Efficient usage and construction of QMC methods

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Some point sets ...

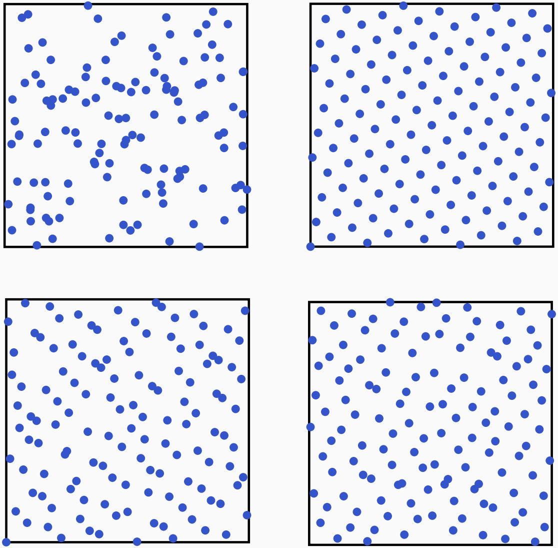


Figure 1: A collection of point sets in $[0,1]^s$

Table of contents

Introduction

Goal of numerical integration

Approximate the integral of the s-variate function f

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

over the s-dimensional unit cube by a quadrature rule, i.e.,

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

with points $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{N-1}\} \subseteq [0,1]^s$ and weights $w_0, \ldots, w_{N-1} \in [0,1]$.

Quasi-Monte Carlo method

A *quasi-Monte Carlo (QMC) method* is a quadrature rule

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

with deterministic quadrature points $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{N-1}\} \subseteq [0,1]^s$.

Worst-case integration error

Quality measure of choice:

Worst-case error

Let $Q_{N,s}$ be a quasi-Monte Carlo rule with underlying point-set $P = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{N-1}\} \subseteq [0,1]^s$ and $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ be a normed function space. The *worst-case error* of $Q_{N,s}$ w.r.t. $\mathcal{H}$ is defined as

$$e_{N,s}(Q_{N,s}, \mathcal{H}) = \sup_{\|f\|_{\mathcal{H}} \leq 1} \left| \int_{[0,1]^s} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{N} \sum_{i=0}^{N-1} f(\boldsymbol{x}_i) \right| .$$

Problem: The quantity $e_{N,s}(Q_{N,s}, \mathcal{H})$ is hard to compute (includes supremum over the unit ball $B = \{f \in \mathcal{H} : \|f\|_{\mathcal{H}} \leq 1\}$).

Reproducing kernel Hilbert spaces

Special function space class:

Reproducing kernel Hilbert space (RKHS)

Let $\mathcal{H}$ be a Hilbert space of real-valued functions $f : [0,1]^s \to \mathbb{R}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. Then $\mathcal{H}$ is called a *reproducing kernel Hilbert space* if there exists a kernel $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$ s.t.

- $K(\cdot, \boldsymbol{x}) \in \mathcal{H}$ for all $\boldsymbol{x} \in [0,1]^s$,
- $f(\boldsymbol{x}) = \langle f, K(\cdot, \boldsymbol{x}) \rangle_{\mathcal{H}}$ for all $f \in \mathcal{H}$ and for all $\boldsymbol{x} \in [0,1]^s$.

Here, we consider integrands f belonging to some RKHS $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$.

Examples for RKHS:

- Korobov space of smoothness $\alpha > 1$
- Sobolev spaces of dominating mixed smoothness α
- Walsh function spaces

Worst-case error expression in RKHS

Explicit formula for the squared worst-case error:

Theorem (worst-case error expression)

Let $\mathcal{H}(K)$ be a reproducing kernel Hilbert space with kernel function $K : [0,1]^s \times [0,1]^s \to \mathbb{R}$ such that the integration functional $\mathcal{I}(f)$ is continuous. Then the squared worst-case error of a quasi-Monte Carlo rule $Q_{N,s}$ with quadrature points $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{N-1}\}$ takes the form

$$e^2_{N,s}(Q_{N,s}, \mathcal{H}) = \int_{[0,1]^{2s}} K(\boldsymbol{x}, \boldsymbol{y}) \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} - \frac{2}{N} \sum_{i=0}^{N-1} \int_{[0,1]^s} K(\boldsymbol{x}_i, \boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} + \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} K(\boldsymbol{x}_i, \boldsymbol{x}_j) \, .$$

Weighted function spaces

Idea of weighted RKHS:

- based on the concept of effective dimension for high dimensions
- coordinate directions x_j of a function $f : [0,1]^s \to \mathbb{R}$ may have a varying importance w.r.t. their impact on the function value $f(\boldsymbol{x})$
- quantify this importance by assigning a positive number $\gamma_{\mathfrak{u}}$ to each group of variables $\boldsymbol{x}_{\mathfrak{u}}$ which reflects their importance

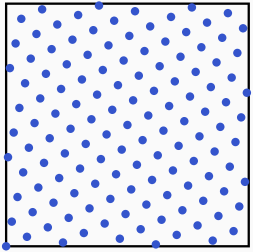
Introduce weighted function spaces[1] with incorporated weight sequence $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \in \{1:s\}}$ for each subset $\mathfrak{u} \subseteq \{1, \ldots, s\} =: \{1 : s\}$

Common weight types:

- product weights: $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ with weights $\gamma_1, \ldots, \gamma_s$
- order-dependent weights: $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|}$ with weights $\Gamma_1, \ldots, \Gamma_s$
- POD weights: $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j$ being a combination of the two

[1] See Sloan, Woźniakowski (1998)

Lattice rules in weighted RKHS



Rank-one lattice rule

A *rank-one lattice rule* is a quasi-Monte Carlo rule with underlying point set $P_N \subseteq [0,1]^s$ of the form

$$P_N = \left\{ \frac{k\,\boldsymbol{z} \bmod N}{N} \;:\; 0 \le k < N \right\} \subseteq [0,1]^s\,,$$

where $\boldsymbol{z} \in \mathbb{Z}^s$ is called the generating vector of the lattice rule.

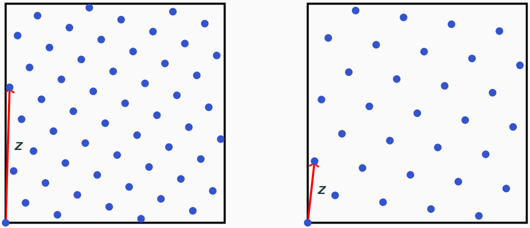


Figure 2: Fibonacci lattice with $N = 55$ and $\boldsymbol{z} = (1, 34)$ (left) and a rank-one lattice with $N = 32$ and $\boldsymbol{z} = (1, 9)$ constructed by the CBC construction (right)

Function space setting

Let $\mathbb{Z}_* := \mathbb{Z} \setminus \{0\}$ and define $r_\alpha(h) := 1/|h|^\alpha$ and $r_\alpha(\boldsymbol{h}) := \prod_{j=1}^{s} r_\alpha(h_j)$ for $h \in \mathbb{Z}_*$ and $\boldsymbol{h} = (h_1, \ldots, h_s) \in \mathbb{Z}_*^s$, respectively.

Consider weighted Korobov space $\mathcal{H}(K_{s,\alpha,\boldsymbol{\gamma}})$ which is RKHS with kernel

$$K_{s,\alpha,\boldsymbol{\gamma}}(\boldsymbol{x}, \boldsymbol{y}) = 1 + \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \sum_{\boldsymbol{h}_{\mathfrak{u}} \in \mathbb{Z}_*^{|\mathfrak{u}|}} r_\alpha(\boldsymbol{h}_{\mathfrak{u}}) \exp(2\pi i \boldsymbol{h}_{\mathfrak{u}} \cdot (\boldsymbol{x}_{\mathfrak{u}} - \boldsymbol{y}_{\mathfrak{u}})),$$

with smoothness $\alpha > 1$ and corresponding inner-product

$$\langle f, g \rangle_{K_{s,\alpha,\boldsymbol{\gamma}}} = \sum_{\mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{-1} \sum_{\boldsymbol{h}_{\mathfrak{u}} \in \mathbb{Z}_*^{|\mathfrak{u}|}} r_\alpha^{-1}(\boldsymbol{h}_{\mathfrak{u}}) \, \widehat{f}(\boldsymbol{h}_{\mathfrak{u}}) \overline{\widehat{g}(\boldsymbol{h}_{\mathfrak{u}})}$$

with $\widehat{f}(\boldsymbol{h}_{\mathfrak{u}})$ being the $\boldsymbol{h}_{\mathfrak{u}}$-th Fourier coefficient of f given by

$$\widehat{f}(\boldsymbol{h}_{\mathfrak{u}}) = \int_{[0,1]^s} f(\boldsymbol{x}) \exp(-2\pi i \boldsymbol{h}_{\mathfrak{u}} \cdot \boldsymbol{x}_{\mathfrak{u}}) \, \mathrm{d}\boldsymbol{x}.$$

Connection to the worst-case error

Let $\boldsymbol{z} \in \mathbb{Z}^s$ be the generating vector of a rank-1 lattice rule $\Lambda_{N,s}$ in the weighted Korobov space $\mathcal{H}(K_{s,\alpha,\boldsymbol{\gamma}})$. The squared worst-case error reads

$$e_{N,s}^2(\boldsymbol{z}) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}} \sum_{\boldsymbol{h}_{\mathfrak{u}} \in \mathcal{D}_{\mathfrak{u}}} r_\alpha(\boldsymbol{h}_{\mathfrak{u}})$$

where

$$\mathcal{D}_{\mathfrak{u}} := \left\{ \boldsymbol{h}_{\mathfrak{u}} \in \mathbb{Z}_*^{|\mathfrak{u}|} \ : \ \boldsymbol{h}_{\mathfrak{u}} \cdot \boldsymbol{z}_{\mathfrak{u}} \equiv 0 \pmod N \right\}.$$

There are connections between the worst-case error of the Korobov space $\mathcal{H}(K_{s,2,\boldsymbol{\gamma}})$ and the (root mean square) worst-case error for QMC integration in a weighted (anchored or unanchored) Sobolev space $\mathcal{H}_{s,\gamma}^{\text{sob}}$ using randomly shifted lattice rules or using tent-transformed lattice rules.

Component-by-component type constructions

The component-by-component construction

The component-by-component (CBC) algorithm[2] chooses the components z_i of the generating vector $\boldsymbol{z}$ one component at a time, keeping all previously chosen components fixed.

Algorithm 1 Component-by-component algorithm in RKHS

for $d = 1$ **to** s **do**
    for all $z_d \in \mathbb{U}_N$ **do**
        Calculate $e^2_{N,d}(z_1, z_2, \ldots, z_{d-1}, z_d)$
    end for
    $z_d = \underset{z \in \mathbb{U}_N}{\operatorname{argmin}}\ e^2_{N,d}(z_1, z_2, \ldots, z_{d-1}, z)$
end for

Notation:

$$\begin{aligned} \mathbb{U}_N &= \{z \in \{1, \ldots, N-1\} : \gcd(z, N) = 1\} \\ &= \{1, \ldots, N-1\} \text{ for } N \text{ prime} \end{aligned}$$

[2]See Sloan, Reztsov (2001) or Korobov (1959)

The successive coordinate search construction

Based on an initial vector $\boldsymbol{z}^0$, the successive coordinate search (SCS) algorithm[3] iterates through the components z_i keeping all other components of $\boldsymbol{z}$ and the dimension s fixed.

Algorithm 2 Successive coordinate search (SCS) algorithm

Input: $\boldsymbol{z}^0 \in \mathbb{Z}_N^s$
Output: $\boldsymbol{z} \in \mathbb{U}_N^s$

for $j = 1$ **to** s **do**
  for all $z_j \in \mathbb{U}_N$ **do**
    Calculate $e^2_{N,s}(z_1, \ldots, z_{j-1}, z_j, z^0_{j+1}, \ldots, z^0_s)$
  end for
  $z_j = \operatorname*{argmin}_{z \in \mathbb{U}_N} e^2_{N,s}(z_1, \ldots, z_{j-1}, z_j, z^0_{j+1}, \ldots, z^0_s)$
end for

Note that here: $\boldsymbol{z}^0 \in \mathbb{Z}_N^s = \{0, 1, \ldots N-1\}^s$

[3]See E., Leövey, Nuyens (2018) (to appear in MCQMC 2016 proceedings)

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

$\boldsymbol{z}$

The successive coordinate search algorithm:

$\boldsymbol{z}$

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

z

The successive coordinate search algorithm:

z

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

$\boldsymbol{z}$ z_1 z_2

The successive coordinate search algorithm:

$\boldsymbol{z}$ z_1 z_2 z_3 z_4 z_5 z_6 z_7

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

$\boldsymbol{z}$ $\quad z_1 \quad z_2 \quad z_3$

The successive coordinate search algorithm:

$\boldsymbol{z}$ $\quad z_1 \quad z_2 \quad z_3 \quad z_4 \quad z_5 \quad z_6 \quad z_7$

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

$\boldsymbol{z}$ | z_1 | z_2 | z_3 | z_4

The successive coordinate search algorithm:

$\boldsymbol{z}$ | z_1 | z_2 | z_3 | z_4 | z_5 | z_6 | z_7

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

$\boldsymbol{z}$ z_1 z_2 z_3 z_4 z_5

The successive coordinate search algorithm:

$\boldsymbol{z}$ z_1 z_2 z_3 z_4 z_5 z_6 z_7

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Error convergence behavior

Assumptions:

- $N = b^m$ with b prime, $m \in \mathbb{N}$ and general weights $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$
- $\boldsymbol{z}^0 \in \mathbb{Z}_N^s$ arbitrary initial vector for the SCS algorithm
- $\boldsymbol{z}_{\text{cbc}}$ and $\boldsymbol{z}_{\text{scs}}$ generating vectors constructed by CBC/SCS algorithm

[4] See, e.g., Dick, Kuo, Sloan (2014) - Acta Numerica review article

[5] See E., Leövey, Nuyens (2018) and E., Kritzer (2018) (submitted)

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Let $\alpha > 1$, then $\forall \lambda \in (\frac{1}{\alpha}, 1]$ the worst-case error satisfies:

CBC construction[4]

$$e^2_{N,s}(\boldsymbol{z}_{\text{cbc}}) \le \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \frac{2(2\zeta(\alpha\lambda))^{|\mathfrak{u}|}}{b^m} \right)^{\frac{1}{\lambda}}$$

SCS algorithm[5]

$$e^2_{N,s}(\boldsymbol{z}_{\text{scs}}) \le \left(\sum_{j=1}^{s} \sum_{j \in \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \frac{2(2\zeta(\alpha\lambda))^{|\mathfrak{u}|}}{b^m} \right)^{\frac{1}{\lambda}}$$

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For product weights $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ the error is $\mathcal{O}(N^{-\alpha/2+\delta})$ with constant independent of the dimension s provided that $\sum_{j=1}^{\infty} \gamma_j^{\frac{1}{\alpha - 2\delta}} < \infty$.

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[5] See E., Leövey, Nuyens (2018) and E., Kritzer (2018) (submitted)

Computational complexity

The CBC and the SCS construction can both be implemented in a fast way[6] by exploiting the (block-)circulant structure of the matrix

$$\Omega_N := \left[\omega\left(\frac{kz \bmod N}{N}\right)\right]_{\substack{z\in\mathbb{U}_N\\ k=0,\ldots,N-1}}$$

to perform a fast matrix-vector multiplication using FFT.

Complexity for $\gamma_{\mathfrak{u}}$ of the form $\prod_{j\in\mathfrak{u}}\gamma_j$

- The fast versions of the algorithms allow for the construction of generating vectors using $\mathcal{O}(s\,N\,\log(N))$ operations.
- The computation in the SCS algorithm is slightly more expensive than in the CBC algorithm since the involved quantities have to be initialized and updated using $\boldsymbol{z}^0$.

[6] See Fast CBC construction by Nuyens and Cools (2006)

Construction method for the SCS algorithm

We consider the following construction methods in order to find generating vectors $\boldsymbol{z}$ with a small worst-case error $e_{N,s}(\boldsymbol{z})$:

1. Uniform random vectors + SCS algorithm:
Choose q initial vectors $\boldsymbol{z}^0 \in \mathbb{Z}_N^s$ at random, apply the fast SCS algorithm to them and then select the one that minimizes $e_{N,s}(\boldsymbol{z})$.
<u>Computational cost (product weights):</u> $\mathcal{O}(q\, s\, N \log(N))$

2. Korobov-type generating vector + SCS algorithm:

Choose q Korobov-type* generating vectors as initial vectors $\boldsymbol{z}^0$, apply the fast SCS algorithm to them and then select the one that minimizes $e_{N,s}(\boldsymbol{z})$.
<u>Computational cost (product weights):</u> $\mathcal{O}(q\, s\, N \log(N))$

*Korobov construction: For a generator $a \in \mathbb{Z}_n$, define the corresponding generating vector by $\boldsymbol{z} = \boldsymbol{z}(a) := (1, a, a^2, \ldots, a^{s-1}) \mod N$.

Reduced CBC type constructions

The reduced construction

Assumptions:

- $N = b^m$ with b prime, $m \in \mathbb{N}$ and general weights $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u} \subseteq \{1:s\}}$
- $w_1, \ldots, w_s \in \mathbb{N}_0$ with $w_1 \leq w_2 \leq \ldots \leq w_s$ and $Y_j = b^{w_j}$ for all j

$$\mathcal{Z}_{N,w_j} := \begin{cases} \{z \in \{1, 2, \ldots, b^{m-w_j} - 1\} : \gcd(z, N) = 1\} & \text{if } w_j < m \\ \{1\} & \text{if } w_j \geq m \end{cases}$$

[7] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

[8] See E., Kritzer (2018) - (submitted for publication - available on arXiv)

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Reduced CBC construction[7]

- Set $z_1 = 1$.
- **For $d = 2$ to s:**

  ◇ Assume that $z_1, \ldots, z_{d-1}$ have already been found.

  ◇ Choose $z_d \in \mathcal{Z}_{N,w_d}$ such that

  $$e^2_{N,d}((Y_1 z_1, \ldots, Y_{d-1} z_{d-1}, Y_d z_d))$$

  is minimized as a function of z_d.
- Obtain the generating vector $\boldsymbol{z} = (Y_1 z_1, \ldots, Y_s z_s)$.

Reduced SCS algorithm[8]

- **Input:** Starting vector $\boldsymbol{z}^0$ with $\boldsymbol{z}^0 = (z_1^0, \ldots, z_s^0) \in \mathbb{Z}_N^s$.
- **For $j = 1$ to s:**

  ◇ Assume that $z_1, \ldots, z_{j-1}$ have already been selected.

  ◇ Choose $z_j \in \mathcal{Z}_{N,w_j}$ such that

  $$e^2_{N,s}((Y_1 z_1, \ldots, Y_{j-1} z_{j-1}, Y_j z_j, z^0_{j+1:s}))$$

  is minimized as a function of z_j.
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Error convergence behavior

Let $\boldsymbol{z}_{\text{cbc}} = (Y_1 z_1, \ldots, Y_s z_s)$ and $\boldsymbol{z}_{\text{scs}} = (Y_1 \bar{z}_1, \ldots, Y_s \bar{z}_s)$ be constructed by the reduced CBC or reduced SCS algorithm with arbitrary initial vector $\boldsymbol{z}^0 \in \mathbb{Z}_N^s$, respectively. Let $\alpha > 1$, then $\forall \lambda \in (\frac{1}{\alpha}, 1]$ the worst-case error satisfies:

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Reduced CBC construction[9]

$$e_{N,s}^2(\boldsymbol{z}_{\text{cbc}}) \leq \left(\sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \frac{2(2\zeta(\alpha\lambda))^{|\mathfrak{u}|}}{b^{\max(0, m - \max_{j \in \mathfrak{u}} w_j)}} \right)^{\frac{1}{\lambda}}$$

Reduced SCS algorithm[10]

$$e_{N,s}^2(\boldsymbol{z}_{\text{scs}}) \leq \left(\sum_{j=1}^{s} \sum_{j \in \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}^{\lambda} \frac{2(2\zeta(\alpha\lambda))^{|\mathfrak{u}|}}{b^{\max(0, m - w_j)}} \right)^{\frac{1}{\lambda}}$$

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For product weights $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ the error is $\mathcal{O}(N^{-\alpha/2+\delta})$ with constant independent of the dimension s provided that

$$\sum_{j=1}^{\infty} \gamma_j^{\frac{1}{\alpha - 2\delta}} b^{w_j} < \infty.$$

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Computational complexity of the reduced constructions

As before, the reduced CBC and SCS constructions can be implemented in a fast way in the spirit of Nuyens and Cools. This is based on the fact that the (block-)circulant matrix

$$\Omega_{b^m} := \left[\omega\left(\frac{kz \bmod N}{N}\right)\right]_{\substack{z\in\mathbb{U}_N \\ k=0,\dots,N-1}}$$

maintains its (block-)circulant structure upon the substitution $\bar{z} = b^w z$ with $z \in \mathcal{Z}_{N,w}$, i.e.,

$$\Omega_{b^m,w} := \left[\omega\left(\frac{kb^w z \bmod N}{N}\right)\right]_{\substack{z\in\mathcal{Z}_{N,w} \\ k=0,\dots,N-1}}$$

with potentially smaller circulant blocks.

Computational complexity of the reduced constructions

Assumptions:

- $N = b^m$ with b prime, $w_1, \ldots, w_s \in \mathbb{N}_0$ with $w_1 \leq w_2 \leq \ldots \leq w_s$
- s^* is the largest integer such that $w_{s^*} < m$

Reduced CBC construction[11] | **Reduced SCS algorithm**[12]

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

[11] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

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Computational complexity of the reduced constructions

Assumptions:

- $N = b^m$ with b prime, $w_1, \dots, w_s \in \mathbb{N}_0$ with $w_1 \le w_2 \le \dots \le w_s$
- s^* is the largest integer such that $w_{s^*} < m$

Reduced CBC construction[11] | **Reduced SCS algorithm**[12]

$\boxed{\textbf{Product weights } \gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j}$

$$\mathcal{O}\left(N \log N + \min(s, s^*) N + \sum_{j=1}^{\min(s,s^*)} (m - w_j) b^{m - w_j}\right)$$

[11] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

[12] See E., Kritzer (2018) - (submitted for publication - available on arXiv)

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[11] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

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$$\mathcal{O}\left(N \log N + \min(s, s^*)^2 N + \sum_{j=1}^{\min(s,s^*)} (m - w_j) b^{m - w_j} \right)$$

[11] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

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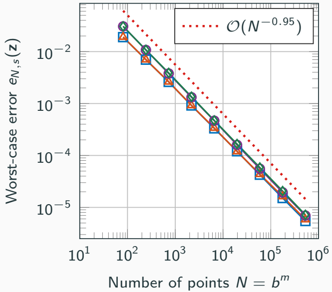
Unreduced construction: $\mathcal{O}(s\, N \log N + s^2 N)$

[11] See Dick, Kritzer, Leobacher, Pillichshammer (2015)

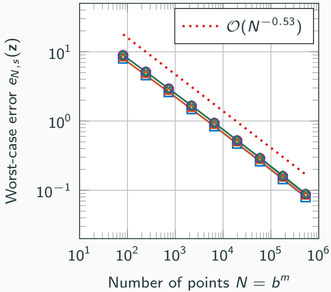
[12] See E., Kritzer (2018) - (submitted for publication - available on arXiv)

Numerical results for product and POD weights

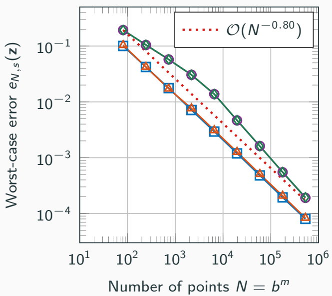
Error convergence for Korobov space with $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$, $s = 100$, $\alpha = 2$, $b = 3$, $w_j = \lfloor 2 \log_b j \rfloor$



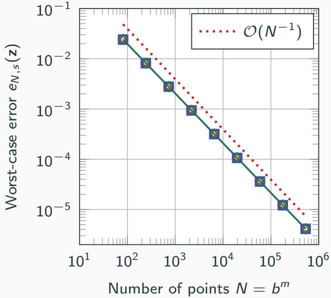
(a) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = (0.2)^j$



(b) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = (0.8)^j$



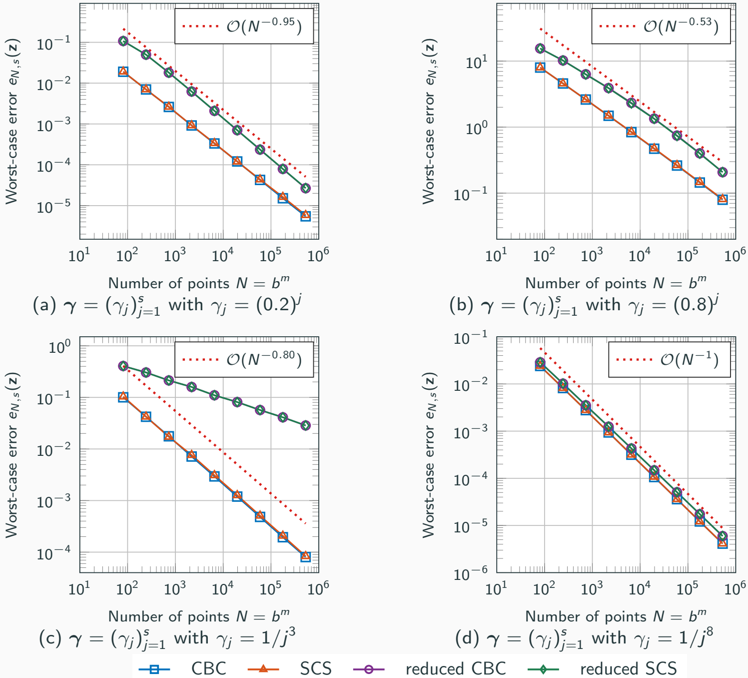
(c) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = 1/j^3$



(d) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = 1/j^8$

CBC SCS reduced CBC reduced SCS

Error convergence for Korobov space with $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$, $s = 100$, $\alpha = 2$, $b = 3$, $w_j = \lfloor \frac{7}{2} \log_b j \rfloor$



(a) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = (0.2)^j$

(b) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = (0.8)^j$

(c) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = 1/j^3$

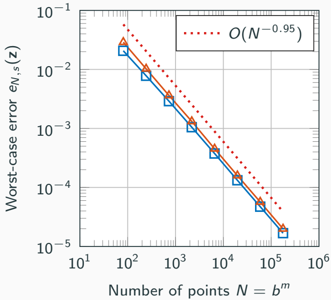
(d) $\boldsymbol{\gamma} = (\gamma_j)_{j=1}^s$ with $\gamma_j = 1/j^8$

Computation times

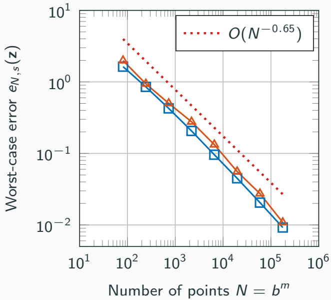
Table 1: Computation times (in seconds) for constructing generating vectors $\boldsymbol{z}$ via the unreduced (normal font) and reduced SCS (**bold font**) algorithm. Constructed for Korobov space with $\gamma_{\mathfrak{u}} = \prod_{j\in\mathfrak{u}} \gamma_j$, $\alpha = 2$, $b = 2$, $\gamma_j = (0.7)^j$ and $w_j = \lfloor 3 \log_b j \rfloor$.

	$s = 50$	$s = 100$	$s = 500$	$s = 1000$	$s = 2000$
$m = 10$	0.0275 **0.00408**	0.0516 **0.00327**	0.256 **0.00354**	0.516 **0.00347**	1.03 **0.00329**
$m = 12$	0.0418 **0.00592**	0.0751 **0.00504**	0.383 **0.00612**	0.756 **0.00516**	1.56 **0.00794**
$m = 14$	0.0792 **0.014**	0.14 **0.0136**	0.767 **0.0163**	1.39 **0.0138**	2.82 **0.0138**
$m = 16$	0.204 **0.0441**	0.388 **0.0434**	2.09 **0.0434**	4.05 **0.0423**	8.04 **0.0462**
$m = 18$	0.686 **0.16**	1.35 **0.177**	6.89 **0.182**	13.7 **0.183**	26.8 **0.187**
$m = 20$	3.28 **0.843**	6.71 **1.4**	34.4 **1.51**	67.4 **1.37**	132 **1.36**

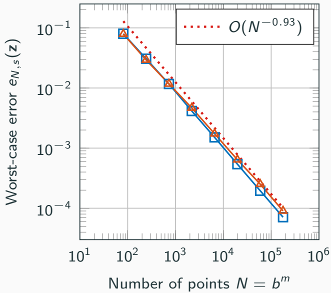
Convergence for Korobov space with $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j$, $s = 500$, $\alpha = 2$, $b = 3$, $w_j = \lfloor 3 \log_b j \rfloor$



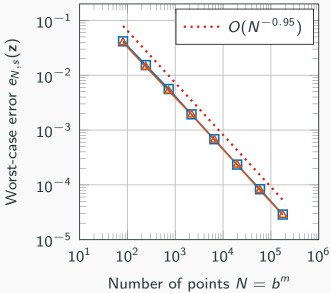
(a) $\Gamma_j = j^4$ and $\gamma_j = (0.1)^j$



(b) $\Gamma_j = j^4$ and $\gamma_j = (0.5)^j$



(c) $\Gamma_j = j^4$ and $\gamma_j = j^{-6}$



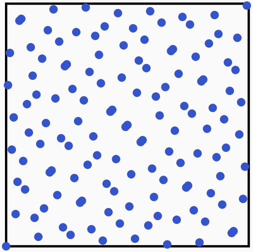
(d) $\Gamma_j = j^4$ and $\gamma_j = j^{-8}$

Computation times

Table 2: Computation times (in seconds) for constructing the generating vector $\boldsymbol{z}$ using the unreduced (normal font) and reduced CBC (**bold font**) construction. The associated lattice can be used for integration in the Korobov space with $\alpha = 2$, $b = 2$ and $w_j = \lfloor 3 \log_b j \rfloor$ with POD weights $\gamma_{\mathfrak{u}} = \Gamma_{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} \gamma_j$ where $\Gamma_j = j^4, \gamma_j = j^{-6}$.

	$s = 50$	$s = 100$	$s = 200$	$s = 500$	$s = 1000$
$m = 8$	0.136 **0.00393**	0.493 **0.00229**	1.87 **0.00229**	12.1 **0.0021**	44.3 **0.00326**
$m = 10$	0.239 **0.00672**	0.709 **0.00558**	2.72 **0.00654**	16.3 **0.00683**	63 **0.00733**
$m = 12$	0.296 **0.0179**	1.05 **0.0184**	3.91 **0.0167**	24 **0.0227**	95.2 **0.0274**
$m = 14$	0.552 **0.0757**	2.03 **0.0876**	7.49 **0.0932**	45.8 **0.115**	180 **0.157**
$m = 16$	1.62 **0.576**	6.31 **0.583**	24.2 **0.576**	148 **0.631**	589 **0.585**
$m = 18$	5.77 **3.3**	21.8 **4.86**	83.8 **4.85**	512 **4.85**	2013 **5.26**
$m = 20$	27.8 **17.4**	103 **59.9**	401 **61.4**	2452 **58.9**	9791 **61.7**

Digital net constructions



Digital construction scheme

Assumptions:

- b prime, $\mathbb{Z}_b := \mathbb{Z}/b\mathbb{Z} = \{0, 1, \ldots, b-1\}$
- $C_1, \ldots, C_s \in \mathbb{Z}_b^{m \times m}$, i.e., m-by-m generating matrices with entries in $\mathbb{Z}_b$
- $P_N = P_{b^m} = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{b^m-1}\}$ with $\boldsymbol{x}_i = (x_{i,1}, \ldots, x_{i,s})$ for $i = 0, \ldots, b^m - 1$

Construction scheme: For each $i = 0, \ldots, b^m - 1$ consider the following steps:

1. Compute the base b expansion of $i = i_1 + i_2 b + \ldots + i_m b^m$.
2. For $j = 1, \ldots, s$ compute $y_1^{(j)}, \ldots, y_m^{(j)}$ (with operations in $\mathbb{Z}_b$) via
$$\begin{pmatrix} y_1^{(j)} \\ y_2^{(j)} \\ \vdots \\ y_m^{(j)} \end{pmatrix} = C_j \begin{pmatrix} i_1 \\ i_2 \\ \vdots \\ i_m \end{pmatrix}.$$
3. Define the component $x_{i,j}$ by
$$x_{i,j} = \sum_{k=1}^{m} y_k^{(j)} b^{-k} = \frac{y_1^{(j)}}{b} + \frac{y_2^{(j)}}{b^2} + \ldots + \frac{y_m^{(j)}}{b^m}.$$

Then $P_{b^m} = \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{b^m-1}\}$ is called a digital net in base b.

QMC software and generators

1. Software on Dirk Nuyens' webpage to apply quasi-Monte Carlo:
   - The Magic Point Shop!:
     `https://www.cs.kuleuven.be/~dirkn/qmc-generators/`
   - QMC4PDE:
     `https://www.cs.kuleuven.be/~dirkn/qmc4pde/`

2. Git repositories with C++, Python, Matlab code on Bitbucket:
   - `https://bitbucket.org/dnuyens/qmc-generators`
   - `https://bitbucket.org/dnuyens/qmc4pde/`

3. Git repository with software for presented CBC type lattice constructions (Matlab) and digital net generator:
   - `https://bitbucket.org/adrian_ebert/digital_sequences/`

Specification for using the digital net point generator

Command line generator `digitalseq_b2g` with the following inputs:

- s – number of dimensions s
- m – number of points given by $N = 2^m$
- C (via file) – generating matrices $C_1, \ldots, C_s$ given in column format

$$C_j = [c_1^{(j)}, c_2^{(j)}, \ldots, c_m^{(j)}] := \begin{pmatrix} c_{1,1}^{(j)} & c_{2,1}^{(j)} & \cdots & c_{m,1}^{(j)} \\ c_{1,2}^{(j)} & c_{2,2}^{(j)} & \cdots & c_{m,2}^{(j)} \\ \vdots & \vdots & & \vdots \\ c_{1,m}^{(j)} & c_{2,m}^{(j)} & \cdots & c_{m,m}^{(j)} \end{pmatrix}$$

with $c_i^{(j)} = \sum_{k=1}^m c_{i,k}^{(j)} 2^k \in \{0, 1, \ldots, N-1\}$ for $i = 1, \ldots, m$.

Features available with this digital net point generator:

- Generation of digital sequence points based on C
- Digital randomization techniques (see following slide)
- Adaptable state of the sequence generator
- Digital interlacing of factor α (via separate programme)

Digital shifting and scrambling

The digital generator comes with the following two randomization techniques:

1. Digital shift:
   - $\Delta \in [0,1]^s$ with base b expansion $\Delta_j = \sum_{k=1}^{\infty} d_k^{(j)} b^{-k}$
   - $P_{b^m} = \{\boldsymbol{x}_0 \oplus \Delta, \ldots, \boldsymbol{x}_{b^m-1} \oplus \Delta\}$ with component-wise digit-wise addition in base b
2. Linear Matousek scrambling:
   - Consider point $\boldsymbol{x} \in [0,1]^s$ with components $x_j = \sum_{k=1}^{\infty} x_k^{(j)} b^{-k}$
   - Linear matrix scramble: $x_j \to \bar{x}_j = \sum_{k=1}^{\infty} \bar{x}_k^{(j)} b^{-k}$ with

$$\bar{x}_k^{(j)} = \sum_{i=1}^{k} M_{ki} x_i^{(j)}.$$

   - Expressible via generating matrices: Set $\bar{C}_j := M_j \cdot C_j$ with

$$M_j = \begin{pmatrix} u_{1,1} & 0 & \cdots & 0 \\ r_{2,1} & u_{2,2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ r_{m,1} & \cdots & r_{m,m-1} & u_{m,m} \end{pmatrix}$$

and uniform random numbers $u_{k,i} \in \mathbb{Z}_b \setminus \{0\}$ and $r_{k,i} \in \mathbb{Z}_b$.

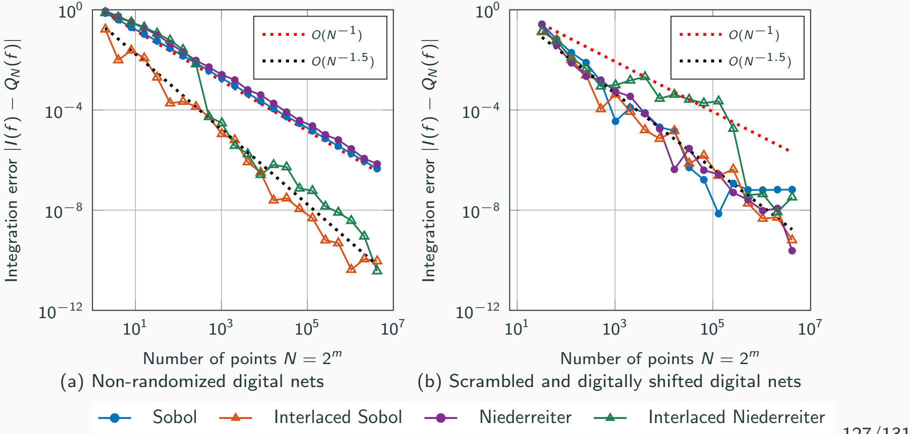
Demo of the digital net point generator

Terminal demo

Numerical example 1

Function $f(x) = \exp(c\sum_{j=1}^{s} \frac{x^j}{j^\beta})$ with integral $I(f) = \prod_{j=1}^{s} \frac{\exp(c\,j^{-\beta})-1}{c\,j^{-\beta}}$.

- $N = 2^m, s = 50, \beta = 2, c = 1$ and we consider digital interlacing of factor $\alpha = 2$.
- We consider $t = 2^4$ affine matrix scrambles and $Q_N(f) := \frac{1}{t}\sum_{i=1}^{t} Q_{2^{m-4}}(f)$.
- In this example, we first interlace and then randomize the digital sequence.



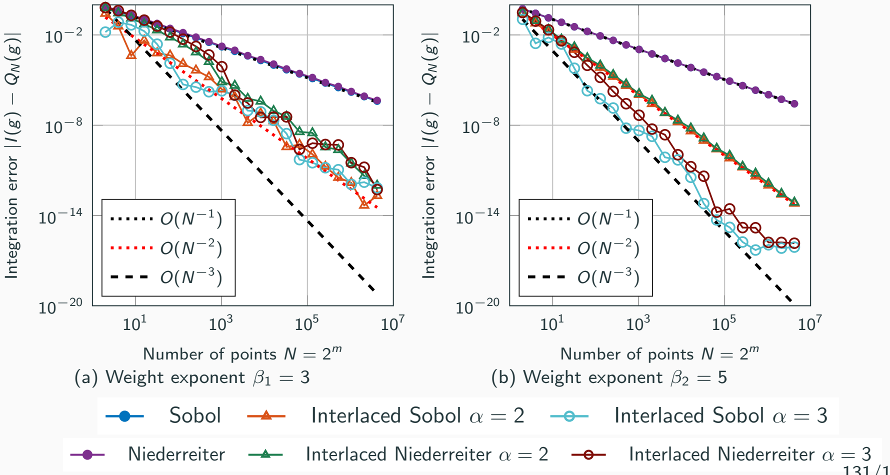
(a) Non-randomized digital nets

(b) Scrambled and digitally shifted digital nets

Numerical example 2

Function $g(\boldsymbol{x}) = \prod_{j=1}^{s} \left(1 + \frac{2x_j - a}{j^\beta}\right)$ with integral $I(g) = \prod_{j=1}^{s} \left(1 + \frac{1-a}{j^\beta}\right)$.

- $N = 2^m$, $s = 100$, $a = 0$ and we consider digital interlacing of factor $\alpha \in \{2, 3\}$.
- We consider two different weight exponents $\beta_1 = 3$ and $\beta_2 = 5$.



(a) Weight exponent $\beta_1 = 3$

(b) Weight exponent $\beta_2 = 5$

Thank you for your attention!

Introduction
Lattice rules
CBC type constructions
Reduced CBC
Numerical results
Digital construction