Efficient usage and construction of QMC methods

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Some point sets ...

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

Approximate the integral of the $s$-variate function $f$

$$I(f) := \int_{[0,1]^s} f(x) \, dx$$

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

$$\int_{[0,1]^s} f(x) \, dx \approx \sum_{i=0}^{N-1} w_i f(x_i),$$

with points $\{x_0, \ldots, x_{N-1}\} \subseteq [0,1]^s$ 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

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

with deterministic quadrature points $\{x_0, \ldots, x_{N-1}\} \subseteq [0,1]^s$. 
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 $P = \{x_0, \ldots, x_{N-1}\} \subseteq [0, 1]^s$ 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

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

**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.

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

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 $\alpha$
- 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 $\{x_0, \ldots, x_{N-1}\}$ takes the form

$$e_{N,s}^2(Q_{N,s}, \mathcal{H}) = \int_{[0,1]^2s} K(x, y) \, dx \, dy - \frac{2}{N} \sum_{i=0}^{N-1} \int_{[0,1]^s} K(x_i, x) \, dx$$

$$+ \frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} K(x_i, x_j).$$
Weighted function spaces

Idea of weighted RKHS:

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

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

Common weight types:

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

\(^1\)See Sloan, Woźniakowski (1998)
Lattice rules in weighted RKHS
A rank-one lattice rule is a quasi-Monte Carlo rule with underlying point set $P_N \subseteq [0, 1]^s$ of the form

$$P_N = \left\{ \frac{k \ z \ \text{mod} \ N}{N} : 0 \leq k < N \right\} \subseteq [0, 1]^s,$$

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

**Figure 2:** Fibonacci lattice with $N = 55$ and $z = (1, 34)$ (left) and a rank-one lattice with $N = 32$ and $z = (1, 9)$ constructed by the CBC construction (right).
Let $\mathbb{Z}_* := \mathbb{Z} \setminus \{0\}$ and define $r_\alpha(h) := 1/|h|^\alpha$ and $r_\alpha(h) := \prod_{j=1}^s r_\alpha(h_j)$ for $h \in \mathbb{Z}_*$ and $h = (h_1, \ldots, h_s) \in \mathbb{Z}_*^s$, respectively.

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

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

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

$$\langle f, g \rangle_{K_{s,\alpha,\gamma}} = \sum_{u \subseteq \{1:s\}} \gamma_u^{-1} \sum_{h_u \in \mathbb{Z}_*^{|u|}} r_\alpha^{-1}(h_u) \hat{f}(h_u) \overline{\hat{g}(h_u)}$$

with $\hat{f}(h_u)$ being the $h_u$-th Fourier coefficient of $f$ given by

$$\hat{f}(h_u) = \int_{[0,1]^s} f(x) \exp(-2\pi i h_u \cdot x_u) \, dx.$$
Let $z \in \mathbb{Z}^s$ be the generating vector of a rank-1 lattice rule $\Lambda_{N,s}$ in the weighted Korobov space $\mathcal{H}(K_s,\alpha,\gamma)$. The squared worst-case error reads

$$e_{N,s}^2(z) = \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u \sum_{h_u \in D_u} r_\alpha(h_u)$$

where

$$D_u := \left\{ h_u \in \mathbb{Z}_{\ast}^{\left| u \right|} : h_u \cdot z_u \equiv 0 \pmod{N} \right\}.$$ 

There are connections between the worst-case error of the Korobov space $\mathcal{H}(K_s,2,\gamma)$ 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 \(z\) one component at a time, keeping all previously chosen components fixed.

Algorithm 1 Component-by-component algorithm in RKHS

\[
\begin{align*}
\text{for } d = 1 \text{ to } s & \text{ do} \\
\quad \text{for all } z_d \in \mathbb{U}_N & \text{ do} \\
\quad & \text{Calculate } e_{N,d}^2(z_1, z_2, \ldots, z_{d-1}, z_d) \\
\quad & z_d = \arg\min_{z \in \mathbb{U}_N} e_{N,d}^2(z_1, z_2, \ldots, z_{d-1}, z) \\
\text{end for} \\
\text{end for}
\end{align*}
\]

Notation: \(\mathbb{U}_N = \{z \in \{1, \ldots, N - 1\} : \gcd(z, N) = 1\}\)
\(= \{1, \ldots, N - 1\} \text{ for } N \text{ prime}\)

\(^2\)See Sloan, Reztsov (2001) or Korobov (1959)
The successive coordinate search construction

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

**Algorithm 2** Successive coordinate search (SCS) algorithm

\begin{align*}
\text{Input: } & z^0 \in \mathbb{Z}^s_N \\
\text{Output: } & z \in \mathbb{U}^s_N \\
\text{for } j = 1 \text{ to } s \text{ do} & \\
\text{for all } & z_j \in \mathbb{U}_N \text{ do} \\
& \text{Calculate } e^2_{N,s}(z_1, \ldots, z_{j-1}, z_j, z^0_j, z_{j+1}, \ldots, z^0_s) \\
& \text{end for} \\
& z_j = \arg\min_{z \in \mathbb{U}_N} e^2_{N,s}(z_1, \ldots, z_{j-1}, z_j, z^0_j, z_{j+1}, \ldots, z^0_s) \\
\text{end for} \\
\end{align*}

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

Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

\[ z \]

\[ Z_1 \]

The successive coordinate search algorithm:

\[ z \]

\[ Z_1 \quad Z_2 \quad Z_3 \quad Z_4 \quad Z_5 \quad Z_6 \quad Z_7 \]
Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

\[ z \]

\[ z_1 \]

The successive coordinate search algorithm:

\[ z \]

\[ z_1 \]
\[ z_2 \]
\[ z_3 \]
\[ z_4 \]
\[ z_5 \]
\[ z_6 \]
\[ z_7 \]
Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

The successive coordinate search algorithm:
Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

\[ z \]

\[ Z_1 \quad Z_2 \quad Z_3 \]

The successive coordinate search algorithm:

\[ z \]

\[ Z_1 \quad Z_2 \quad Z_3 \quad Z_4 \quad Z_5 \quad Z_6 \quad Z_7 \]
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\begin{align*}
z & \quad Z_1 & \quad Z_2 & \quad Z_3 & \quad Z_4 & \quad Z_5 & \quad Z_6 \\
\end{align*}
\]

The successive coordinate search algorithm:

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z & \quad Z_1 & \quad Z_2 & \quad Z_3 & \quad Z_4 & \quad Z_5 & \quad Z_6 & \quad Z_7 \\
\end{align*}
\]
Comparison between both constructions

Schema for both constructions:

The component-by-component algorithm:

The successive coordinate search algorithm:
Error convergence behavior

Assumptions:

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

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4 See, e.g., Dick, Kuo, Sloan (2014) - Acta Numerica review article
**Error convergence behavior**

**Assumptions:**

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

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

\[
\begin{align*}
\text{CBC construction}^4 & : e_{N,s}^2(z_{cbc}) \leq \left( \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha\lambda))|u|}{b^m} \right)^{\frac{1}{\lambda}} \\
\text{SCS algorithm}^5 & : e_{N,s}^2(z_{scs}) \leq \left( \sum_{j=1}^s \sum_{j \in u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha\lambda))|u|}{b^m} \right)^{\frac{1}{\lambda}}
\end{align*}
\]

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^4 See, e.g., Dick, Kuo, Sloan (2014) - Acta Numerica review article
Assumptions:
- \( N = b^m \) with \( b \) prime, \( m \in \mathbb{N} \) and general weights \( \gamma = (\gamma_u)_{u \subseteq \{1:s\}} \)
- \( z^0 \in \mathbb{Z}_N^s \) arbitrary initial vector for the SCS algorithm
- \( z_{\text{cbc}} \) and \( z_{\text{scs}} \) generating vectors constructed by CBC/SCS algorithm

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

**CBC construction** \(^4\)

\[
e^2_{N,s}(z_{\text{cbc}}) \leq \left( \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^{\lambda} \frac{2(2\zeta(\alpha \lambda)) |u|}{b^m} \right)^{\frac{1}{x}}
\]

**SCS algorithm** \(^5\)

\[
e^2_{N,s}(z_{\text{scs}}) \leq \left( \sum_{j=1}^{s} \sum_{j \in u \subseteq \{1:s\}} \gamma_u^{\lambda} \frac{2(2\zeta(\alpha \lambda)) |u|}{b^m} \right)^{\frac{1}{x}}
\]

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

\(^4\) See, e.g., Dick, Kuo, Sloan (2014) - Acta Numerica review article
The CBC and the SCS construction can both be implemented in a fast way\(^6\) by exploiting the (block-)circulant structure of the matrix

\[
\Omega_N := \left[ \omega \left( \frac{kz \mod N}{N} \right) \right]_{k=0,\ldots,N-1}
\]

to perform a fast matrix-vector multiplication using FFT.

**Complexity for \(\gamma_u\) of the form \(\prod_{j \in u} \gamma_j\)**

- The fast versions of the algorithms allow for the construction of generating vectors using \(O(s N \log(N))\) 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 \(z^0\).

Construction method for the SCS algorithm

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

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

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

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

Assumptions:

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

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

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7See Dick, Kritzer, Leobacher, Pillichshammer (2015)
8See E., Kritzer (2018) - (submitted for publication - available on arXiv)
The reduced construction

Assumptions:

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

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

Reduced CBC construction\(^7\)

- Set \( z_1 = 1 \).
- **For** \( d = 2 \) **to** \( s \):
  - \( \diamond \) Assume that \( z_1, \ldots, z_{d-1} \) have already been found.
  - \( \diamond \) Choose \( z_d \in Z_{N,w_d} \) such that
    \[ e_{N,d}^2((Y_1 z_1, \ldots, Y_{d-1} z_{d-1}, Y_d z_d)) \]
    is minimized as a function of \( z_d \).
- Obtain the generating vector \( z = (Y_1 z_1, \ldots, Y_s z_s) \).

Reduced SCS algorithm\(^8\)

- **Input:** Starting vector \( z^0 \) with \( z^0 = (z^0_1, \ldots, z^0_s) \in \mathbb{Z}_N^s \).
- **For** \( j = 1 \) **to** \( s \):
  - \( \diamond \) Assume that \( z_1, \ldots, z_{j-1} \) have already been selected.
  - \( \diamond \) Choose \( z_j \in Z_{N,w_j} \) such that
    \[ e_{N,s}^2((Y_1 z_1, \ldots, Y_{j-1} z_{j-1}, Y_j z_j, z^0_{j+1:s})) \]
    is minimized as a function of \( z_j \).
- Obtain the generating vector \( z = (Y_1 z_1, \ldots, Y_s z_s) \).

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\(^7\) See Dick, Kritzer, Leobacher, Pillichshammer (2015)
\(^8\) See E., Kritzer (2018) - (submitted for publication - available on arXiv)
Let \( z_{\text{cbc}} = (Y_1z_1, \ldots, Y_sz_s) \) and \( z_{\text{scs}} = (Y_1\bar{z}_1, \ldots, Y_s\bar{z}_s) \) be constructed by the reduced CBC or reduced SCS algorithm with arbitrary initial vector \( z^0 \in \mathbb{Z}_N^s \), respectively. Let \( \alpha > 1 \), then \( \forall \lambda \in (\frac{1}{\alpha}, 1] \) the worst-case error satisfies:

\[
\begin{align*}
\text{Reduced CBC construction} & \quad \mathbb{E}(e_N, s(z_{\text{cbc}})) \leq \left( \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma^u \lambda^{|u|} b_{\max(0, m - \max_{j \in u} w_j)} \right)^{1/\lambda} \\
\text{Reduced SCS algorithm} & \quad \mathbb{E}(e_N, s(z_{\text{scs}})) \leq \left( \sum_{j=1}^{s} \sum_{u \subseteq \{1:s\}} \gamma^u \lambda^{|u|} b_{\max(0, m - w_j)} \right)^{1/\lambda}
\end{align*}
\]

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

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9 See Dick, Kritzer, Leobacher, Pillichshammer (2015)
10 See E., Kritzer (2018) - (submitted for publication - available on arXiv)
Error convergence behavior

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

**Reduced CBC construction**

\[
e_{N,s}^2(z_{cbc}) \leq \left( \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha \lambda))^{\lvert u \rvert}}{b_{\max(0,m-\max_{j \in u} w_j)}} \right)^{\frac{1}{\lambda}}
\]

**Reduced SCS algorithm**

\[
e_{N,s}^2(z_{scs}) \leq \left( \sum_{j=1}^{s} \sum_{j \in u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha \lambda))^{\lvert u \rvert}}{b_{\max(0,m-w_j)}} \right)^{\frac{1}{\lambda}}
\]

---

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

**Reduced CBC construction** \(^9\)

\[
e^{2}_{N,s}(z_{\text{cbc}}) \leq \left( \sum_{\emptyset \neq u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha \lambda)) |u|}{b^{\max(0,m-\max_{j \in u} w_j)}} \right)^{\frac{1}{\lambda}}
\]

**Reduced SCS algorithm** \(^10\)

\[
e^{2}_{N,s}(z_{\text{scs}}) \leq \left( \sum_{j=1}^{s} \sum_{j \in u \subseteq \{1:s\}} \gamma_u^\lambda \frac{2(2\zeta(\alpha \lambda)) |u|}{b^{\max(0,m-w_j)}} \right)^{\frac{1}{\lambda}}
\]

For product weights \( \gamma_u = \prod_{j \in u} \gamma_j \) the error is \( O(N^{-\alpha/2+\delta}) \) 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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\(^10\)See E., Kritzer (2018) - (submitted for publication - available on arXiv)
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

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

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

\[
\Omega_{b^m,w} := \left[ \omega \left( \frac{k b^w z \mod N}{N} \right) \right]_{z \in \mathbb{Z}_{N,w}}^{k=0,\ldots,N-1}
\]

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** \( \gamma_u = \prod_{j \in u} \gamma_j \)

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\(^{11}\text{See Dick, Kritzer, Leobacher, Pillichshammer (2015)}\)

\(^{12}\text{See E., Kritzer (2018) - (submitted for publication - available on arXiv)}\)
Computational complexity of the reduced constructions

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<table>
<thead>
<tr>
<th>Reduced CBC construction$^{11}$</th>
<th>Reduced SCS algorithm$^{12}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product weights</strong> $\gamma_u = \prod_{j \in u} \gamma_j$</td>
<td></td>
</tr>
<tr>
<td>$O \left( N \log N + \min(s, s^<em>) N + \sum_{j=1}^{\min(s, s^</em>)} (m - w_j) b^{m-w_j} \right)$</td>
<td></td>
</tr>
</tbody>
</table>

$^{11}$See Dick, Kritzer, Leobacher, Pillichshammer (2015)
$^{12}$See E., Kritzer (2018) - (submitted for publication - available on arXiv)
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** $\gamma_u = \prod_{j \in u} \gamma_j$

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

Unreduced constructions: $O \left( s N \log N \right)$

---

\(^{11}\)See Dick, Kritzer, Leobacher, Pillichshammer (2015)

\(^{12}\)See E., Kritzer (2018) - (submitted for publication - available on arXiv)
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\(^1\)

| Product weights $\gamma_u = \prod_{j \in u} \gamma_j$

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

Unreduced constructions: $O \left( s \, N \log N \right)$

Reduced SCS algorithm\(^2\)

| POD weights $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$

---

\(^1\)See Dick, Kritzer, Leobacher, Pillichshammer (2015)
\(^2\)See E., Kritzer (2018) - (submitted for publication - available on arXiv)
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\(^{11}\)  

**Product weights** \( \gamma_u = \prod_{j \in u} \gamma_j \)

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

Unreduced constructions: \( \mathcal{O} (s N \log N) \)

Reduced SCS algorithm\(^{12}\)  

**POD weights** \( \gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j \)

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

\(^{11}\)See Dick, Kritzer, Leobacher, Pillichshammer (2015)  
\(^{12}\)See E., Kritzer (2018) - (submitted for publication - available on arXiv)
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 $w_{s^*} < m$

<table>
<thead>
<tr>
<th>Reduced CBC construction$^{11}$</th>
<th>Reduced SCS algorithm$^{12}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product weights</strong> $\gamma_u = \prod_{j \in u} \gamma_j$</td>
<td><strong>Product weights</strong> $\gamma_u = \prod_{j \in u} \gamma_j$</td>
</tr>
<tr>
<td>$\mathcal{O} \left( N \log N + \min(s, s^<em>) N + \sum_{j=1}^{\min(s, s^</em>)} (m - w_j) b^{m-w_j} \right)$</td>
<td>$\mathcal{O} \left( N \log N + \min(s, s^<em>) N + \sum_{j=1}^{\min(s, s^</em>)} (m - w_j) b^{m-w_j} \right)$</td>
</tr>
</tbody>
</table>

Unreduced constructions: $\mathcal{O}(s N \log N)$

| POD weights $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$ | POD weights $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$ |
| $\mathcal{O} \left( N \log N + \min(s, s^*)^2 N + \sum_{j=1}^{\min(s, s^*)} (m - w_j) b^{m-w_j} \right)$ | $\mathcal{O} \left( N \log N + \min(s, s^*)^2 N + \sum_{j=1}^{\min(s, s^*)} (m - w_j) b^{m-w_j} \right)$ |

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 $\gamma_u = \prod_{j \in u} \gamma_j, s = 100, \alpha = 2, b = 3, w_j = \lfloor 2 \log_b j \rfloor$

Number of points $N = b^m$
(a) $\gamma = (\gamma_j)^s_{j=1}$ with $\gamma_j = (0.2)^j$
(b) $\gamma = (\gamma_j)^s_{j=1}$ with $\gamma_j = (0.8)^j$
(c) $\gamma = (\gamma_j)^s_{j=1}$ with $\gamma_j = 1/j^3$
(d) $\gamma = (\gamma_j)^s_{j=1}$ with $\gamma_j = 1/j^8$
Error convergence for Korobov space with \( \gamma_u = \prod_{j \in u} \gamma_j \), \( s = 100 \), \( \alpha = 2 \), \( b = 3 \), \( w_j = \lfloor \frac{7}{2} \log_b j \rfloor \)

Number of points \( N = b^m \)

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

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

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

(d) \( \gamma = (\gamma_j)_{j=1}^s \) with \( \gamma_j = 1/j^8 \)
Table 1: Computation times (in seconds) for constructing generating vectors $z$ via the unreduced (normal font) and reduced SCS (bold font) algorithm. Constructed for Korobov space with $\gamma_u = \prod_{j \in u} \gamma_j$, $\alpha = 2$, $b = 2$, $\gamma_j = (0.7)^j$ and $w_j = \lfloor 3 \log_b j \rfloor$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$s = 50$</th>
<th>$s = 100$</th>
<th>$s = 500$</th>
<th>$s = 1000$</th>
<th>$s = 2000$</th>
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<tbody>
<tr>
<td>10</td>
<td>0.0275</td>
<td>0.0516</td>
<td>0.256</td>
<td>0.516</td>
<td>1.03</td>
</tr>
<tr>
<td></td>
<td><strong>0.00408</strong></td>
<td><strong>0.00327</strong></td>
<td><strong>0.00354</strong></td>
<td><strong>0.00347</strong></td>
<td><strong>0.00329</strong></td>
</tr>
<tr>
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<td>0.383</td>
<td>0.756</td>
<td>1.56</td>
</tr>
<tr>
<td></td>
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<td><strong>0.00504</strong></td>
<td><strong>0.00612</strong></td>
<td><strong>0.00516</strong></td>
<td><strong>0.00794</strong></td>
</tr>
<tr>
<td>14</td>
<td>0.0792</td>
<td>0.14</td>
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<td>2.82</td>
</tr>
<tr>
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<td><strong>0.0136</strong></td>
<td><strong>0.0163</strong></td>
<td><strong>0.0138</strong></td>
<td><strong>0.0138</strong></td>
</tr>
<tr>
<td>16</td>
<td>0.204</td>
<td>0.388</td>
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</tr>
<tr>
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<td><strong>0.0434</strong></td>
<td><strong>0.0434</strong></td>
<td><strong>0.0423</strong></td>
<td><strong>0.0462</strong></td>
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<tr>
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<td>6.89</td>
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<tr>
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<td><strong>0.843</strong></td>
<td><strong>1.4</strong></td>
<td><strong>1.51</strong></td>
<td><strong>1.37</strong></td>
<td><strong>1.36</strong></td>
</tr>
</tbody>
</table>
Convergence for Korobov space with \( \gamma_u = |u| \prod_{j \in u} \gamma_j \), \( s = 500 \), \( \alpha = 2 \), \( b = 3 \), \( w_j = \lceil 3 \log_b j \rceil \).
Computation times

Table 2: Computation times (in seconds) for constructing the generating vector $z$ 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 $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$ where $\Gamma_j = j^4$, $\gamma_j = j^{-6}$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$s = 50$</th>
<th>$s = 100$</th>
<th>$s = 200$</th>
<th>$s = 500$</th>
<th>$s = 1000$</th>
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<td><strong>0.0184</strong></td>
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<td>180</td>
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<tr>
<td></td>
<td><strong>0.0757</strong></td>
<td><strong>0.0876</strong></td>
<td><strong>0.0932</strong></td>
<td><strong>0.115</strong></td>
<td><strong>0.157</strong></td>
</tr>
<tr>
<td>16</td>
<td>1.62</td>
<td>6.31</td>
<td>24.2</td>
<td>148</td>
<td>589</td>
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<tr>
<td></td>
<td><strong>0.576</strong></td>
<td><strong>0.583</strong></td>
<td><strong>0.576</strong></td>
<td><strong>0.631</strong></td>
<td><strong>0.585</strong></td>
</tr>
<tr>
<td>18</td>
<td>5.77</td>
<td>21.8</td>
<td>83.8</td>
<td>512</td>
<td>2013</td>
</tr>
<tr>
<td></td>
<td><strong>3.3</strong></td>
<td><strong>4.86</strong></td>
<td><strong>4.85</strong></td>
<td><strong>4.85</strong></td>
<td><strong>5.26</strong></td>
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<tr>
<td>20</td>
<td>27.8</td>
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<tr>
<td></td>
<td><strong>17.4</strong></td>
<td><strong>59.9</strong></td>
<td><strong>61.4</strong></td>
<td><strong>58.9</strong></td>
<td><strong>61.7</strong></td>
</tr>
</tbody>
</table>
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 $\mathbb{Z}_b$
- $P_N = P_{b^m} = \{x_0, \ldots, x_{b^m-1}\}$ with $x_i = (x_{i,1}, \ldots, x_{i,s})$ 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 $P_{b^m} = \{x_0, \ldots, x_{b^m-1}\}$ is called a digital net in base $b$. 

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QMC software and generators

1. Software on Dirk Nuyens’ webpage to apply quasi-Monte Carlo:
   • The Magic Point Shop!:
   • 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

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

with $c_{i,k}^{(j)} = \sum_{k=1}^{m} c_{i,k}^{(j)} 2^k \in \{0, 1, \ldots, N - 1\}$ 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 $\alpha$ (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 $\Delta_j = \sum_{k=1}^{\infty} d_k^{(j)} b^{-k}$
   - $P_{b^m} = \{x_0 \oplus \Delta, \ldots, x_{b^m-1} \oplus \Delta\}$ with component-wise digit-wise addition in base $b$

2. Linear Matousek scrambling:
   - Consider point $x \in [0, 1]^s$ with components $x_j = \sum_{k=1}^{\infty} x_k^{(j)} b^{-k}$
   - Linear matrix scramble: $x_j \rightarrow \tilde{x}_j = \sum_{k=1}^{\infty} \tilde{x}_k^{(j)} b^{-k}$ with

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

   - Expressible via generating matrices: Set $\tilde{C}_j := M_j \cdot C_j$ 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.
Numerical example 2

Function $g(x) = \prod_{j=1}^{s} \left( 1 + \frac{2x_j - a}{j^\beta} \right)$ 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 $\beta_2 = 5$.

![Graphs showing integration error vs. number of points for different orderings of points and weight exponents.](image-url)
Thank you for your attention!