Uncertainty Quantification and Quasi-Monte Carlo

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Today's lecture follows the survey article

J. Dick, F. Y. Kuo, and I. H. Sloan. High-dimensional integration: The quasi-Monte Carlo way. *Acta Numer.* **22**:133–288, 2013. https://doi.org/10.1017/S0962492913000044

Notations

- $\{1:s\} := \{1, 2, \ldots, s\}$ for $s \in \mathbb{N}$. We use fraktur letters to denote subsets $\mathfrak{u} \subseteq \{1:s\}$. We use $|\mathfrak{u}|$ to denote the cardinality of set $\mathfrak{u}$.
- For $x \geq 0$, we define the fractional part $\{x\} := x - \lfloor x \rfloor = \mathrm{mod}(x, 1)$. For $x < 0$, $\{x\} := x + \lfloor |x| \rfloor$. For $\boldsymbol{x} \in \mathbb{R}^s$, we define

$$\{\boldsymbol{x}\} := (\{x_1\}, \{x_2\}, \ldots, \{x_s\}).$$

  For example, $\{(1.2, 0.5, 2.77)\} = (0.2, 0.5, 0.77)$.
- For $\mathfrak{u} \subseteq \{1:s\}$, we define $\boldsymbol{x}_\mathfrak{u} = (x_j)_{j \in \mathfrak{u}}$ and

$$\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_\mathfrak{u}} f(\boldsymbol{x}) := \prod_{j \in \mathfrak{u}} \frac{\partial}{\partial x_j} f(\boldsymbol{x}).$$

  For example, with $\mathfrak{u} = \{1, 2, 4\}$, we have $|\mathfrak{u}| = 3$, $\boldsymbol{x}_\mathfrak{u} = (x_1, x_2, x_4)$, and

$$\frac{\partial^{|\mathfrak{u}|}}{\partial \boldsymbol{x}_\mathfrak{u}} f(\boldsymbol{x}) = \frac{\partial^3}{\partial x_1 \partial x_2 \partial x_4} f(\boldsymbol{x}).$$

Quasi-Monte Carlo methods

Let $f \in C([0,1]^s)$. We consider the problem of approximating the high-dimensional integral

$$I_s f = \int_{[0,1]^s} f(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}.$$

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

$$Q_{n,s} f = \frac{1}{n} \sum_{i=0}^{n-1} f(\boldsymbol{t}_i),$$

where $(\boldsymbol{t}_i)_{i=0}^{n-1}$ is an ensemble of *deterministic* nodes in $[0,1]^s$ (**not** a random sample of $\mathcal{U}([0,1]^s)$).

QMC methods exploit the smoothness and anisotropy of an integrand in order to achieve better-than-Monte Carlo cubature convergence rates.

Rank-1 lattice rules

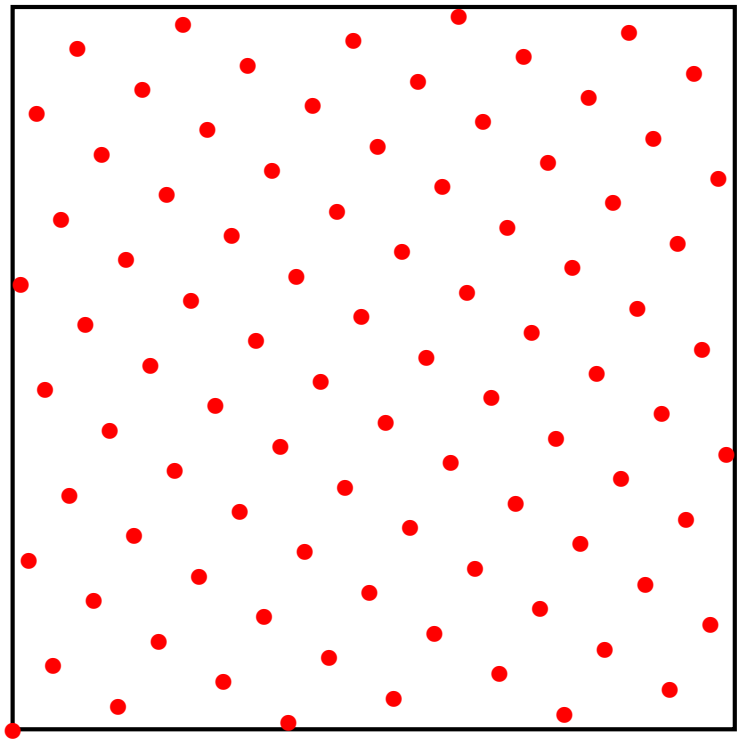
Rank-1 lattice rules

$$Q_{n,s} f = \frac{1}{n} \sum_{i=0}^{n-1} f(\boldsymbol{t}_i)$$

have the points

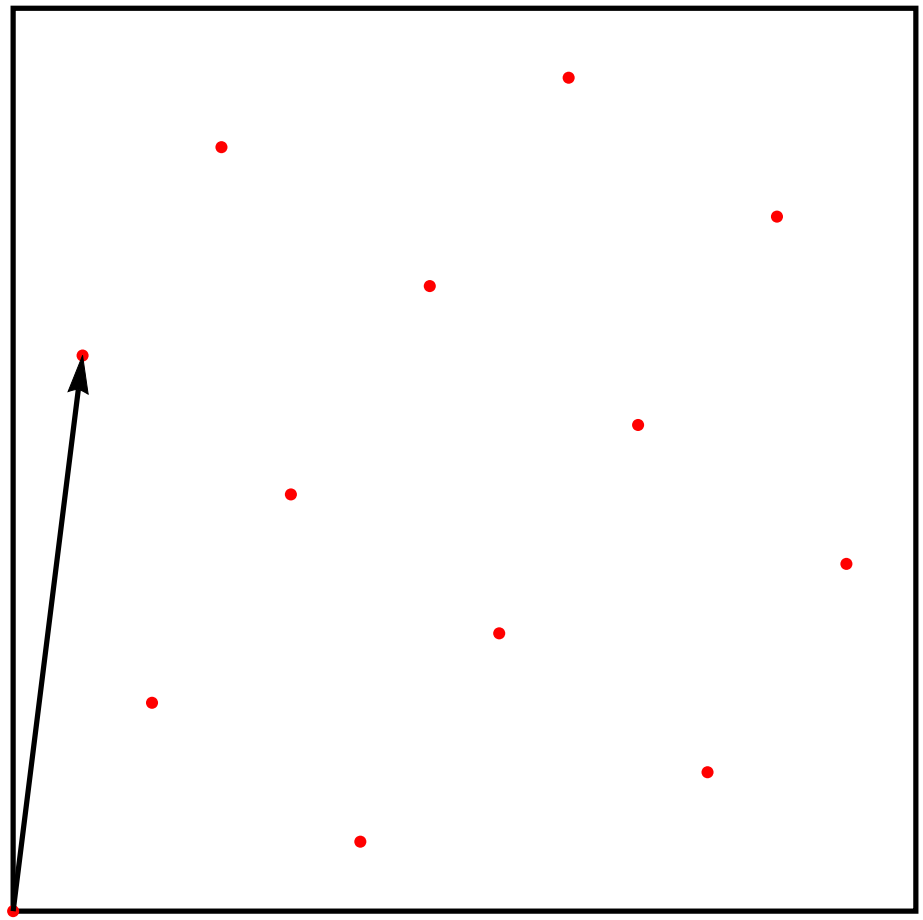
$$\boldsymbol{t}_i = \mathrm{mod}\left(\frac{i\boldsymbol{z}}{n}, 1\right), \quad i \in \{0, \ldots, n-1\},$$

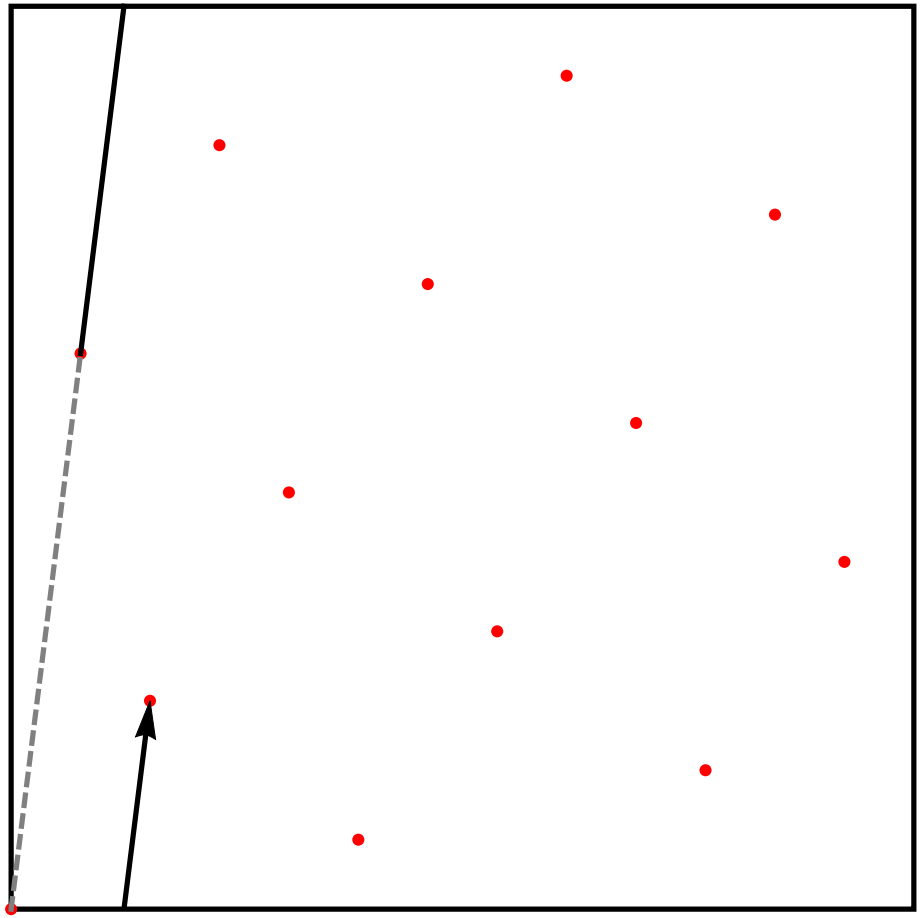
where the entire point set is determined by the *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$, with all components *coprime* to n.

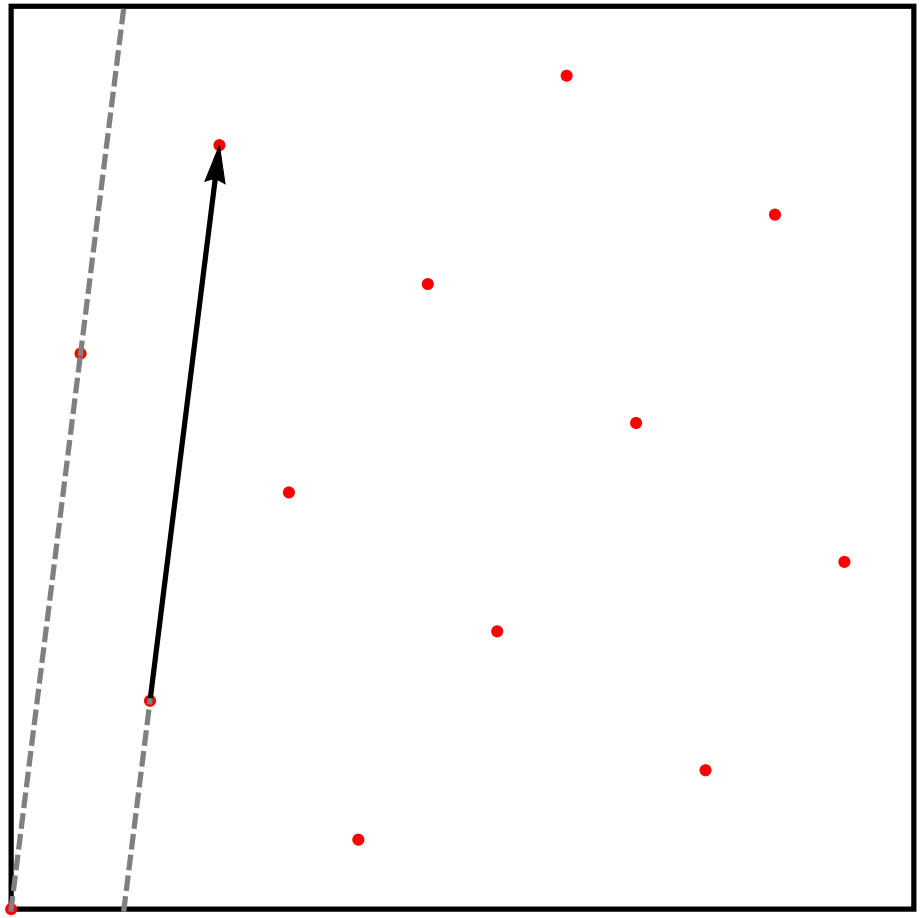


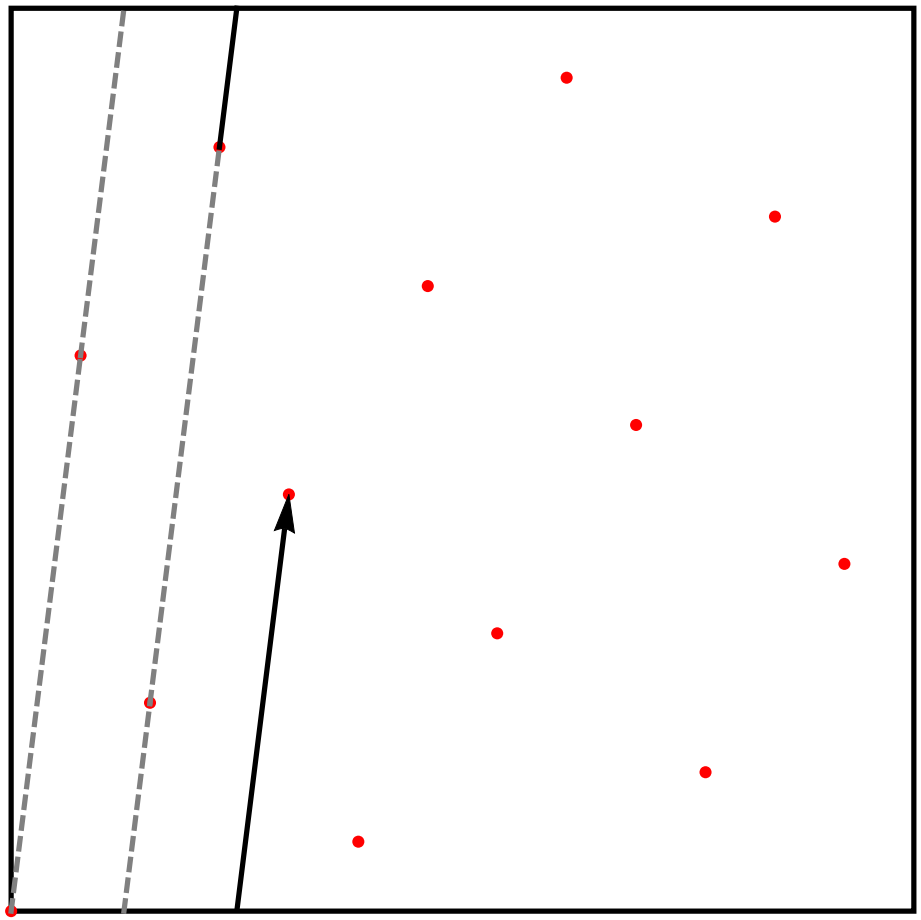
Lattice rule with $\boldsymbol{z} = (1, 55)$ and $n = 89$ nodes in $[0, 1]^2$

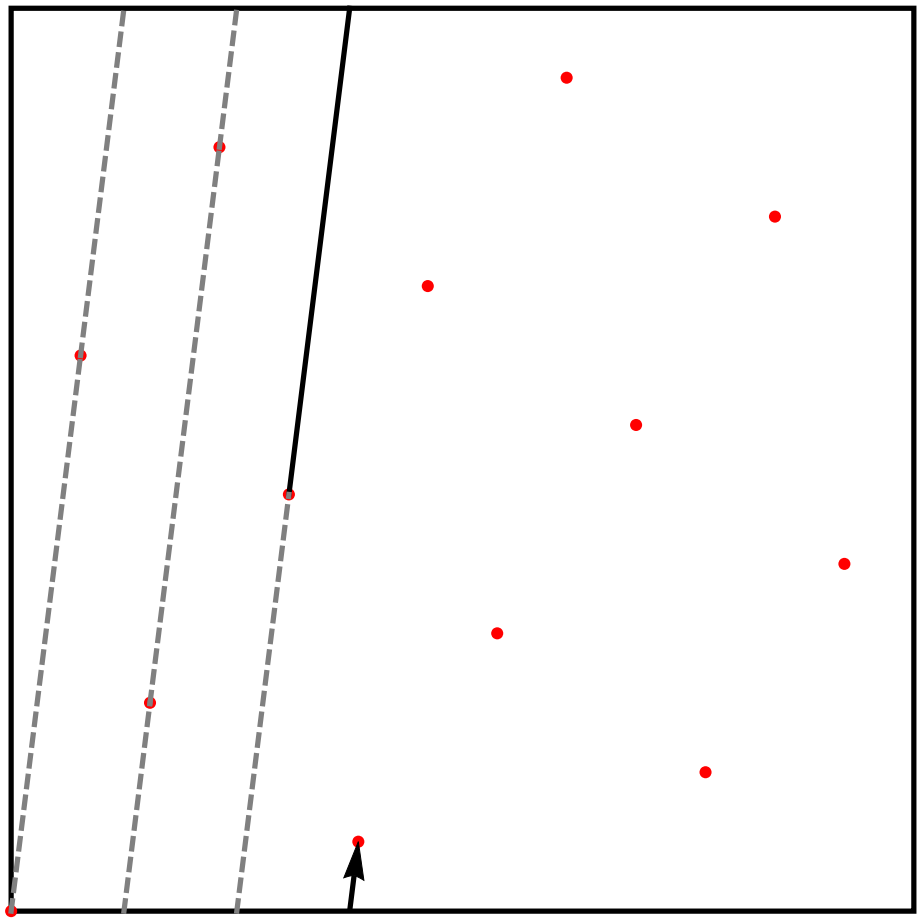
The quality of the lattice rule is determined by the generating vector

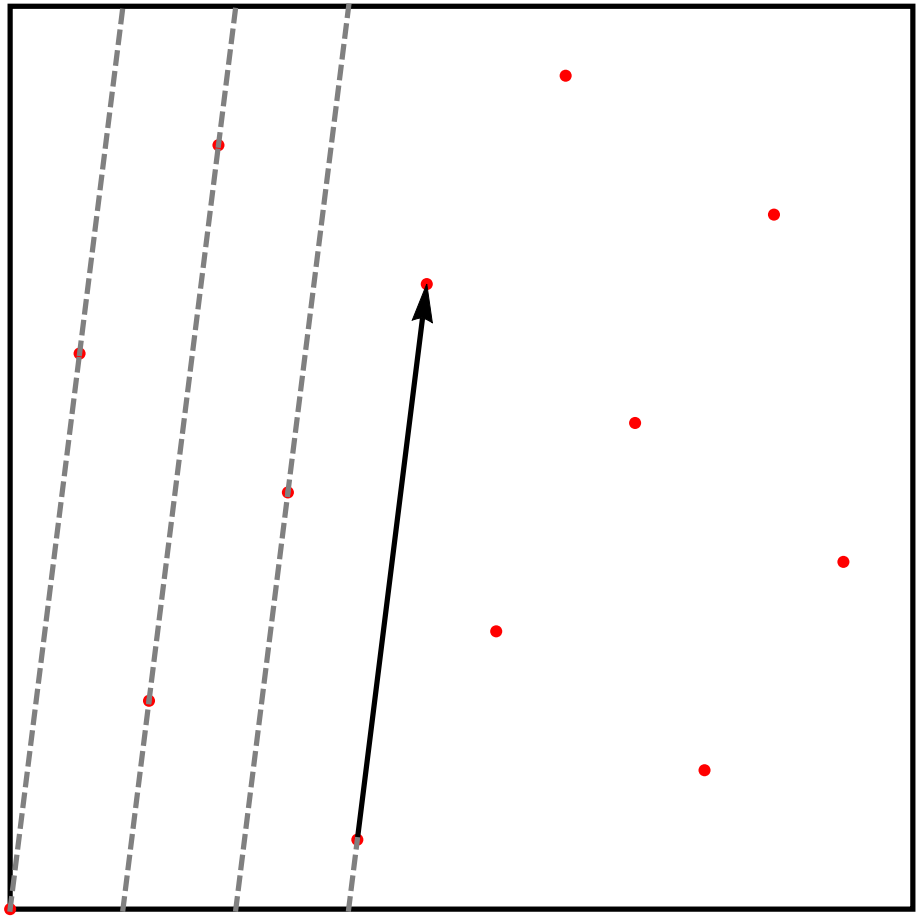


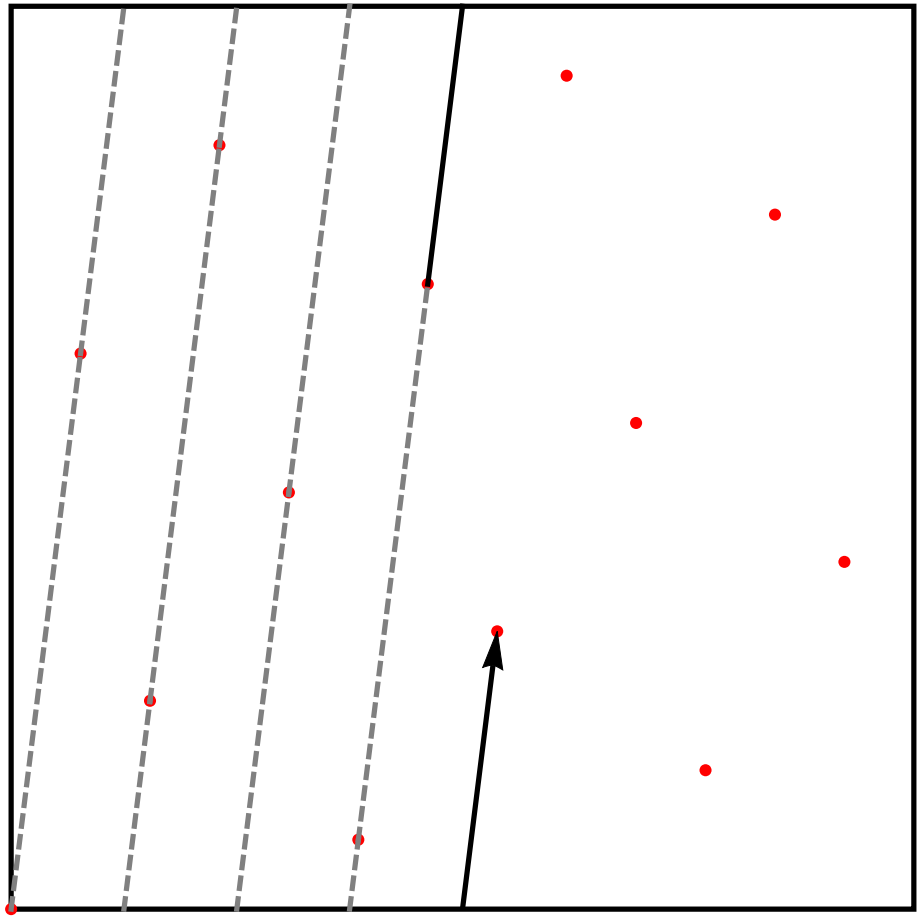


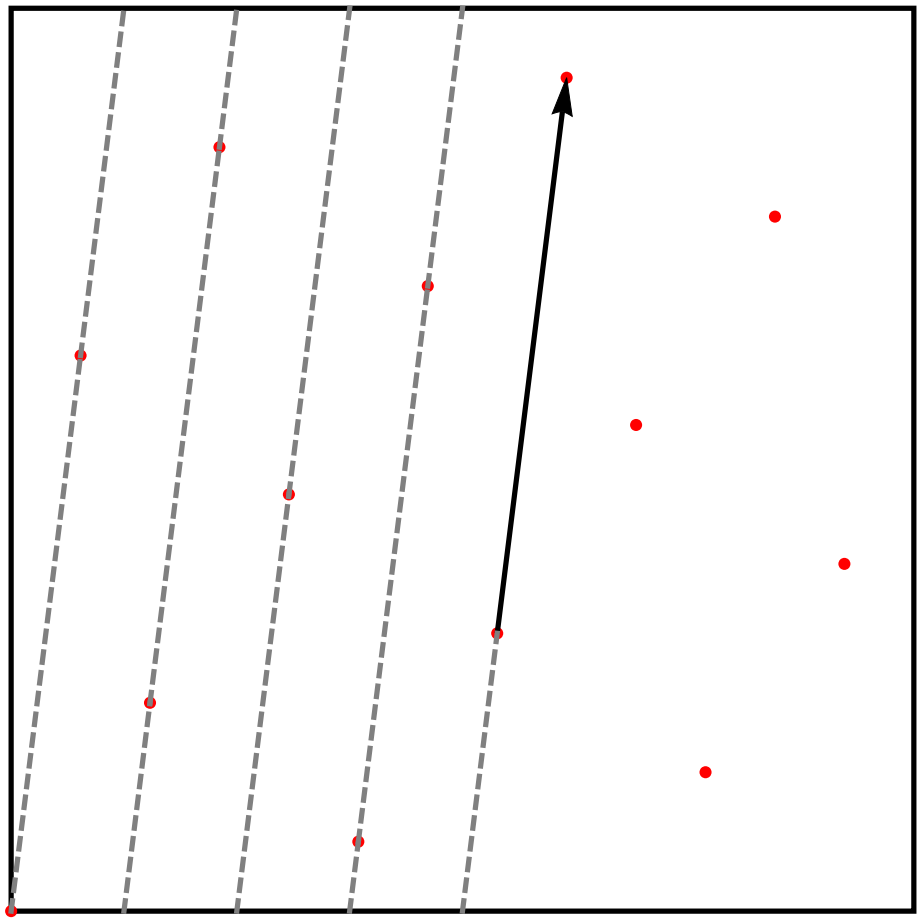


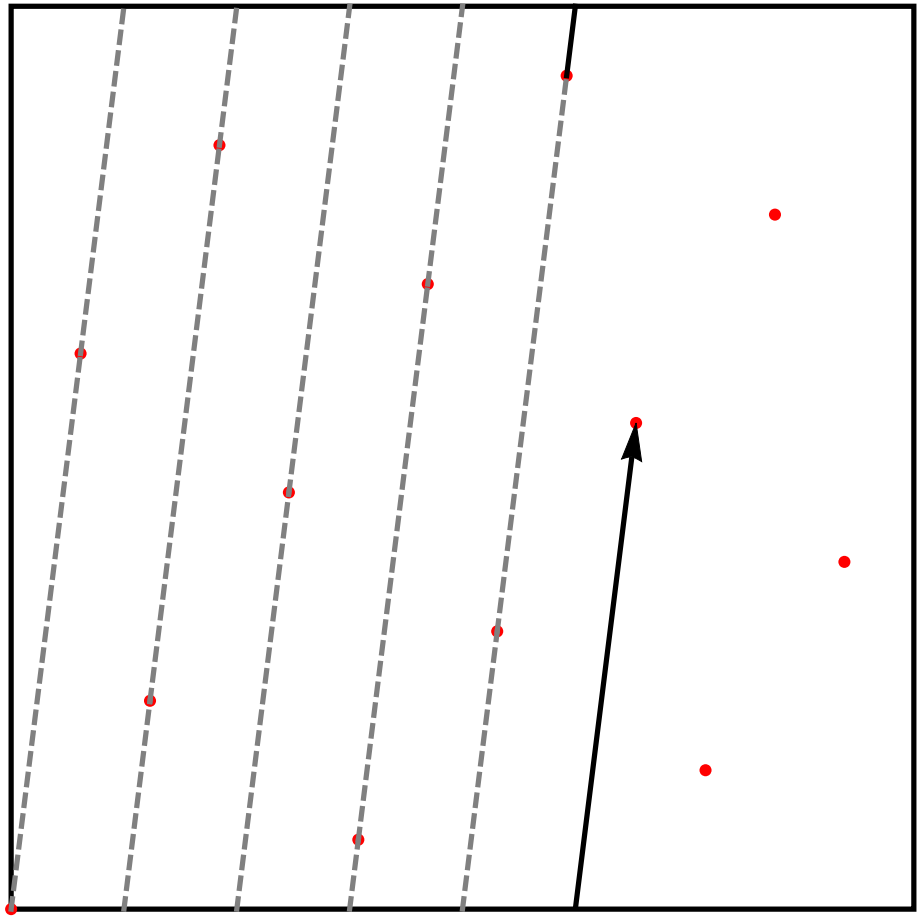


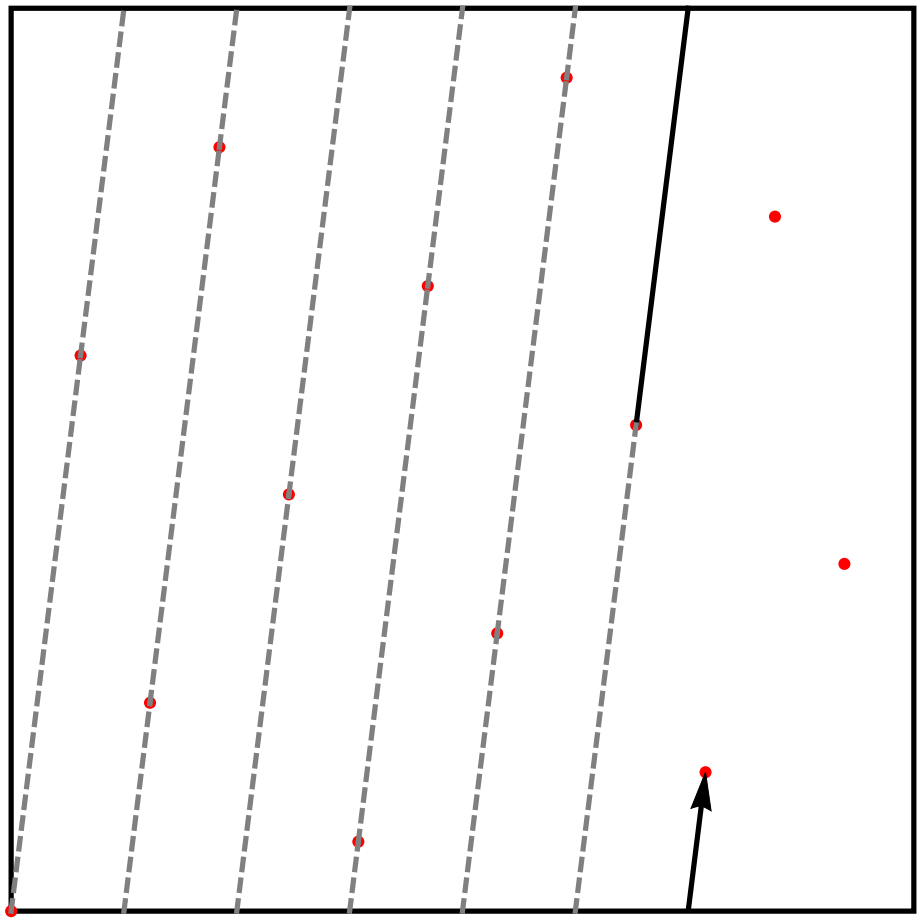


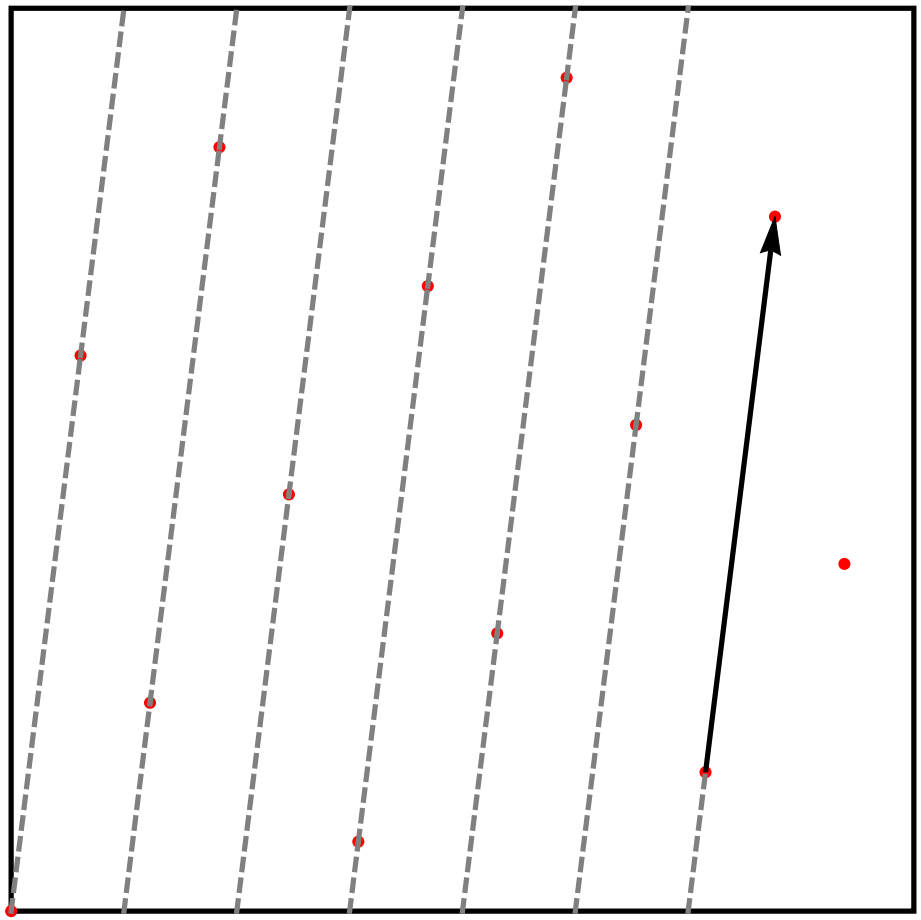


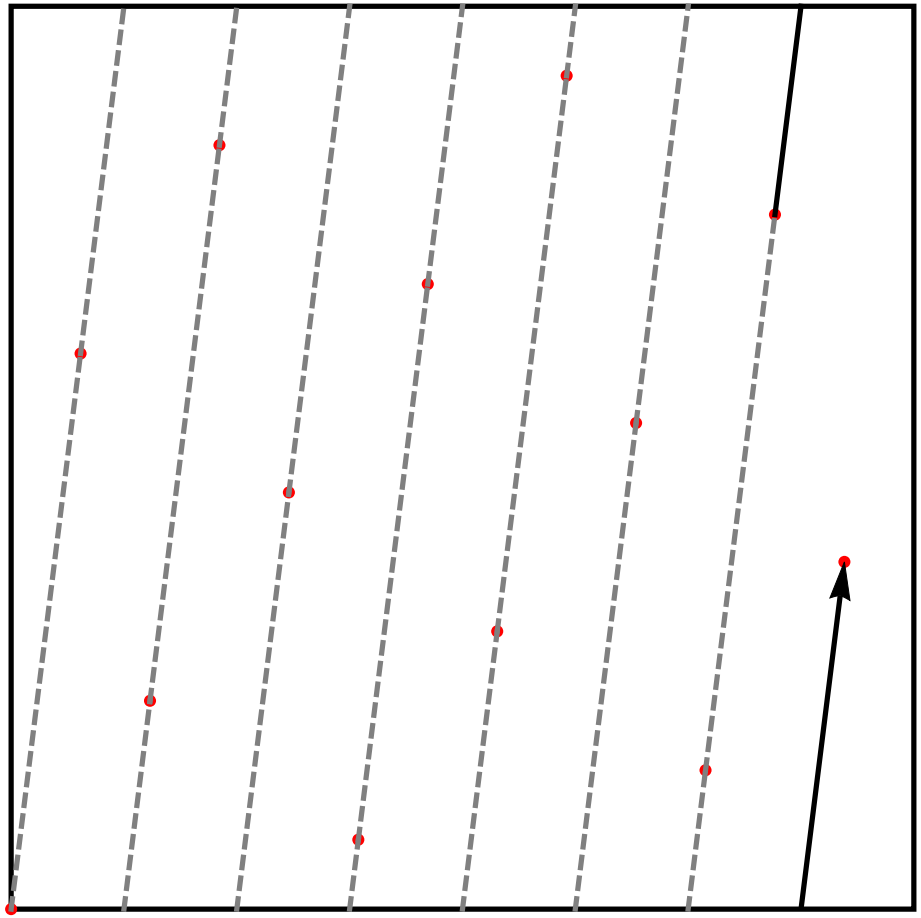












Historical remarks on the development of lattice rules

- Number theorists (Korobov, Zaremba, Hua) in the 1950s and 60s.
- Lattice rules for multiple integration (Sloan and Kachoyan 1987; Sloan and Joe 1994).
- Weighted spaces (Sloan and Woźniakowski 1998; Hickernell 1996).
- Component-by-component (CBC) construction of lattice rules (Kuo, Joe, Sloan 2002).
- Fast CBC algorithm (Cools and Nuyens 2006; Kuo, Cools, and Nuyens 2006).
- Uncertainty quantification of PDEs using QMC methods (Kuo, Schwab, Sloan 2012).

and of course many, many others! (Dick, Giles, Goda, Graham, Kritzer, Niederreiter, Pillichshammer, Wasilkowski, ...)

Brief introduction to the classical theory of lattice rules

Let $f : [0,1]^s \to \mathbb{R}$ be an absolutely continuous and 1-periodic function, i.e.,

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

with an *absolutely convergent Fourier series*

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h} \in \mathbb{Z}^s} \widehat{f}(\boldsymbol{h}) \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h} \cdot \boldsymbol{x}}, \quad \widehat{f}(\boldsymbol{h}) := \int_{[0,1]^s} f(\boldsymbol{x}) \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{h} \cdot \boldsymbol{x}} \, \mathrm{d}\boldsymbol{x}.$$

Then the lattice rule error is precisely the sum of the integrand's Fourier coefficients over the so-called *dual lattice*.

Theorem (Rank-1 lattice rule error)

Under the aforementioned conditions on $f : [0,1]^s \to \mathbb{R}$, there holds

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

where the dual lattice

$$\Lambda^\perp := \{\boldsymbol{h} \in \mathbb{Z}^s \mid \boldsymbol{h} \cdot \boldsymbol{z} \equiv 0 \pmod{n}\}$$

is determined entirely by the generating vector $\boldsymbol{z} \in \mathbb{N}^s$ and $n \in \mathbb{N}$.

For future convenience, let us prove a couple of helpful auxiliary identities.

Lemma

Let $\boldsymbol{h} = (h_1, \ldots, h_s) \in \mathbb{Z}^s$ and $n \in \mathbb{N}$. Then

$$\int_{[0,1]^s} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{x}} \,\mathrm{d}\boldsymbol{x} = \begin{cases} 1 & \text{if } \boldsymbol{h} = \boldsymbol{0} \\ 0 & \text{otherwise} \end{cases}$$

$$\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n} = \begin{cases} 1 & \text{if } \boldsymbol{h}\cdot\boldsymbol{z} \equiv 0 \pmod{n} \\ 0 & \text{otherwise.} \end{cases}$$

Proof. By Fubini's theorem

$$\int_{[0,1]^s} \mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{x}} \,\mathrm{d}\boldsymbol{x} = \prod_{j=1}^{s} \int_0^1 \mathrm{e}^{2\pi \mathrm{i} h_j x_j} \,\mathrm{d}x_j, \tag{1}$$

where

$$\int_0^1 \mathrm{e}^{2\pi \mathrm{i} h_j x_j} \,\mathrm{d}x_j = \begin{cases} \int_0^1 \mathrm{d}x_j & \text{if } h_j = 0 \\ \left[\frac{\mathrm{e}^{2\pi \mathrm{i} h_j x_j}}{2\pi \mathrm{i} h_j}\right]_{x_j=0}^{x_j=1} & \text{if } h_j \neq 0 \end{cases} = \begin{cases} 1 & \text{if } h_j = 0 \\ 0 & \text{if } h_j \neq 0. \end{cases}$$

Thus the expression (1) is zero unless $h_1 = h_2 = \cdots = h_s = 0$.

To prove the second claim

$$\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n} = \begin{cases} 1 & \text{if } \boldsymbol{h}\cdot\boldsymbol{z} \equiv 0 \pmod{n} \\ 0 & \text{otherwise} \end{cases}$$

consider two cases:

- If $\boldsymbol{h}\cdot\boldsymbol{z}$ is a multiple of n, i.e., $\boldsymbol{h}\cdot\boldsymbol{z} \equiv 0 \pmod{n}$, then clearly

$$\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n} = \frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{0} = 1.$$

- If $\boldsymbol{h}\cdot\boldsymbol{z}$ is not a multiple of n, then by the geometric sum formula

$$\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi \mathrm{i} k \boldsymbol{h}\cdot\boldsymbol{z}/n} = \frac{1}{n}\sum_{k=0}^{n-1} \left(\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{z}/n}\right)^{k} = \frac{1}{n}\frac{1-\left(\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{z}/n}\right)^{n}}{1-\mathrm{e}^{2\pi \mathrm{i} \boldsymbol{h}\cdot\boldsymbol{z}/n}} = 0.$$

This yields the assertion. □

Proof (Rank-1 lattice rule error). Using the Fourier series representation

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{h}\in\mathbb{Z}^s} \widehat{f}(\boldsymbol{h})\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\cdot\boldsymbol{x}}, \quad \widehat{f}(\boldsymbol{h}) := \int_{[0,1]^s} f(\boldsymbol{x})\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{h}\cdot\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x},$$

and noting that $\mathrm{e}^{2\pi\mathrm{i}\left\{\frac{k\boldsymbol{z}}{n}\right\}\cdot\boldsymbol{h}} = \mathrm{e}^{2\pi\mathrm{i}k\boldsymbol{z}\cdot\boldsymbol{h}/n}$, we can change the order of the series (note that the Fourier series is absolutely convergent!) to obtain

$$\begin{aligned}
Q_{n,s}(f) - I_s(f) &= \frac{1}{n}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\boldsymbol{z}}{n}\right\}\right) - \int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
&= \frac{1}{n}\sum_{k=0}^{n-1}\sum_{\boldsymbol{h}\in\mathbb{Z}^s} \widehat{f}(\boldsymbol{h})\mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\cdot\boldsymbol{x}/n} - \widehat{f}(\boldsymbol{0}) \\
&= \sum_{\boldsymbol{h}\in\mathbb{Z}^s} \widehat{f}(\boldsymbol{h}) \underbrace{\frac{1}{n}\sum_{k=0}^{n-1} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\cdot\boldsymbol{x}/n}}_{\substack{=1 \text{ if } \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n \\ =0 \text{ otherwise}}} - \widehat{f}(\boldsymbol{0}) \\
&= \sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^s \\ \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n}} \widehat{f}(\boldsymbol{h}) - \widehat{f}(\boldsymbol{0}) = \sum_{\substack{\boldsymbol{h}\in\mathbb{Z}^s\setminus\{\boldsymbol{0}\} \\ \boldsymbol{h}\cdot\boldsymbol{z}\equiv 0 \pmod n}} \widehat{f}(\boldsymbol{h}). \qquad \square
\end{aligned}$$

Ultimately, we are interested in applying lattice rules for *non-periodic*, smooth functions. We will need to put in a bit more effort to make this method work in the non-periodic setting...

Worst-case error and reproducing kernel Hilbert space (RKHS)

Worst-case error

In the classical study of quadrature and cubature rules, we usually consider the so-called *worst-case error*. Suppose that $f \in H$, where H is a Hilbert space continuously embedded in $C([0,1]^s)$. Let $I_s : H \to \mathbb{R}$ be an integral operator

$$I_s f := \int_{[0,1]^s} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$

and let $Q_{n,s} : H \to \mathbb{R}$ be a QMC rule

$$Q_{n,s} f := \frac{1}{n} \sum_{i=0}^{n-1} f(\boldsymbol{t}_i),$$

where $P := \{\boldsymbol{t}_i \in [0,1]^s \mid 0 \le i \le n-1\}$ is a collection of cubature nodes. The worst-case error of cubature rule $Q_{n,s}$ in H is defined by

$$e_{n,s}(P; H) := \sup_{\substack{f \in H \\ \|f\|_H \le 1}} |I_s f - Q_{n,s} f|.$$

Note that this is precisely the operator norm of $\|I_s - Q_{n,s}\|_{H \to \mathbb{R}}$.

Since the worst-case error is just the operator norm of $I_s - Q_{n,s}$, we can express the cubature error as

$$|I_s f - Q_{n,s} f| \leq e_{n,s}(P; H)\|f\|_H.$$

Worst-case errors are in general hard to compute – except for the special case, when H is a *reproducing kernel Hilbert space* (RKHS).

Our strategy will be to *choose* the Hilbert space H (where our integrand f lives) to be such that it is possible to write down the expression for $e_{n,s}(P; H)$ *explicitly* given a family of QMC rules. This allows us to analyze the dependence of the cubature error w.r.t. n and s.

We will end up taking H as an *unanchored, weighted Sobolev space* since this choice turns out to be "compatible" with the family of (randomly shifted) lattice rules!

Reproducing kernel Hilbert space (RKHS)

Let H be a Hilbert space of functions on $D \subseteq \mathbb{R}^s$, with the property that *every point evaluation is a bounded linear functional*. That is, for any $\boldsymbol{y} \in D$, let

$$T_{\boldsymbol{y}}(f) := f(\boldsymbol{y}) \quad \text{for all } f \in H.$$

Then, since $T_{\boldsymbol{y}}$ is a bounded linear functional, by Riesz representation theorem there exists a unique representer $a_{\boldsymbol{y}} := K(\cdot, \boldsymbol{y}) \in H$ such that

$$T_{\boldsymbol{y}}(f) = \langle f, a_{\boldsymbol{y}} \rangle = \langle f, K(\cdot, \boldsymbol{y}) \rangle \quad \text{for all } f \in H.$$

The function $K(\boldsymbol{x}, \boldsymbol{y})$ is known as the *reproducing kernel* of H.

Definition (Reproducing kernel)

A *reproducing kernel* of a Hilbert space H of functions on $D \subseteq \mathbb{R}^s$ is a function $K : D \times D \to \mathbb{R}$ which satisfies

$$K(\cdot, \boldsymbol{y}) \in H \quad \text{for all } \boldsymbol{y} \in D$$
$$\text{and } f(\boldsymbol{y}) = \langle f, K(\cdot, \boldsymbol{y}) \rangle \quad \text{for all } f \in H \text{ and } \boldsymbol{y} \in D.$$

The latter property is known as the *reproducing property*.

Remarks

- A *reproducing kernel Hilbert space* (RKHS) is a Hilbert space equipped with a reproducing kernel, or equivalently, it is a Hilbert space in which *every point evaluation is a bounded linear functional*.
- For any other bounded linear functional $A\colon H \to \mathbb{R}$, its representer $a \in H$ satisfying $A(f) = \langle f, a\rangle$ for all $f \in H$ is given by

$$a(\boldsymbol{y}) = \langle a, K(\cdot, \boldsymbol{y})\rangle = \langle K(\cdot, \boldsymbol{y}), a\rangle = A(K(\cdot, \boldsymbol{y})) \quad \text{for all } \boldsymbol{y} \in D.$$

- Any reproducing kernel $K(\boldsymbol{x}, \boldsymbol{y})$ is symmetric in its arguments:

$$K(\boldsymbol{x}, \boldsymbol{y}) = K(\boldsymbol{y}, \boldsymbol{x}) \quad \text{for all } \boldsymbol{x}, \boldsymbol{y} \in D.$$

Proof. For fixed $\boldsymbol{y} \in D$, apply the reproducing property to the function $f = K(\cdot, \boldsymbol{y})$ to get

$$\begin{aligned} K(\boldsymbol{x}, \boldsymbol{y}) = f(\boldsymbol{x}) &= \langle f, K(\cdot, \boldsymbol{x})\rangle = \langle K(\cdot, \boldsymbol{y}), \langle K(\cdot, \boldsymbol{x})\rangle \\ &= \langle K(\cdot, \boldsymbol{x}), K(\cdot, \boldsymbol{y})\rangle = K(\boldsymbol{y}, \boldsymbol{x}). \quad \square \end{aligned}$$

Example

Suppose that we have a Hilbert space containing continuous functions on $[0,1]$ with square-integrable first order derivatives, equipped with the inner product

$$\langle f, g\rangle = \left(\int_0^1 f(x)\,\mathrm{d}x\right)\left(\int_0^1 g(x)\,\mathrm{d}x\right) + \int_0^1 f'(x)g'(x)\,\mathrm{d}x.$$

Then this space has the *reproducing kernel*

$$K(x,y) = 1 + \eta(x,y),\ \eta(x,y) = \tfrac{1}{2}B_2(|x-y|) + (x-\tfrac{1}{2})(y-\tfrac{1}{2}),$$

where $B_2(x) := x^2 - x + \frac{1}{6}$ denotes the *Bernoulli polynomial of degree 2*.

That is, we claim that

$$\langle f, K(\cdot, y)\rangle = f(y) \quad \text{for all } y \in [0,1].$$

Example (continued)

By observing that

$$\int_0^1 K(x,y)\,\mathrm{d}x = 1 \quad \text{and} \quad \frac{\partial}{\partial x}K(x,y) = x - \frac{1}{2} - \frac{1}{2}\mathrm{sign}(x-y),$$

there holds

$$\langle f, K(\cdot,y)\rangle = \Big(\int_0^1 f(x)\,\mathrm{d}x\Big)\underbrace{\Big(\int_0^1 K(x,y)\,\mathrm{d}x\Big)}_{=1} + \int_0^1 f'(x)\Big(x - \frac{1}{2} - \frac{1}{2}\mathrm{sign}(x-y)\Big)\,\mathrm{d}x$$

$$= \int_0^1 f(x)\,\mathrm{d}x + \int_0^1 f'(x)x\,\mathrm{d}x - \frac{1}{2}\int_0^1 f'(x)\,\mathrm{d}x + \frac{1}{2}\int_0^y f'(x)\,\mathrm{d}x - \frac{1}{2}\int_y^1 f'(x)\,\mathrm{d}x$$

$$= \cancel{\int_0^1 f(x)\,\mathrm{d}x} + \cancel{f(1)} - \cancel{\int_0^1 f(x)\,\mathrm{d}x} - \cancel{\frac{1}{2}f(1)} + \cancel{\frac{1}{2}f(0)} + \frac{1}{2}f(y) - \cancel{\frac{1}{2}f(0)} - \cancel{\frac{1}{2}f(1)} + \frac{1}{2}f(y)$$

$$= f(y)$$

for all $y \in [0,1]$, as desired.

Theorem

Let $H := H_s(K)$ be an RKHS and let $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$ be a reproducing kernel that satisfies

$$\int_{[0,1]^s} \int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} < \infty.$$

Then

$$e^2_{n,s}(P; H_s(K)) = \int_{[0,1]^s} \int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} - \frac{2}{n} \sum_{i=0}^{n-1} \int_{[0,1]^s} K(\boldsymbol{t}_i, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} K(\boldsymbol{t}_i, \boldsymbol{t}_j). \tag{2}$$

Proof. For $f \in H$, we apply the reproducing property $f(\boldsymbol{t}_k) = \langle f, K(\cdot, \boldsymbol{t}_k)\rangle_H$ and average the results to obtain

$$Q_{n,s} f = \frac{1}{n}\sum_{k=0}^{n-1} f(\boldsymbol{t}_k) = \frac{1}{n}\sum_{k=0}^{n-1}\langle f, K(\cdot, \boldsymbol{t}_k)\rangle_H = \left\langle f, \frac{1}{n}\sum_{k=0}^{n-1} K(\cdot, \boldsymbol{t}_k)\right\rangle_H. \quad (3)$$

Similarly, we find that

$$I_s f = \int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{[0,1]^s}\langle f, K(\cdot, \boldsymbol{x})\rangle_H\,\mathrm{d}\boldsymbol{x} = \left\langle f, \int_{[0,1]^s} K(\cdot, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\right\rangle_H, \quad (4)$$

which holds provided that $\int_{[0,1]^s} K(\cdot, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \in H$. However, this is guaranteed by our assumption since

$$\begin{aligned}\left\| \int_{[0,1]^s} K(\cdot, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\right\|_H^2 &= \int_{[0,1]^s}\int_{[0,1]^s}\langle K(\cdot, \boldsymbol{x}), K(\cdot, \boldsymbol{y})\rangle_H\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} \\ &= \int_{[0,1]^s}\int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} < \infty,\end{aligned}$$

which will hold for all the kernels we shall consider.

Taking the difference of (3) and (4) yields

$$I_s f - Q_{n,s} f = \left\langle f, \int_{[0,1]^s} K(\cdot, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{n} \sum_{i=0}^{n-1} K(\cdot, \boldsymbol{t}_i) \right\rangle_H = \langle f, \xi \rangle_H,$$

where

$$\xi(\boldsymbol{y}) := \int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{n} \sum_{i=0}^{n-1} K(\boldsymbol{y}, \boldsymbol{t}_i), \quad \boldsymbol{y} \in [0,1]^s$$

is called the *representer* of the integration error since

$$e_{n,s}(P; H) = \sup_{\|f\| \leq 1} |\langle f, \xi \rangle_H| = \|\xi\|_H.$$

Especially, the supremum is attained by $f = \xi / \|\xi\| \in H$ and we obtain

$$e_{n,s}^2(P; H) = \left\| \int_{[0,1]^s} K(\cdot, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{n} \sum_{i=0}^{n-1} K(\boldsymbol{x}, \boldsymbol{t}_i) \right\|^2$$

$$= \int_{[0,1]^s} \int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} - \frac{2}{n} \sum_{i=0}^{n-1} \int_{[0,1]^s} K(\boldsymbol{x}, \boldsymbol{t}_i) \, \mathrm{d}\boldsymbol{x} + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} K(\boldsymbol{t}_i, \boldsymbol{t}_j),$$

as desired. □

Randomly shifted rank-1 lattice points

In what follows, we will discuss randomly shifted QMC rules.

Consider the rank-1 lattice point set $\boldsymbol{t}_k := \{\frac{k\boldsymbol{z}}{n}\}$ for some generating vector $z \in \mathbb{N}^s$ and fixed $n \in \mathbb{N}$. Given a vector $\boldsymbol{\Delta} \in [0,1]^s$, known as the *shift*, the $\boldsymbol{\Delta}$-shift of the QMC points $\boldsymbol{t}_0, \ldots, \boldsymbol{t}_{n-1}$ is defined as the point set

$$\{\boldsymbol{t}_k + \boldsymbol{\Delta}\}, \quad k = 0, \ldots, n-1.$$

Shifting preserves the lattice structure. In practice, we will generate a number of independent random shifts $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{R-1}$ from $\mathcal{U}([0,1]^s)$ and take the average of $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{R-1}$-shifted QMC rules as our approximation of I_s.

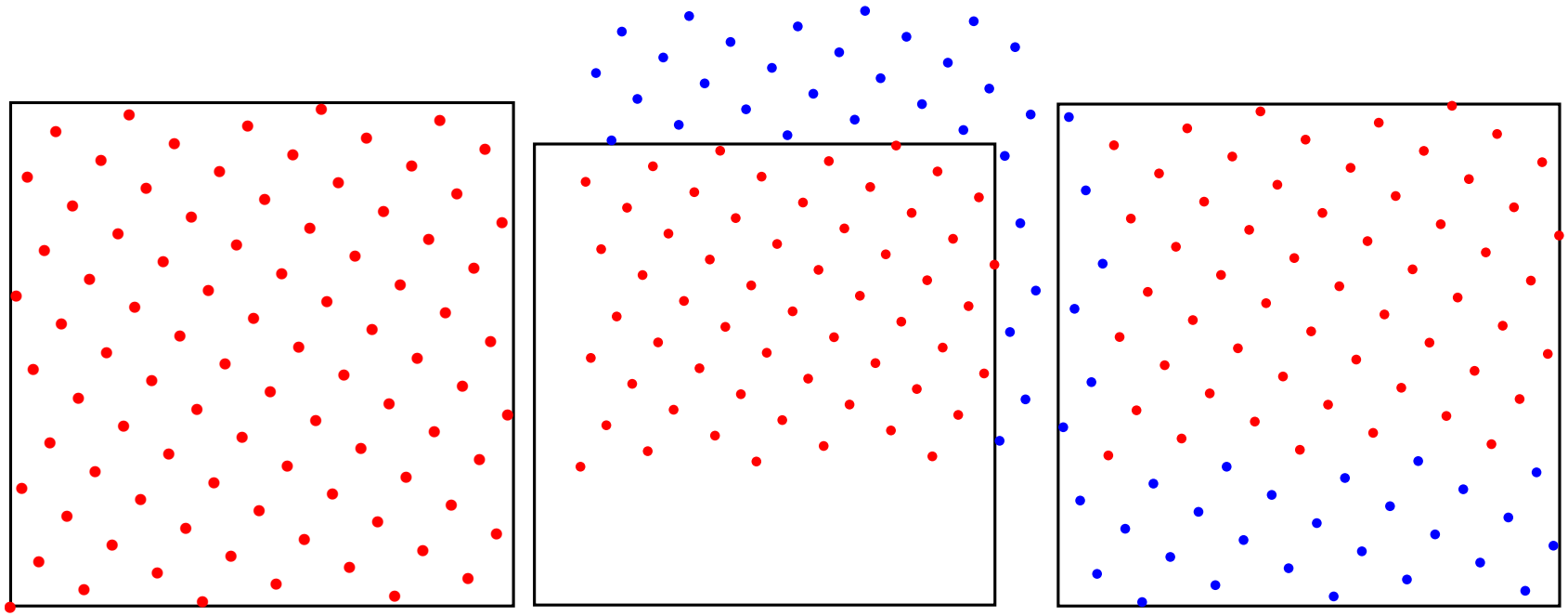
Advantages:

- Leads to a shift-invariant kernel (advantageous for high-dimensional computation).
- Randomization yields an unbiased estimator of the integral.
- Randomization provides a practical error estimate.

Shifted rank-1 lattice rules have points

$$\left\{ \frac{k\boldsymbol{z}}{n} + \boldsymbol{\Delta} \right\}, \quad k = 0, \ldots, n-1.$$

Use a number of random shifts for error estimation.



Lattice rule shifted by $\boldsymbol{\Delta} = (0.1, 0.3)$.

Randomization in practice

- Generate R independent random shifts $\boldsymbol{\Delta}_0, \ldots, \boldsymbol{\Delta}_{R-1}$ from $\mathcal{U}([0,1]^s)$.
- For a given QMC rule with points $(\boldsymbol{t}_i)_{i=0}^{n-1} \subset [0,1]^s$, form the approximations $Q_{n,s}^{(0)} f, \ldots, Q_{n,s}^{(R-1)} f$, where

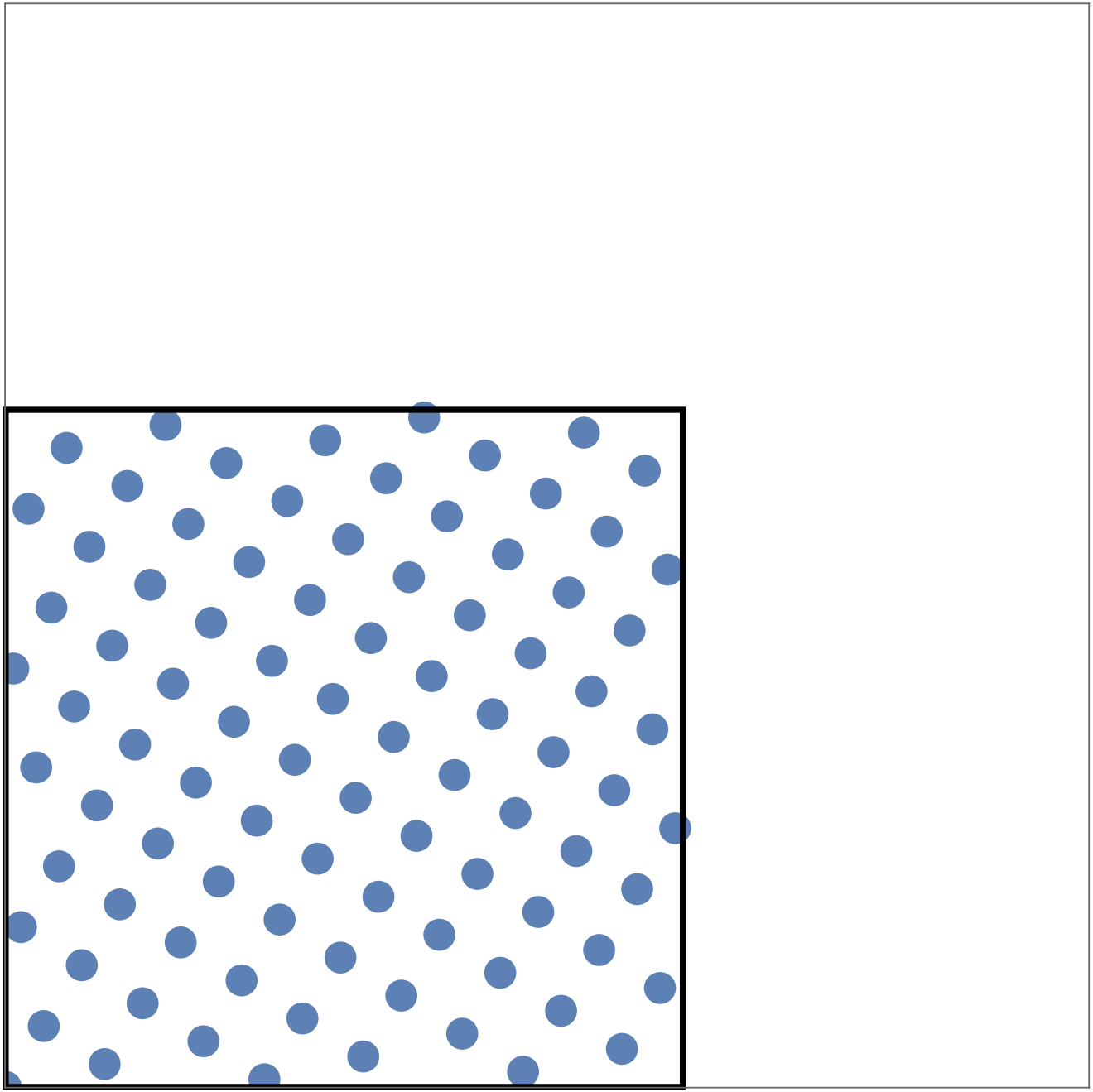
$$Q_{n,s}^{\boldsymbol{\Delta}_r} f = \frac{1}{n} \sum_{i=0}^{n-1} f(\{\boldsymbol{t}_i + \boldsymbol{\Delta}_r\}), \quad r = 0, \ldots, R-1,$$

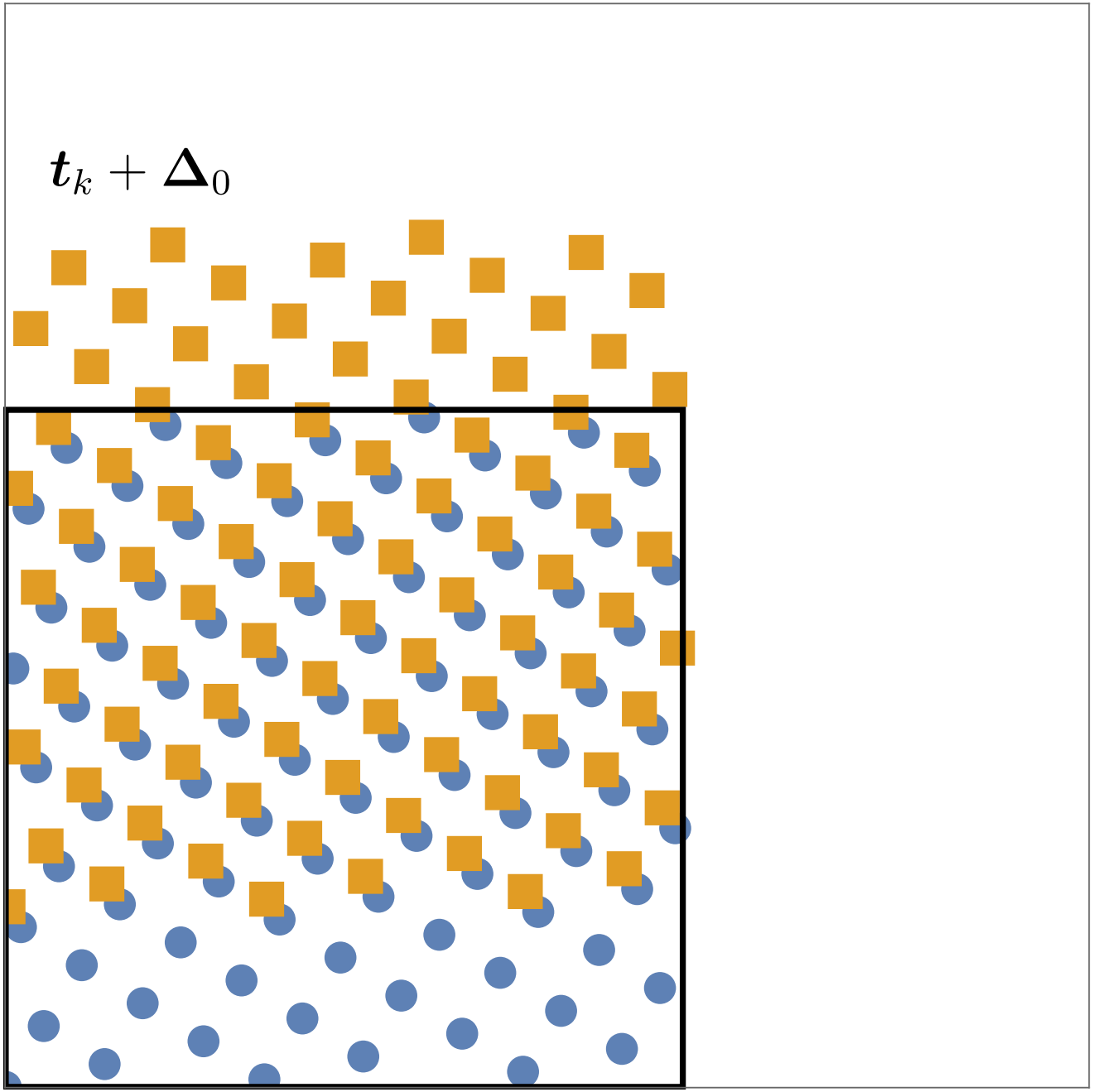
  is the approximation of the integral using a $\boldsymbol{\Delta}_r$-shift of the original QMC rule.
- We take the *average*

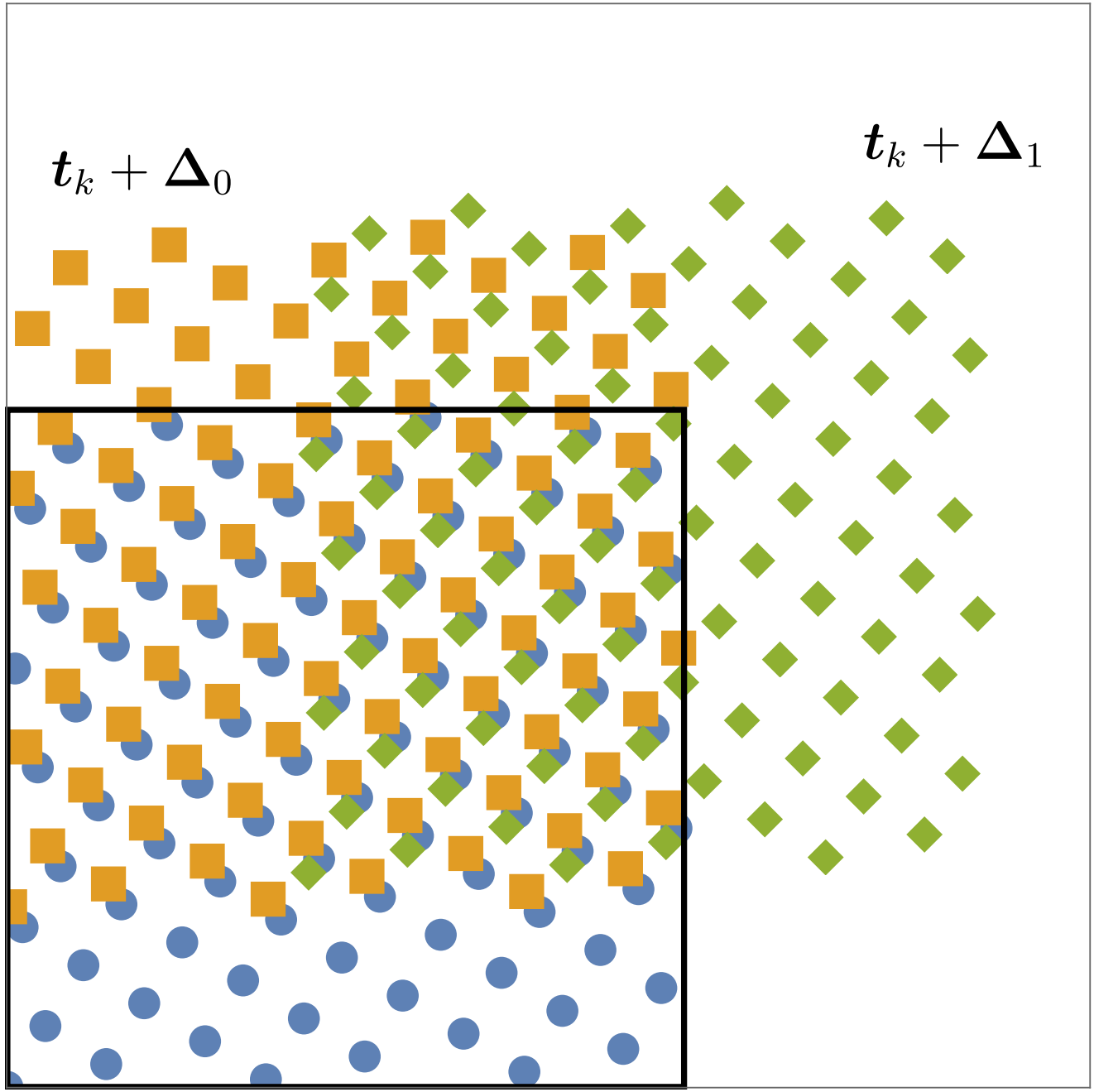
$$\overline{Q}_{n,s,R} f = \frac{1}{R} \sum_{r=0}^{R-1} Q_{n,s}^{\boldsymbol{\Delta}_r} f$$

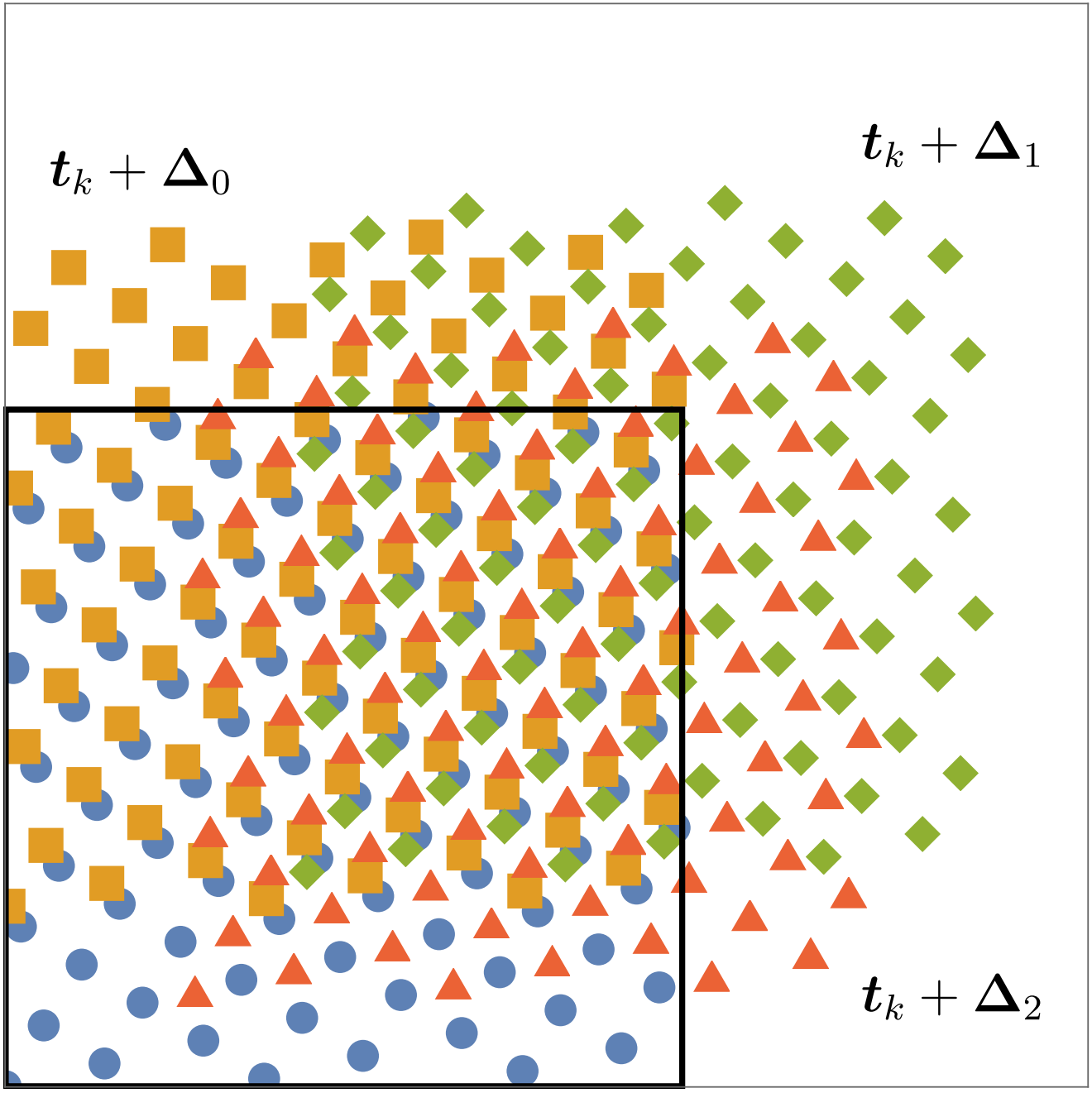
  as our *final* approximation of the integral.
- An *unbiased* estimate for the mean-square error of $\overline{Q}_{n,s,R} f$ is given by

$$\mathbb{E}_{\boldsymbol{\Delta}} |I_s f - Q_{n,s}^{\boldsymbol{\Delta}} f|^2 \approx \frac{1}{R(R-1)} \sum_{r=0}^{R-1} (Q_{n,s}^{\boldsymbol{\Delta}_r} f - \overline{Q}_{n,s,R} f)^2.$$

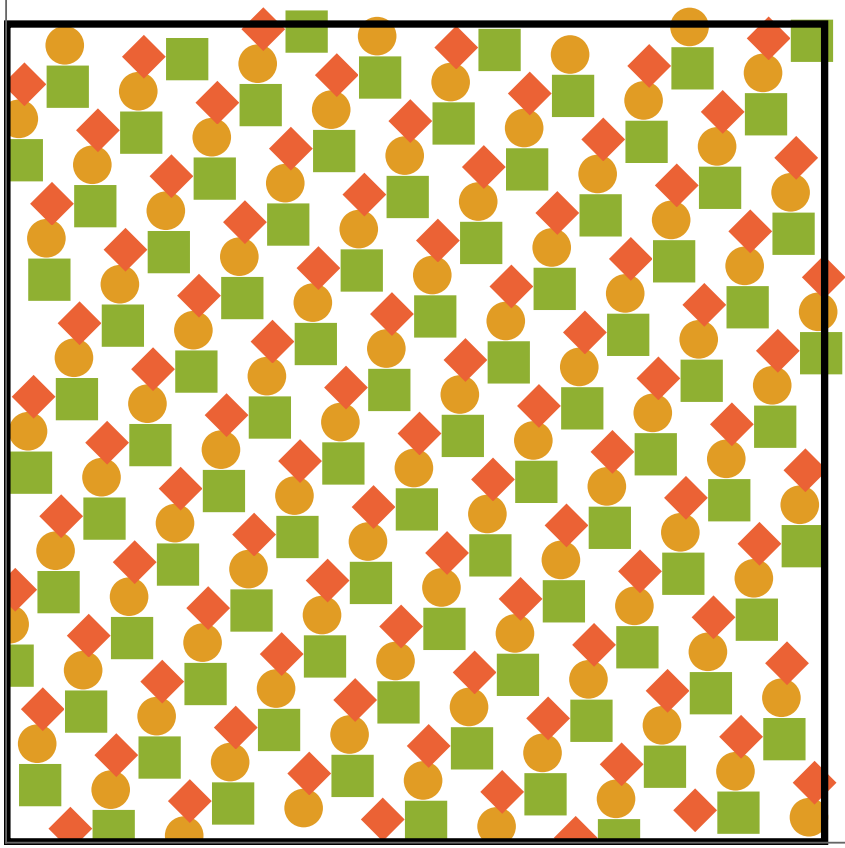



$t_k + \Delta_0$


$t_k + \Delta_0$
$t_k + \Delta_1$


$t_k + \Delta_0$
$t_k + \Delta_1$
$t_k + \Delta_2$

$$\{\{\boldsymbol{t}_k + \boldsymbol{\Delta}_0\}, \{\boldsymbol{t}_k + \boldsymbol{\Delta}_1\}, \{\boldsymbol{t}_k + \boldsymbol{\Delta}_2\}\}$$



$Q_{n,s}^{\boldsymbol{\Delta}_0} f = \frac{1}{n}\sum_{i=0}^{n-1} f(\{\boldsymbol{t}_i + \boldsymbol{\Delta}_0\})$, $Q_{n,s}^{\boldsymbol{\Delta}_1} f = \frac{1}{n}\sum_{i=0}^{n-1} f(\{\boldsymbol{t}_i + \boldsymbol{\Delta}_1\})$, $Q_{n,s}^{\boldsymbol{\Delta}_2} f = \frac{1}{n}\sum_{i=0}^{n-1} f(\{\boldsymbol{t}_i + \boldsymbol{\Delta}_2\})$

QMC approximation with 3 random shifts: $\overline{Q}_{n,s,3} f = \frac{Q_{n,s}^{\boldsymbol{\Delta}_0} f + Q_{n,s}^{\boldsymbol{\Delta}_1} f + Q_{n,s}^{\boldsymbol{\Delta}_2} f}{3}$.

Shift-averaged worst-case error

For any QMC point set $P = \{\boldsymbol{t}_0, \ldots, \boldsymbol{t}_{n-1}\}$ and any shift $\boldsymbol{\Delta} \in [0,1]^s$, let

$$P + \boldsymbol{\Delta} := \{\{\boldsymbol{t}_i + \boldsymbol{\Delta}\} \mid i = 0, 1, \ldots, n-1\}$$

denote the *shifted QMC point set*, and let $Q_{n,s}^{\boldsymbol{\Delta}} f$ denote a corresponding shifted QMC rule (over the point set $P + \boldsymbol{\Delta}$). For any integrand $f \in H$, it follows from the definition of the worst-case error that

$$|I_s f - Q_{n,s}(\boldsymbol{\Delta}; f)| \leq e_{n,s}(P + \boldsymbol{\Delta}; H)\|f\|_H,$$

where $e_{n,s}(P + \boldsymbol{\Delta}; H) := \sup_{\|f\|_H \leq 1} |I_s(f) - Q_{n,s}^{\boldsymbol{\Delta}} f|$. We deduce a bound for the *root-mean-square* error

$$\sqrt{\mathbb{E}_{\boldsymbol{\Delta}} |I_s f - Q_{n,s}^{\boldsymbol{\Delta}} f|^2} \leq e_{n,s}^{\mathrm{sh}}(P; H)\|f\|_H,$$

where the expected value $\mathbb{E}_{\boldsymbol{\Delta}}$ is taken over the random shift $\boldsymbol{\Delta}$ which is uniformly distributed over $[0,1]^s$ and the quantity

$$e_{n,s}^{\mathrm{sh}}(P; H) := \sqrt{\int_{[0,1]^s} e_{n,s}^2(P + \boldsymbol{\Delta}; H)\, \mathrm{d}\boldsymbol{\Delta}}$$

is called the *shift-averaged worst-case error*.

Theorem (Formula for the shift-averaged worst-case error)

$$[e^{\mathrm{sh}}_{n,s}(P; H_s(K))]^2 = -\int_{[0,1]^s}\int_{[0,1]^s} K(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1} K^{\mathrm{sh}}(\boldsymbol{t}_i,\boldsymbol{t}_j),$$

where

$$K^{\mathrm{sh}}(\boldsymbol{x},\boldsymbol{y}) := \int_{[0,1]^s} K(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}, \quad \boldsymbol{x},\boldsymbol{y}\in[0,1]^s.$$

Proof. The definition of shift-averaged WCE and (2) imply

$$\begin{aligned}
[e^{\mathrm{sh}}_{n,s}(P; H_s(K))]^2 &= \int_{[0,1]^s} e^2_{n,s}(P+\boldsymbol{\Delta}; H)\,\mathrm{d}\boldsymbol{\Delta} \\
&= \int_{[0,1]^s}\int_{[0,1]^s} K(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \frac{2}{n}\sum_{i=0}^{n-1}\int_{[0,1]^s}\int_{[0,1]^s} K(\{\boldsymbol{t}_i+\boldsymbol{\Delta}\},\boldsymbol{y})\,\mathrm{d}\boldsymbol{\Delta}\,\mathrm{d}\boldsymbol{y} \\
&\quad + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\int_{[0,1]^s} K(\{\boldsymbol{t}_i+\boldsymbol{\Delta}\},\{\boldsymbol{t}_j+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}.
\end{aligned}$$

The result follows by a change of variables $\boldsymbol{x} = \{\boldsymbol{t}_i + \boldsymbol{\Delta}\}$ in the second term. □

Remarks

$$K^{\mathrm{sh}}(\boldsymbol{x},\boldsymbol{y}) := \int_{[0,1]^s} K(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta}, \quad \boldsymbol{x},\boldsymbol{y}\in[0,1]^s.$$

- The function K^{sh} is actually a reproducing kernel, with the *shift-invariant property*

$$K^{\mathrm{sh}}(\boldsymbol{x},\boldsymbol{y}) = K^{\mathrm{sh}}(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\}) \quad \text{for all } \boldsymbol{x},\boldsymbol{y},\boldsymbol{\Delta}\in[0,1].$$

  Equivalently,

$$K^{\mathrm{sh}}(\boldsymbol{x},\boldsymbol{y}) = K^{\mathrm{sh}}(\{\boldsymbol{x}-\boldsymbol{y}\},\boldsymbol{0}) \quad \text{for all } \boldsymbol{x},\boldsymbol{y}\in[0,1].$$

- The function K^{sh} is called the *shift-invariant kernel associated with* K.

Weighted Sobolev spaces

Unanchored, weighted Sobolev space

For our purposes, the relevant function space setting will be the *unanchored, weighted Sobolev space*. For any given collection $(\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1:s\}}$ of positive numbers (called *weights*), we associate a space $H_{s,\gamma}$ containing continuous functions on $[0,1]^s$ whose *mixed first partial derivatives are square-integrable*. It is defined by the reproducing kernel

$$K_{s,\gamma}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \eta(x_j,y_j), \quad \eta(x,y) := \tfrac{1}{2}B_2(|x-y|)+(x-\tfrac{1}{2})(y-\tfrac{1}{2}),$$

where $B_2(x) := x^2 - x + \frac{1}{6}$ is the Bernoulli polynomial of degree 2.
Norm $\|f\|_{s,\gamma} = \sqrt{\langle f,f\rangle_{s,\gamma}}$ induced by the inner product

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

where $\mathrm{d}\boldsymbol{x}_{\mathfrak{u}} := \prod_{j\in\mathfrak{u}} \mathrm{d}x_j$ and $\mathrm{d}\boldsymbol{x}_{-\mathfrak{u}} := \prod_{j\in\{1:s\}\setminus\mathfrak{u}} \mathrm{d}x_j$.

Remarks

- We sum over all 2^s possible subsets of the indices $\{1:s\}$. By convention, an empty product is 1.
- Each term of the sum corresponds to a subset of variables $\boldsymbol{x}_{\mathfrak{u}} = \{x_j \mid j \in \mathfrak{u}\}$. We refer to these as the "active" variables, and denote the remaining "inactive" variables by $\boldsymbol{x}_{-\mathfrak{u}}$.
- The cardinality $|\mathfrak{u}|$ of the set $\mathfrak{u}$ is referred to as the "order" of the subset of variables $\boldsymbol{x}_{\mathfrak{u}}$. There is a *weight* parameter $\gamma_{\mathfrak{u}}$ associated with every subset of variables $\boldsymbol{x}_{\mathfrak{u}}$. The weights together model the relative importance between different subsets of variables. A small weight $\gamma_{\mathfrak{u}}$ means that the L^2 norm of $\frac{\partial^{|\mathfrak{u}|} f}{\partial \boldsymbol{x}_{\mathfrak{u}}}$ must also be small.
- Note that $\|\cdot\|_{s,\boldsymbol{\gamma}}$ and $\|\cdot\|_{s,c\boldsymbol{\gamma}}$ are equivalent norms for any $c > 0$.[†] Therefore we do not lose any generality by assuming that the weights have been normalized s.t. $\gamma_{\varnothing} = 1$. WLOG, we will *always* use the convention that $\gamma_{\varnothing} := 1$.

[†]Here, $c\boldsymbol{\gamma} = (c\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$.

Special forms of weights

- *Product weights*: we have a sequence of numbers satisfying $\gamma_1 \geq \gamma_2 \geq \cdots$ and we take

$$\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j.$$

  In this case, the reproducing kernel is given by the product

$$K_{s,\gamma}(\boldsymbol{x}, \boldsymbol{y}) = \prod_{j \in \mathfrak{u}} \Big(1 + \gamma_j \eta(x_j, y_j)\Big).$$

- *Finite order weights*: there exists $q \in \mathbb{N}$ s.t. $\gamma_{\mathfrak{u}} = 0$ for all $|\mathfrak{u}| > q$.
- *Order dependent weights*: we have a sequence of numbers $\Gamma_1, \Gamma_2, \ldots$, and take

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}.$$

- *Product-and-order dependent (POD) weights*: we have two sequences $\gamma_1, \gamma_2, \ldots$ and $\Gamma_1, \Gamma_2, \ldots$, and take

$$\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j.$$

Why weighted spaces are interesting

Theorem (Sloan and Woźniakowski 1998)

Consider $H_{s,\boldsymbol{\gamma}}$ equipped with product weights $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$. Then there exist point sets $P_n \subset [0,1]^s$ for $n = 1, 2, \ldots$ such that the worst-case error $e_{n,s}(P_n; H_{s,\boldsymbol{\gamma}})$ is bounded independently of s if and only if

$$\sum_{j=1}^{\infty} \gamma_j < \infty. \tag{5}$$

To be more precise, the result has two parts:

- If condition (5) does *not* hold, then no matter how the points are chosen, the worst-case error is unbounded as $s \to \infty$.
- However, if (5) holds, then "good points" exist (although the result does not say how to find them).

Recall that $H_{s,\gamma}$ is defined via the reproducing kernel

$$K_{s,\gamma}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \eta(x_j,y_j), \quad \eta(x,y) := \tfrac{1}{2}B_2(|x-y|)+(x-\tfrac{1}{2})(y-\tfrac{1}{2}),$$

where $B_2(x) := x^2 - x + \frac{1}{6}$ is the Bernoulli polynomial of degree 2.

Lemma

$$\int_{[0,1]^s} K_{s,\gamma}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = 1,$$
$$\int_{[0,1]^s}\int_{[0,1]^s} K_{s,\gamma}(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} = 1,$$
$$\int_{[0,1]^s} K_{s,\gamma}(\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}}(\tfrac{1}{6})^{|\mathfrak{u}|}.$$

Proof. Left as an exercise. □

Recall that $H_{s,\gamma}$ is defined via the reproducing kernel

$$K_{s,\gamma}(\boldsymbol{x},\boldsymbol{y}) = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \eta(x_j,y_j), \quad \eta(x,y) := \tfrac{1}{2}B_2(|x-y|)+(x-\tfrac{1}{2})(y-\tfrac{1}{2}),$$

where $B_2(x) := x^2 - x + \frac{1}{6}$ is the Bernoulli polynomial of degree 2.

For our analysis, we will need the shift-invariant kernel associated with $K_{s,\gamma}$.

Lemma

$$\begin{aligned} K^{\mathrm{sh}}_{s,\gamma}(\boldsymbol{x},\boldsymbol{y}) &:= \int_{[0,1]^s} K_{s,\gamma}(\{\boldsymbol{x}+\boldsymbol{\Delta}\},\{\boldsymbol{y}+\boldsymbol{\Delta}\})\,\mathrm{d}\boldsymbol{\Delta} \\ &= \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} B_2(|x_j-y_j|). \end{aligned}$$

Proof. This is an immediate consequence of

$$\int_0^1 \eta(\{x+\Delta\},\{y+\Delta\})\,\mathrm{d}\Delta = B_2(|x-y|). \quad \square$$

Let

$$P = \left\{ \left\{ \frac{k\boldsymbol{z}}{n} \right\} \mid k = 0, \ldots, n-1 \right\}$$

be a rank-1 lattice point set corresponding to generating vector $\boldsymbol{z} \in \mathbb{N}^s$ and $n \in \mathbb{N}$.

When dealing with the shift-invariant kernel corresponding to the unanchored, weighted Sobolev space $H_{s,\boldsymbol{\gamma}}$, we use the shorthand notation

$$e^{\mathrm{sh}}_{n,s}(\boldsymbol{z}) := e^{\mathrm{sh}}_{n,s}(P; H_{s,\boldsymbol{\gamma}}).$$

Lemma

The shift-averaged worst-case error for a rank-1 lattice rule in the weighted unanchored Sobolev space satisfies

$$[e^{\mathrm{sh}}_{n,s}(\boldsymbol{z})]^2 = \frac{1}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} B_2\left(\left\{\frac{k z_j}{n}\right\}\right).$$

Proof. Let $\boldsymbol{t}_j = \left\{\frac{j\boldsymbol{z}}{n}\right\}$. We have the kernel

$$K_{s,\gamma}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}} \eta(x_j, y_j), \quad \eta(x, y) := \tfrac{1}{2} B_2(|x-y|) + (x-\tfrac{1}{2})(y-\tfrac{1}{2}),$$

which satisfies $\int_{[0,1]^s} \int_{[0,1]^s} K_{s,\gamma}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} = 1$. We showed that the shift-invariant kernel related to K is given by

$$K^{\mathrm{sh}}_{s,\gamma}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \prod_{k \in \mathfrak{u}} B_2(|x_k - y_k|).$$

Moreover, we showed that the shift-averaged WCE is given by

$$[e^{\mathrm{sh}}_{n,s}(\boldsymbol{z})]^2 = -\int_{[0,1]^s} \int_{[0,1]^s} K_{s,\gamma}(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} + \frac{1}{n^2} \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} K^{\mathrm{sh}}_{s,\gamma}(\boldsymbol{t}_i, \boldsymbol{t}_j).$$

Making the obvious substitutions, we arrive at

$$[e^{\mathrm{sh}}_{n,s}(\boldsymbol{z})]^2 = -1 + \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{k\in\mathfrak{u}} B_2\left(\left\{\frac{(i-j)z_k}{n}\right\}\right) \quad (\gamma_\varnothing := 1)$$

$$= \frac{1}{n^2}\sum_{i=0}^{n-1}\sum_{j=0}^{n-1}\sum_{\varnothing\neq\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{k\in\mathfrak{u}} B_2\left(\left\{\frac{\mathrm{mod}(i-j,n)z_k}{n}\right\}\right).$$

As i and j range from 0 to $n-1$, the values of $\mathrm{mod}(i-j,n)$ are just $0,\ldots,n-1$ in some order (see next slide for illustration), with each value occurring n times. Thus the double sum can be reduced into a single sum:

$$[e^{\mathrm{sh}}_{n,s}(\boldsymbol{z})]^2 = \frac{1}{n}\sum_{\ell=0}^{n-1}\sum_{\varnothing\neq\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{k\in\mathfrak{u}} B_2\left(\left\{\frac{\ell z_k}{n}\right\}\right),$$

as desired. □

An illustration of the counting argument used on the previous slide

i/j	0	1	2	3	4	$\cdots$	$n-1$
0	0	1	2	3	4	$\cdots$	$n-1$
1	$n-1$	0	1	2	3	$\cdots$	$n-2$
2	$n-2$	$n-1$	0	1	2	$\cdots$	$n-3$
3	$n-3$	$n-2$	$n-1$	0	1	$\cdots$	$n-4$
4	$n-4$	$n-3$	$n-2$	$n-1$	0	$\cdots$	$n-5$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$n-1$	1	2	3	4	5	$\cdots$	0

Table of the values $\mathrm{mod}(i-j,n)$, when $i,j \in \{0,1,\ldots,n-1\}$.

By a simple counting argument we can write

$$\sum_{i=0}^{n-1}\sum_{j=0}^{n-1} f(\mathrm{mod}(i-j,n)) = n\sum_{\ell=0}^{n-1} f(\ell)$$

for *any* function $f : \{0,1,\ldots,n-1\} \to \mathbb{R}$.

Two easy technical results

Lemma (Fourier expansion of the Bernoulli polynomial B_2)

$$B_2(x) = \frac{1}{2\pi^2} \sum_{h \in \mathbb{Z}\setminus\{0\}} \frac{\mathrm{e}^{2\pi \mathrm{i} h x}}{h^2}.$$

Proof. Short argument: let $F(x) = \frac{1}{2\pi^2} \sum_{h \in \mathbb{Z}\setminus\{0\}} \frac{\mathrm{e}^{2\pi \mathrm{i} h x}}{h^2}$. Now[†] $F''(x) = 2$, so $F(x) = x^2 + c_1 x + c_0$. Moreover, $F(0) = F(1) = \frac{1}{6}$, so $c_0 = \frac{1}{6}$ and $c_1 = -1$. Hence $F(x) = x^2 - x + \frac{1}{6} = B_2(x)$. □

Lemma ("Jensen-like" inequality)

$$\sum_{k=1}^{\infty} a_k \leq \left(\sum_{k=1}^{\infty} a_k^{\lambda} \right)^{1/\lambda}, \quad a_k \geq 0,\ \lambda \in (0, 1].$$

Proof. Suppose that $\sum_{k=1}^{\infty} a_k^{\lambda} = 1$. Then $a_k \leq 1 \Rightarrow a_k \leq a_k^{\lambda}$ $\Rightarrow \sum_{k=1}^{\infty} a_k \leq \sum_{k=1}^{\infty} a_k^{\lambda} = 1$, and hence $\sum_{k=1}^{\infty} a_k \leq \left(\sum_{k=1}^{\infty} a_k^{\lambda} \right)^{1/\lambda}$. The general case $\sum_{k=1}^{\infty} a_k^{\lambda} = C \in \mathbb{R}_+$ follows by applying the same argument for the scaled sequence $a_k \leftarrow \frac{1}{C^{1/\lambda}} a_k$. □

[†] F is absolutely convergent, so exchanging differentiation and summation is OK.

Component-by-component construction

The components of the generating vector $\boldsymbol{z}$ can be restricted to the set

$$\mathbb{U}_n := \{z \in \mathbb{Z} \mid 1 \leq z \leq n-1 \text{ and } \gcd(z,n) = 1\},$$

whose cardinality is given by the Euler totient function $\varphi(n) := |\mathbb{U}_n|$. When n is prime, $\varphi(n)$ takes its largest value $n-1$.

We know that for $f \in H_{s,\gamma}$, there holds

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

Finding $\boldsymbol{z}^* = \arg\min_{\boldsymbol{z} \in \mathbb{U}_n} e_{n,s}^{\mathrm{sh}}(\boldsymbol{z})$ is not computationally feasible: the search space contains altogether up to $(n-1)^s$ possible choices for $\boldsymbol{z}$. However, the *component-by-component* (*CBC*) *construction* provides a feasible way to obtain good lattice generating vectors.

CBC construction

CBC construction. Given n, s, and weights $(\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1:s\}}$.

1. Set $z_1 = 1$.
2. For $k = 2, 3, \ldots, s$, choose $z_k \in \mathbb{U}_n$ to minimize $[e^{\mathrm{sh}}_{n,k}(z_1, \ldots, z_k)]^2$.

Remarks:

- Note that we have the (in principle computable) expression

$$[e^{\mathrm{sh}}_{n,k}(\boldsymbol{z})]^2 = \frac{1}{n} \sum_{\varnothing\neq\mathfrak{u}\subseteq\{1:k\}} \gamma_{\mathfrak{u}} \sum_{\ell=0}^{n-1} \prod_{j\in\mathfrak{u}} B_2\left(\left\{\frac{\ell z_j}{n}\right\}\right). \tag{6}$$

- We will show that when the weights $(\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1:s\}}$ are so-called *product-and-order dependent* (*POD*) weights, i.e., they can be written in the form

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

  where $\gamma_{\varnothing} := 1$, $(\Gamma_k)_{k=1}^{\infty}$ and $(\gamma_j)_{j=1}^{\infty}$ are sequences of positive numbers, then the value of (6) can be obtained in $\mathcal{O}(s\,n\log n + s^2 n)$ time using the so-called *fast CBC algorithm*. *This is quadratic, not exponential, w.r.t. the dimension s.*
- The CBC algorithm is a greedy algorithm: in general, it will **not** produce a generating vector which minimizes $e^{\mathrm{sh}}_{n,s}(\boldsymbol{z})$. Regardless, we **can** produce an error estimate for the *QMC rule based on a generating vector constructed by the CBC algorithm!*