Uncertainty Quantification and Quasi-Monte Carlo

Wintersemester 2022/23

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Eighth lecture, December 5, 2022

Course practical matters

- The deadline for the 7^{th} exercise sheet will be *extended* until **13.12.**
  - The 7^{th} exercise sheet is extremely important w.r.t. the main theme of the course, so it's worthwhile to discuss it thoroughly. :)
- **Tomorrow's exercise session:** Hints for the 7^{th} exercise sheet, using Python to solve parametric PDEs.
- The 8^{th} **exercise sheet** will be published **next week**, **deadline: 10.1.2023.**
- We'll have **"bonus lectures"** about the fast CBC algorithm on **both 2.1. and 3.1.2023.**

Course schedule

Monday	*Tuesday*
Dec 5	**Dec 6**
Lecture	Hints for 7^{th} exercise sheet, parametric PDEs using Python
Dec 12	**Dec 13**
Lecture	Extended deadline for 7^{th} exercise sheet
Xmas break (2 weeks)	
Jan 2	**Jan 3**
Fast CBC lecture	Fast CBC lecture (continued)
Jan 9	**Jan 10**
Lecture	Deadline for 8^{th} exercise sheet
Jan 16	**Jan 17**
Lecture	Deadline for 9^{th} exercise sheet
Jan 23	**Jan 24**
Lecture	Deadline for 10^{th} exercise sheet
Jan 30	**Jan 31**
Lecture	Deadline for 11^{th} exercise sheet
Feb 6	**Feb 7**
Summary/recap lecture	Deadline for 12^{th} (final) exercise sheet
Feb 13	**Feb 14**
Oral exam day 1	Oral exam day 2 (if necessary)

Recap from last week

We considered *rank-1 lattice rules*, a class of *equal weight (quasi-Monte Carlo) cubature rules*

$$Q_{n,s}f = \frac{1}{n}\sum_{i=0}^{n-1} f(\boldsymbol{t}_i) \approx \int_{[0,1]^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} =: I_s f, \quad \boldsymbol{t}_i := \left\{\frac{i\boldsymbol{z}}{n}\right\},$$

where the point set $P := \left\{\left\{\frac{i\boldsymbol{z}}{n}\right\} : i = 0, \ldots, n-1\right\}$ is determined by a *generating vector* $\boldsymbol{z} \in \mathbb{N}^s$. Note that we can assume the components of $\boldsymbol{z}$ to be coprime with n.

If the integrand f belongs to a Hilbert space H, we can bound the cubature error by

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

where $e_{n,s}(P; H) := \sup_{f \in H,\ \|f\|_H \leq 1} |I_s f - Q_{n,s} f|$ is called the *worst-case error*.

Recap from last week (cont'd)

If H is a *reproducing kernel Hilbert space (RKHS)*, then we can write down an expression for the worst-case error using the reproducing kernel K.

Theorem

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

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

We continue following 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

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 $\boldsymbol{z} \in \mathbb{N}^s$ 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.

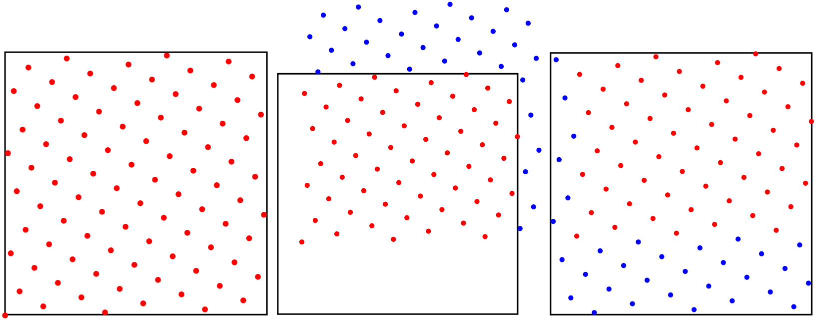
Advantages:

- 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

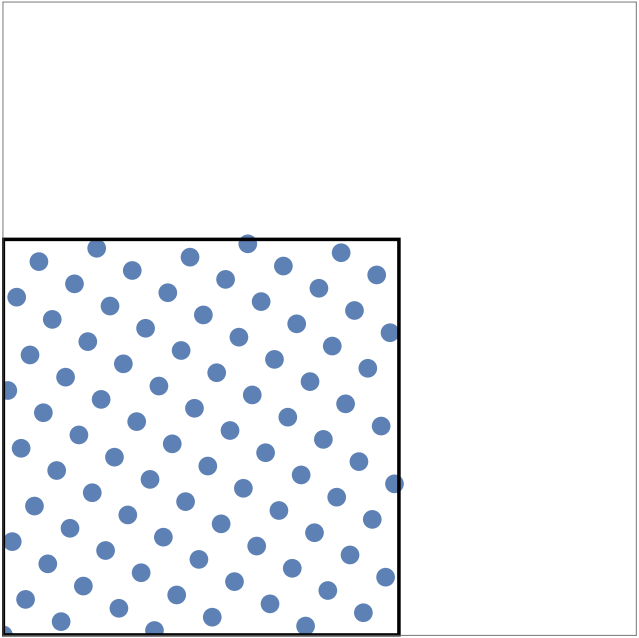
$$Q_{n,s}^{\boldsymbol{\Delta}_r} f = \frac{1}{n} \sum_{i=0}^{n-1} f(\{\boldsymbol{t}_i + \boldsymbol{\Delta}_r\}), \quad r = 0, \ldots, R-1,$$

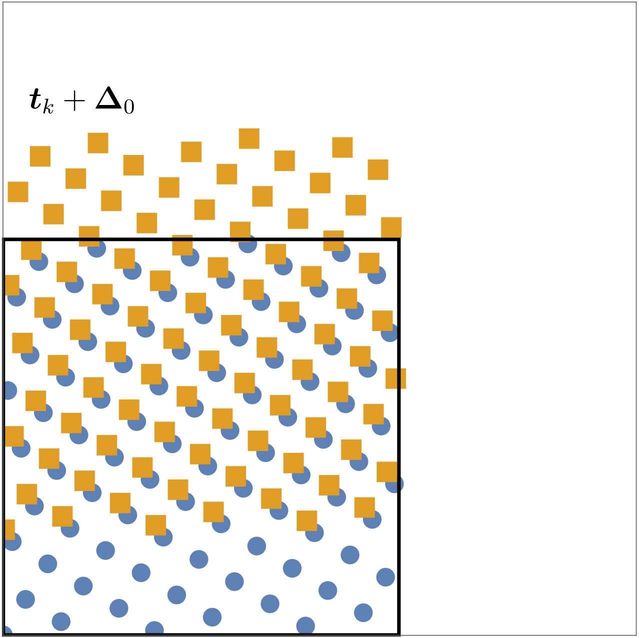
  is the approximation of the integral using a $\boldsymbol{\Delta}_r$-shift of the original QMC rule.
- We take the *average*

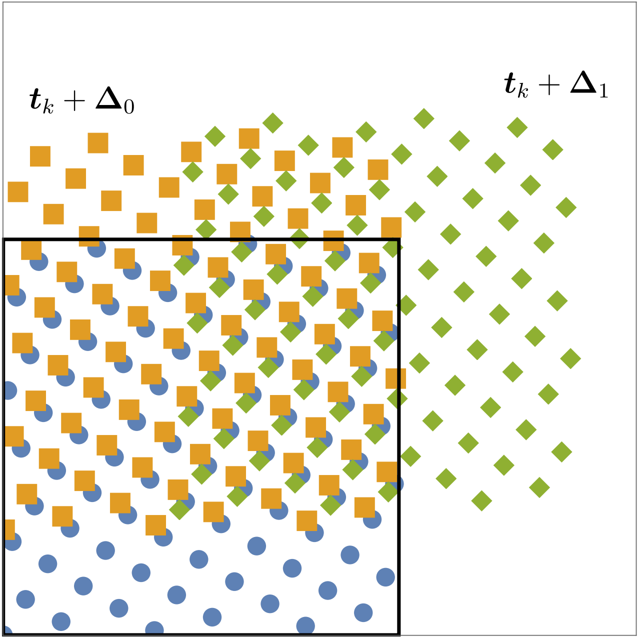
$$\overline{Q}_{n,s,R} f = \frac{1}{R} \sum_{r=0}^{R-1} Q_{n,s}^{\boldsymbol{\Delta}_r} f$$

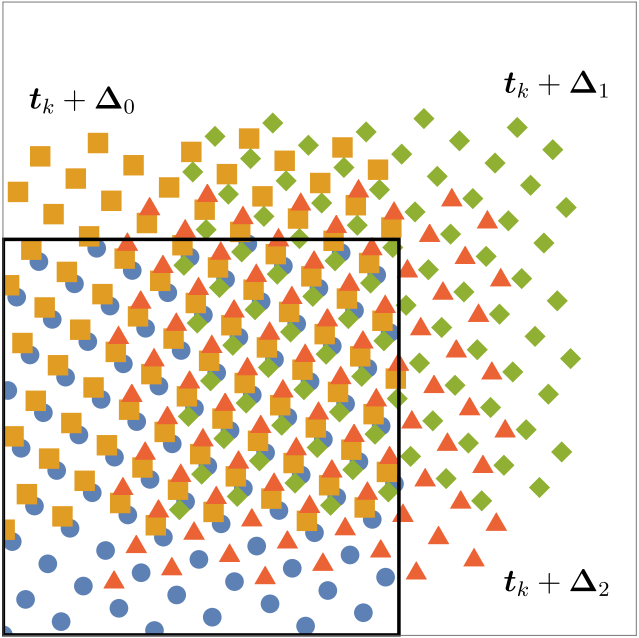
  as our *final* approximation of the integral.
- An *unbiased* estimate for the mean-square error of $\overline{Q}_{n,s,R} f$ is given by

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

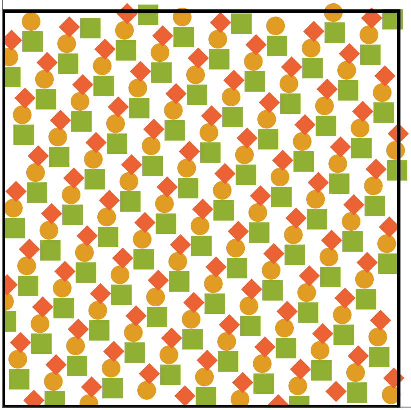



$\boldsymbol{t}_k + \boldsymbol{\Delta}_0$


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


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

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



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

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 (1) 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 $H_{s,\boldsymbol{\gamma}}$ containing continuous functions on $[0,1]^s$ whose *mixed first partial derivatives are square-integrable*. It is defined by the reproducing kernel

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

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

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

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

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

- *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 $H_{s,\gamma}$ *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* $e_{n,s}(P_n; H_{s,\gamma})$ *is bounded independently of* s *if and only if*

$$\sum_{j=1}^{\infty} \gamma_j < \infty. \tag{2}$$

To be more precise, the result has two parts:

- If condition (2) does *not* hold, then no matter how the points are chosen, the worst-case error is unbounded as $s \to \infty$.
- However, if (2) 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

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

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 $H_{s,\gamma}$, we use the shorthand notation

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

Lemma

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

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

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 $\operatorname{mod}(i-j,n)$, when $i,j \in \{0,1,\ldots,n-1\}$.

By a simple counting argument we can write

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

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

Two easy technical results

Lemma (Fourier expansion of the Bernoulli polynomial B_2)

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

Proof. Short argument: let $F(x) = \frac{1}{2\pi^2} \sum_{h\in\mathbb{Z}\setminus\{0\}} \frac{e^{2\pi i h x}}{h^2}$. 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)

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

Proof. Suppose that $\sum_{k=1}^{\infty} a_k^{\lambda} = 1$. Then $a_k \le 1 \Rightarrow a_k \le a_k^{\lambda}$ $\Rightarrow \sum_{k=1}^{\infty} a_k \le \sum_{k=1}^{\infty} a_k^{\lambda} = 1$, and hence $\sum_{k=1}^{\infty} a_k \le \left(\sum_{k=1}^{\infty} a_k^{\lambda} \right)^{1/\lambda}$. 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 $[e^{\rm sh}_{n,k}(z_1, \ldots, z_k)]^2$.

Remarks:

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

$$[e^{\rm sh}_{n,k}(\boldsymbol{z})]^2 = \frac{1}{n} \sum_{\varnothing \neq \mathfrak{u} \subseteq \{1:k\}} \gamma_{\mathfrak{u}} \sum_{\ell=0}^{n-1} \prod_{j \in \mathfrak{u}} B_2\left(\left\{\frac{\ell z_j}{n}\right\}\right). \tag{3}$$

- 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 (3) 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 $e^{\rm sh}_{n,s}(\boldsymbol{z})$. Regardless, we **can** produce an error estimate for the *QMC rule based on a generating vector constructed by the CBC algorithm!*