructed by a CBC algorithm such that

$$\|f - f_n\|_{L^2([0,1]^s)} \leq \frac{\tau}{n^{1/(4\lambda)}} \left(\sum_{\mathbf{u} \subseteq \{1, \dots, s\}} \max\{1, |\mathbf{u}|\} \gamma_{\mathbf{u}}^\lambda (2\zeta(\alpha\lambda))^{|\mathbf{u}|} \right)^{1/\lambda} \|f\|_{H_{s,\alpha,\gamma}}$$

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

Remark: Generalized for composite n by Kuo–Mo–Nuyens (2022+).

Numerical experiment

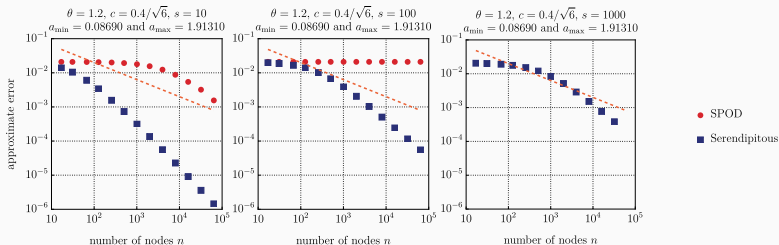
Let us consider the PDE problem

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

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

$$a(\mathbf{x}, \mathbf{y}) = 1 + \sum_{j=1}^s \sin(2\pi y_j) \psi_j(\mathbf{x}), \quad \mathbf{x} \in D, \quad y_j \in [0, 1],$$

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



SPOD: Kernel interpolation using weights derived in [K–Kazashi–Kuo–Nobile–Sloan (2022)].

Serendip.: Kernel interpolation using product weights advocated in [K–Kuo–Sloan (2024)]. 8

Doubling the rate for high-dimensional function approximation

Let $U \subseteq \mathbb{R}^s$ be a nonempty domain such that

- H is a Hilbert space continuously embedded in $L^2(U)$.
- B is a “smoother” normed space continuously embedded in H .

Critical assumption:

$$|\langle f, g \rangle_H| \leq \|f\|_{L^2(U)} \|g\|_B \quad \text{for all } f \in H, g \in B.$$

Theorem (Sloan–K 2023+)

Let P_n be the H -orthogonal projection operator onto a finite-dimensional space $V \subset H$, $n := \dim(V)$. Assume that for some $C, \kappa > 0$, there holds

$$\|f - P_n f\|_{L^2(U)} \leq C n^{-\kappa} \|f\|_H \quad \text{for all } f \in H.$$

Then for all $g \in B$, we have

$$\|g - P_n g\|_{L^2(U)} \leq C^2 n^{-2\kappa} \|g\|_B$$

and

$$\|g - P_n g\|_H \leq C n^{-\kappa} \|g\|_B.$$

Proof. Let $g \in B$.

Since $f = g - P_n g \in H$ and $P_n(g - P_n g) = P_n g - P_n g = 0$, we obtain

$$\begin{aligned} \|g - P_n g\|_{L^2(U)} &= \|(g - P_n g) - P_n(g - P_n g)\|_{L^2(U)} \leq Cn^{-\kappa} \|g - P_n g\|_H \\ \Rightarrow \|g - P_n g\|_{L^2(U)}^2 &\leq C^2 n^{-2\kappa} \|g - P_n g\|_H^2. \end{aligned} \quad (1)$$

Now

$$\begin{aligned} \|g - P_n g\|_H^2 &= \langle g - P_n g, g - P_n g \rangle_H \stackrel{g - P_n g \perp P_n g}{=} \langle g - P_n g, g \rangle_H \\ &\leq \|g - P_n g\|_{L^2(U)} \|g\|_B. \end{aligned} \quad (2)$$

Plugging this into (1) yields

$$\begin{aligned} \|g - P_n g\|_{L^2(U)}^2 &\leq C^2 n^{-2\kappa} \|g - P_n g\|_{L^2(U)} \|g\|_B \\ \Rightarrow \|g - P_n g\|_{L^2(U)} &\leq C^2 n^{-2\kappa} \|g\|_B \end{aligned} \quad (3)$$

as desired.

The inequality $\|g - P_n g\|_H \leq Cn^{-\kappa} \|g\|_B$ follows (in squared form) by plugging (3) into (2). \square

Application to kernel interpolation

For $H = H_{s,\alpha,\gamma}$ and $B = H_{s,2\alpha,\gamma^2}$, there holds

$$|\langle f, g \rangle_{H_{s,\alpha,\gamma}}| \leq \|f\|_{L^2(U)} \|g\|_{H_{s,2\alpha,\gamma^2}}.$$

The kernel interpolant

$$f_n(\mathbf{y}) = \sum_{k=1}^n c_k K(\mathbf{t}_k, \mathbf{y})$$

is precisely the H -orthogonal projection of $f \in H$ onto $V = \text{span}\{K(\mathbf{t}_1, \cdot), \dots, K(\mathbf{t}_n, \cdot)\}$.

\therefore If $f \in B$, then

$$\begin{aligned}\|f - f_n\|_{L^2(U)} &\lesssim n^{-1/(2\lambda)}, \\ \|f - f_n\|_{H_{s,\alpha,\gamma}} &\lesssim n^{-1/(4\lambda)},\end{aligned}$$

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

Application to numerical integration?

- Given a sufficiently smooth function, we are able to obtain twice the approximation rate using our kernel interpolant!
- “Doubling the rate” phenomena known also in the context of numerical integration.
 - E.g., (randomly shifted) rank-1 lattice rules have convergence rate $\mathcal{O}(n^{-1})$ for functions with first-order dominating mixed smoothness, but for a sufficiently smooth integrand we can obtain $\mathcal{O}(n^{-2})$ convergence using *baker’s transform*.
- Can our method be applied to numerical integration?

Idea: Let H be a RKHS over the computational domain $[0, 1]^s$ with kernel K . Let the cubature point set $\mathbf{t}_1, \dots, \mathbf{t}_n \in [0, 1]^s$ be given (e.g., lattice points). We find the weights w_1, \dots, w_n of a cubature rule

$$\sum_{k=1}^n w_k f(\mathbf{t}_k) \approx \int_{[0,1]^s} f(\mathbf{y}) d\mathbf{y}, \quad f \in H,$$

by solving the linear system

$$\begin{cases} w_1 K(\mathbf{t}_1, \mathbf{t}_1) + \dots + w_n K(\mathbf{t}_1, \mathbf{t}_n) = \int_{[0,1]^s} K(\mathbf{t}_1, \mathbf{y}) d\mathbf{y} \\ \vdots \\ w_1 K(\mathbf{t}_n, \mathbf{t}_1) + \dots + w_n K(\mathbf{t}_n, \mathbf{t}_n) = \int_{[0,1]^s} K(\mathbf{t}_n, \mathbf{y}) d\mathbf{y}. \end{cases}$$

Let us focus on the weighted Sobolev space H of **non-periodic** functions $f: [0, 1]^s \rightarrow \mathbb{R}$ with first-order dominating mixed smoothness, with norm

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

and kernel $K(\mathbf{y}, \mathbf{y}') = \sum_{\mathbf{u} \subseteq \{1, \dots, s\}} \gamma_{\mathbf{u}} \prod_{j \in \mathbf{u}} \omega(y_j, y'_j)$, $\mathbf{y}, \mathbf{y}' \in [0, 1]^s$, where $\omega(y, y') = \frac{1}{2} B_2(|y - y'|) + (y - \frac{1}{2})(y' - \frac{1}{2})$, $y, y' \in [0, 1]$.

Essentially, we are “reweighting” an existing cubature rule!

It is not difficult to check that

$$\int_{[0,1]^s} K(\mathbf{x}, \mathbf{y}) \, d\mathbf{y} = 1 \quad \text{for all } \mathbf{x} \in [0, 1]^s.$$

Thus the weights $\mathbf{w} := [w_1, \dots, w_n]^T$ can be obtained from the linear system

$$\mathcal{K} \mathbf{w} = \mathbf{1},$$

where $\mathcal{K} \in \mathbb{R}^{n \times n}$ is defined elementwise by $\mathcal{K}_{i,j} = K(\mathbf{t}_i, \mathbf{t}_j)$.

Unfortunately, in the non-periodic case the system matrix is no longer circulant.

However, the construction of \mathcal{K} is computationally feasible for large dimensions s if the weight structure is suitable.

- For product weights $\gamma_u = \prod_{j \in u} \gamma_j$ (or equal weights), we can use the formula

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

- For POD or SPOD weights, we can assemble the matrix \mathcal{K} using recursion formulae w.r.t. the dimension s (compare with the CBC construction in QMC analysis).

Special case: dimension $s = 1$

For simplicity, let us consider the *unweighted* 1-dimensional case. In this case,

$$\|f\|_H^2 = \left(\int_0^1 f(y) \, dy \right)^2 + \int_0^1 |f'(y)|^2 \, dy$$

with kernel $K(y, y') = 1 + \frac{1}{2} B_2(|y - y'|) + (y - \frac{1}{2})(y' - \frac{1}{2})$.

Let $t_k = \frac{k}{n}$, $k = 0, \dots, n-1$ be the 1d lattice points with $n \geq 2$. (This is precisely a left-Riemann rule.)

We can analytically solve the quadrature weights for our kernel quadrature $Q_n(f) = \sum_{k=0}^{n-1} w_k f(t_k)$ in this case! They are

$$w_0 = \frac{1}{2n} \frac{12n^3}{12n^3 + n + 3},$$

$$w_k = \frac{1}{n} \frac{12n^3}{12n^3 + n + 3}, \quad k \in \{1, \dots, n-2\},$$

$$w_{n-1} = \frac{3}{2n} \frac{12n^3}{12n^3 + n + 3}.$$

Step 1

The quadrature error can be recast as

$$\begin{aligned}\int_0^1 f(y) \, dy - \sum_{k=0}^{n-1} w_k f(t_k) &= \int_0^1 \langle f, K(\cdot, y) \rangle_H \, dy - \sum_{k=0}^{n-1} w_k \langle f, K(\cdot, t_k) \rangle_H \\ &= \left\langle f, \int_0^1 K(\cdot, y) \, dy - \sum_{k=0}^{n-1} w_k K(\cdot, t_k) \right\rangle_H \\ &= \langle f, h - h_n \rangle_H,\end{aligned}$$

where $h := \int_0^1 K(\cdot, y) \, dy = 1$ and $h_n := \sum_{k=0}^{n-1} w_k K(\cdot, t_k)$ is the kernel interpolant of h .

Step 2

Let us assume that $f \in B$, where B is a Sobolev space of functions with dominating mixed smoothness of order 2.

Since

$$\langle f, h - h_n \rangle_H = \left(\int_0^1 f(y) \, dy \right) \left(\int_0^1 (h(y) - h_n(y)) \, dy \right) + \int_0^1 f'(y)(h'(y) - h'_n(y)) \, dy,$$

we can use integration by parts to obtain

$$\begin{aligned} & \int_0^1 f'(y)(h'(y) - h'_n(y)) \, dy \\ &= f'(1) \underbrace{(h(1) - h_n(1))}_{=\frac{6n}{12n^3+n+3}} - f'(0) \underbrace{(h(0) - h_n(0))}_{=0} - \int_0^1 f''(y)(h(y) - h_n(y)) \, dy \\ &\leq \frac{6n}{12n^3 + n + 3} f'(1) + \|f''\|_{L^2(0,1)} \|h - h_n\|_{L^2(0,1)}. \end{aligned}$$

Therefore

$$|\langle f, h - h_n \rangle_H| \leq \underbrace{\frac{6n}{12n^3 + n + 3} f'(1)}_{=O(n^{-2})} + \|h - h_n\|_{L^2(0,1)} (\|f\|_{L^2(0,1)} + \|f''\|_{L^2(0,1)}).$$

It remains to assess the convergence rate of $\|h - h_n\|_{L^2(0,1)}$.

Step 3

Making use of the identities

$$\sum_{k=0}^{n-1} w_k = \frac{24n^2}{12n^3 + n + 3} + \frac{12n^2(n-2)}{12n^3 + n + 3},$$

$$\begin{aligned} \sum_{k=0}^{n-1} \sum_{\ell=0}^{n-1} w_k w_\ell \left(\frac{46}{45} - \frac{1}{6} t_k^2 + \frac{1}{12} t_k^3 - \frac{1}{24} t_k^4 + \frac{1}{4} t_k^2 t_\ell - \frac{1}{6} t_\ell^2 \right. \\ \left. + \frac{1}{4} t_k t_\ell^2 - \frac{1}{4} t_k^2 t_\ell^2 + \frac{1}{12} t_\ell^3 - \frac{1}{24} t_\ell^4 + \frac{1}{12} |t_k - t_\ell|^3 \right) = \frac{720n^6 + n^2 + 60n - 45}{5(12n^3 + n + 3)^2}, \end{aligned}$$

where the latter identity is valid for $n \geq 2$, we obtain

$$\begin{aligned} \|h - h_n\|_{L^2(0,1)}^2 &= \int_0^1 \left(1 - \sum_{k=0}^{n-1} w_k K(x, t_k) \right)^2 dx \\ &= \int_0^1 \left(1 - 2 \sum_{k=0}^{n-1} w_k K(x, t_k) + \sum_{k=0}^{n-1} \sum_{\ell=0}^{n-1} w_k w_\ell K(x, t_k) K(x, t_\ell) \right) dx \\ &= 1 - 2 \sum_{k=0}^{n-1} w_k + \sum_{k=0}^{n-1} \sum_{\ell=0}^{n-1} w_k w_\ell \left(\frac{46}{45} - \frac{1}{6} t_k^2 + \frac{1}{12} t_k^3 - \frac{1}{24} t_k^4 + \frac{1}{4} t_k^2 t_\ell - \frac{1}{6} t_\ell^2 \right. \\ &\quad \left. + \frac{1}{4} t_k t_\ell^2 - \frac{1}{4} t_k^2 t_\ell^2 + \frac{1}{12} t_\ell^3 - \frac{1}{24} t_\ell^4 + \frac{1}{12} |t_k - t_\ell|^3 \right) = \dots = \frac{6n(n+15)}{5(12n^3 + n + 3)^2} \end{aligned}$$

for $n \geq 2$.

$\therefore \|h - h_n\|_{L^2(0,1)} = \mathcal{O}(n^{-2})$ as desired.

Generalization to higher dimensions?

- It seems difficult to generalize the 1d argument to higher dimensions.
- Not clear if the result even holds for general $s > 1$ (does the “compatibility condition” $|\langle f, g \rangle_H| \leq \|f\|_{L^2} \|g\|_B$ hold, how to control $\sum_{k=1}^n w_k$, etc.?)
- Nevertheless, it is easy to implement the method numerically even in high dimensions.

$$\int_{[0,1]^s} \frac{1}{1 + \sum_{j=1}^s j^{-2} y_j} d\mathbf{y}$$

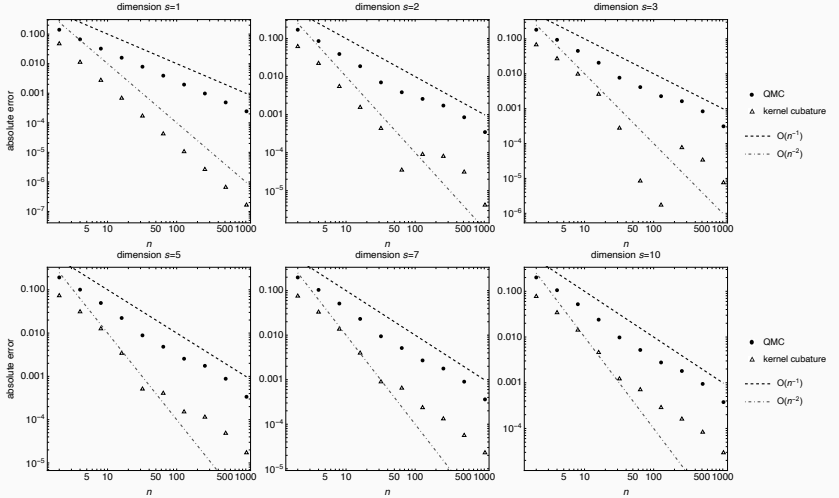


Figure 1: QMC vs. kernel cubature constructed using the weights

$$\gamma_u = (|u|! \prod_{j \in u} \frac{b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^\lambda}})^{\frac{2}{1+\lambda}}, \quad \lambda = \frac{1}{2-2\delta}, \quad \delta = 0.05, \quad \text{for all } u \subseteq \{1, \dots, s\}.$$

Let us consider the PDE problem

$$-\nabla \cdot (a(\mathbf{x}, \mathbf{y}) \nabla u(\mathbf{x}, \mathbf{y})) = x_1, \quad u(\cdot, \mathbf{y})|_{\partial D} = 0,$$

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

$$a(\mathbf{x}, \mathbf{y}) = 1 + \sum_{j=1}^s y_j \psi_j(\mathbf{x}), \quad \mathbf{x} \in D, \quad y_j \in [-\frac{1}{2}, \frac{1}{2}],$$

where $\psi_j(\mathbf{x}) = 0.1j^{-2} \sin(j\pi x_1) \sin(j\pi x_2)$. We compute $\mathbb{E}[G(u)]$ using both QMC and “reweighted” QMC, where $G(v) = \int_D v(\mathbf{x}) d\mathbf{x}$.

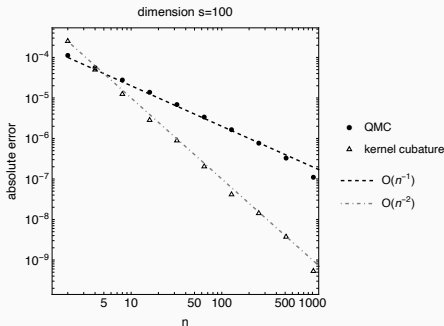


Figure 2: QMC vs. kernel cubature with $s = 100$ constructed using the weights

$$\gamma_u = (|u|! \prod_{j \in u} \frac{b_j}{\sqrt{2\zeta(2\lambda)/(2\pi^2)^\lambda}})^{\frac{2}{1+\lambda}}, \quad \lambda = \frac{1}{2-2\delta}, \quad \delta = 0.05, \quad \text{for all } u \subseteq \{1, \dots, s\}.$$

Conclusions

- Doubling the rate for kernel approximation.
- Preliminary work commenced to explore a similar phenomenon in numerical integration (1d case OK, but higher dimensions unclear).



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Thank you for your attention!