

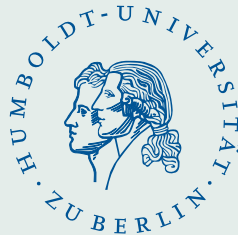
# Convergence of randomized Quasi-Monte Carlo methods for mixed-integer two-stage stochastic programs

H. Leövey und W. Römisch

Axpo, Baden, Switzerland

Humboldt-University Berlin

<http://www.math.hu-berlin.de/~romisch>



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## Introduction

- A breakthrough was obtained for computing high-dimensional integrals by means of randomized Quasi-Monte Carlo (RQMC) methods for integrands with mixed first derivatives (Kuo-Sloan 05).
- RQMC methods for the numerical quadrature in stochastic optimization models replace the stochastic parameter by a finite number of (random) scenarios having equal probabilities and lead to large scale approximating programs.
- Stochastic two-stage mixed-integer optimization models lead to discontinuous integrands, where the specific structure of polyhedral continuity regions and discontinuity facets is hidden.
- For RQMC methods on discontinuous integrands of the form  $g(x)\mathbf{1}_B(x)$  on  $[0, 1]^d$ , where  $g$  has finite HK variation and  $B$  is convex polyhedral, He-Wang 15 obtained the convergence rate

$$O\left(n^{-\frac{1}{2} - \frac{1}{4d_* - 2} + \delta}\right)$$

where  $d_*$  is the number of coordinate axes which are not parallel to the discontinuity faces of  $B$  and  $\delta > 0$  is small.

## Mixed-integer two-stage stochastic programs

$$\min \left\{ \langle c, x \rangle + \int_{\mathbb{R}^d} \Phi(q(\xi), h(\xi) - Vx) \rho(\xi) d\xi : x \in X \right\},$$

$$\Phi(u, t) := \inf \left\{ \langle u_1, y_1 \rangle + \langle u_2, y_2 \rangle : W_1 y_1 + W_2 y_2 \leq t, y_1 \in \mathbb{R}^{m_1}, y_2 \in \mathbb{Z}^{m_2} \right\}$$

for all  $(u, t) \in \mathbb{R}^{m_1+m_2} \times \mathbb{R}^r$ , with  $c \in \mathbb{R}^m$ , a closed subset  $X$  of  $\mathbb{R}^m$ ,  $(r, m_1)$  and  $(r, m_2)$ -matrices  $W_1$  and  $W_2$ ,  $(r, m)$ -matrix  $V$ , affine functions  $q(\xi) \in \mathbb{R}^{m_1+m_2}$ ,  $h(\xi) \in \mathbb{R}^r$ , and a probability density  $\rho$  on  $\mathbb{R}^d$ .

### Assumptions:

**(B1)** The matrices  $W_1$  and  $W_2$  have only rational elements.

**(B2)** For each pair  $(x, \xi) \in X \times \mathbb{R}^d$  it holds that  $h(\xi) - Vx \in \mathcal{T}$ , where

$$\mathcal{T} := \{t \in \mathbb{R}^r : \exists (y_1, y_2) \in \mathbb{R}^{m_1} \times \mathbb{Z}^{m_2} \text{ such that } W_1 y_1 + W_2 y_2 \leq t\}.$$

**(B3)** For each  $\xi \in \mathbb{R}^d$  the recourse cost  $q(\xi)$  belongs to the dual feasible set

$$\mathcal{U} := \{u = (u_1, u_2) \in \mathbb{R}^{m_1+m_2} : \exists v \in \mathbb{R}_-^r \text{ such that } W_1^\top v = u_1, W_2^\top v = u_2\}.$$

**(B4)** The number of integer decisions is finite.

### Proposition:

Assume (B1)–(B4). The function  $\Phi$  is finite and lower semicontinuous on  $\mathcal{U} \times \mathcal{T}$  and there exists finitely many Borel sets  $U_\nu \times B_\nu$ ,  $\nu \in \mathcal{N}$ , covering  $\mathcal{U} \times \mathcal{T}$  such that their closure is convex polyhedral and  $\Phi$  is bilinear in  $(u, t)$  on each  $U_\nu \times B_\nu$ .  $\Phi$  may have points of discontinuity at the boundaries of  $U_\nu \times B_\nu$ .

**Example:** (Schultz-Stougie-van der Vlerk 98)

**Stochastic multi-knapsack problem:**

$\min \rightarrow \max$ ,  $m = 2$ ,  $m_1 = 0$ ,  $m_2 = 4$ ,  $d = s = 2$ ,  $X = [-5, 5]^2$ ,  
 $c = (1.5, 4)$ ,  $h(\xi) = \xi$ ,  $q(\xi) \equiv q = (16, 19, 23, 28)$ ,  $y_i \in \{0, 1\}$ ,  
 $i = 1, 2, 3, 4$ ,  $P \sim U(\{5, 10, 15\}^2)$  (discrete)

$$V(\xi) \equiv V = \begin{pmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} \end{pmatrix} \quad W = \begin{pmatrix} 2 & 3 & 4 & 5 \\ 6 & 1 & 3 & 2 \end{pmatrix}$$

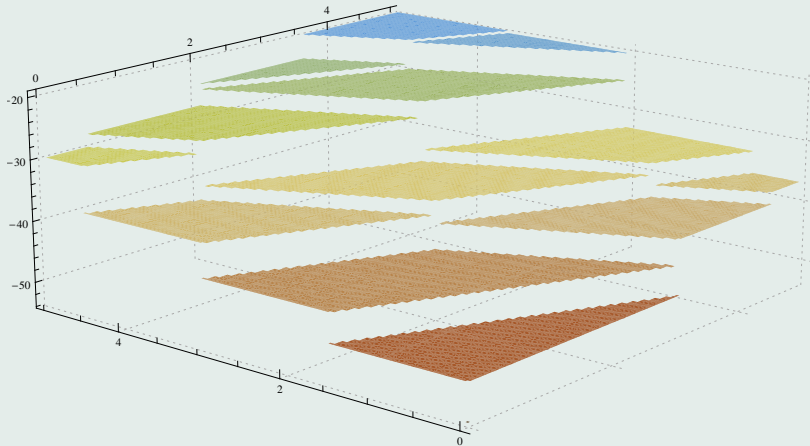


Illustration of the expected recourse function with discrete uniform probability distribution

## Quasi-Monte Carlo methods

We consider the approximate computation of

$$I_d(g) = \int_{[0,1]^d} g(x) dx$$

by a Quasi-Monte Carlo (QMC) method

$$Q_n(g) = \frac{1}{n} \sum_{j=1}^n g(x^j)$$

with (deterministic) points  $x^j$ ,  $j = 1, \dots, n$ , from  $[0, 1]^d$ .

Worst-case quadrature error in a normed space  $(\mathbb{G}_d, \|\cdot\|)$ :

$$e_n(\mathbb{G}_d) = \sup_{\|g\| \leq 1} |Q_n(g) - I_d(g)|$$

The convergence rate  $e_n(\mathbb{G}_d) = O(n^{-1}(\log n)^{d-1})$  can be achieved in suitable normed spaces  $\mathbb{G}_d$  like  $\text{BV}_{\text{HK}}([0, 1]^d)$ .

Quasi-Monte Carlo methods often have good convergence properties if the integrands have **low effective dimension**.

# Randomized QMC methods

Randomized versions of QMC point sets have the properties that

(Owen 95, L'Ecuyer-Lemieux 02, Dick-Pillichshammer 10)

- (i) each point of the randomized point set has a uniform distribution over  $[0, 1)^d$  (**uniformity**), and
- (ii) the QMC properties are preserved under the randomization with probability one (**equidistribution**).

Examples of randomization techniques are

- (a) **random shifts** of lattice rules,
- (b) **scrambling**, i.e., random permutations of the integers in  $\mathbb{Z}_b = \{0, 1, \dots, b-1\}$  applied to the digits in  $b$ -adic representation,
- (c) **affine scrambling** which generates random digits by random linear transformations of the original digits, where the elements of all matrices and vectors are chosen randomly, independently and uniformly over  $\mathbb{Z}_b$ .

Properties (i) and (ii) enable error estimates and lead to improved convergence results compared to the original QMC method.

## Weighted tensor product Sobolev spaces

$$\mathbb{G}_d = \mathcal{W}_{2,\gamma,\text{mix}}^{(1,\dots,1)}([0, 1]^d) = \bigotimes_{i=1}^d W_{2,\gamma_i}^1([0, 1]),$$

where  $W_{2,\gamma_i}^1([0, 1])$  is the Sobolev space of absolutely continuous functions  $h$  on  $[0, 1]$  with derivative  $h' \in L_2([0, 1])$ . Its inner product is

$$\langle h, \tilde{h} \rangle = \left( \int_0^1 h(t) dt \right) \left( \int_0^1 \tilde{h}(t) dt \right) + \gamma_i^{-1} \int_0^1 h'(t) \tilde{h}'(t) dt.$$

The weighted norm  $\|g\|_\gamma = \sqrt{\langle g, g \rangle_\gamma}$  and inner product of  $\mathbb{G}_d$  are given by

$$\langle g, \tilde{g} \rangle_\gamma = \sum_{u \subseteq \mathfrak{D}} \gamma_u^{-1} \int_{[0,1]^{|u|}} I_u g(t^u) I_u \tilde{g}(t^u) dt^u,$$

where  $\mathfrak{D} = \{1, \dots, d\}$ , the weights  $\gamma_i$  are positive nonincreasing, and

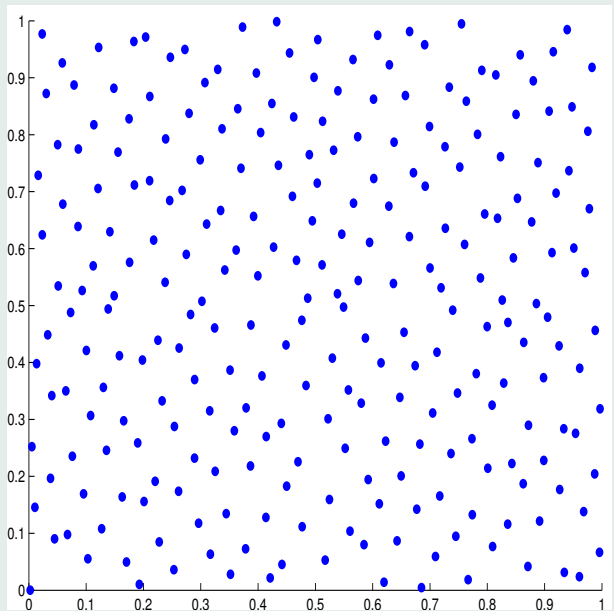
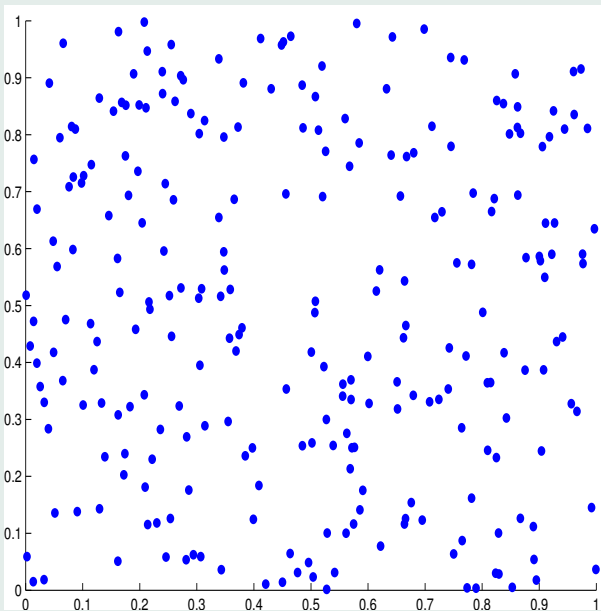
$$I_u g(t^u) = \int_{[0,1]^{d-|u|}} \frac{\partial^{|u|}}{\partial t^u} g(t) dt^{-u} \quad \text{and} \quad \gamma_u = \prod_{i \in u} \gamma_i$$

for  $u \subseteq \mathfrak{D}$ , where  $\gamma_\emptyset = 1$ . For  $u \subseteq \mathfrak{D}$  we use the notation  $|u|$  for its cardinality,  $-u$  for  $\mathfrak{D} \setminus u$  and  $t^u$  for the  $|u|$ -dimensional vector with components  $t_j$ ,  $j \in u$ .

Moreover,  $\mathbb{G}_d$  is a **reproducing kernel Hilbert space with the kernel**

$$K_{d,\gamma}(t, s) = \prod_{i=1}^d \left( 1 + \gamma_i (0.5 B_2(|t_i - s_i|) + B_1(t_i) B_1(s_i)) \right) \quad (t, s \in [0, 1]^d),$$

where  $B_1(t) = t - \frac{1}{2}$  and  $B_2(t) = t^2 - t + \frac{1}{6}$ .



Comparison of  $n = 2^7$  MC Mersenne Twister points and randomly binary shifted Sobol' points in dimension  $d = 500$ , projection onto the 8. and 9. components

**Randomly scrambled Sobol' sequences** admits the following convergence rate of the root mean square error on  $\mathcal{W}_{2,\gamma,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$

$$\sup_{\|g\|_{\gamma} \leq 1} \sqrt{\mathbb{E}|Q_n(\omega)(g) - I_d(g)|^2} \leq C_d n^{-\frac{3}{2}} (\log n)^{\frac{d-1}{2}}.$$

(Dick-Pillichshammer 10)

Usually a rate close to  $O(n^{-1})$  is observable unless the sample sizes become huge.



## Randomly shifted lattice rules

Is the random vector  $\Delta$  uniformly distributed on  $[0, 1]^d$ , we consider

$$Q_n(\omega)(g) = \frac{1}{n} \sum_{j=1}^n g\left(\left\{\frac{(j-1)}{n}\mathbf{g} + \Delta(\omega)\right\}\right).$$

$\{\{z\}\}$  means taking componentwise the fractional part of  $z$

Let  $n \in \mathbb{N}$  be prime and  $g \in \mathcal{W}_{2,\gamma,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$ .

Then  $\mathbf{g} \in \mathbb{Z}_+^d$  can be constructed componentwise such that for each  $\delta \in (0, \frac{1}{2}]$  there exists a constant  $C(\delta) > 0$  with

$$\sup_{\|g\|_\gamma \leq 1} \sqrt{\mathbb{E}|Q_n(\omega)(g) - I_d(g)|^2} \leq C(\delta) n^{-1+\delta},$$

where the constant  $C(\delta)$  increases if  $\delta$  decreases, but does not depend on the dimension  $d$  if the sequence  $(\gamma_j)$  satisfies

$$\sum_{j=1}^{\infty} \gamma_j^{\frac{1}{2(1-\delta)}} < \infty \quad (\text{e.g. } \gamma_j = \frac{1}{j^3}).$$

(Sloan-Kuo-Joe 02, Kuo 03, Nuyens-Cools 06)

# Transformation of integrals for general densities $\rho$

We consider the function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  and the integral

$$\int_{\mathbb{R}^d} f(\xi) \rho(\xi) d\xi.$$

Although there are general distributional transforms for probability distributions from  $\mathbb{R}^d$  to  $[0, 1]^d$  based on using conditional distributions (Rosenblatt 52, Rüschendorf 09) we consider here a more restrictive two-step procedure:

**Step 1:** Transformation of the multivariate density function  $\rho$  on  $\mathbb{R}^d$  into a product-density  $\rho(\xi) = \prod_{k=1}^d \rho_k(\xi_k)$  with  $d$  independent one-dimensional marginal densities  $\rho_k$ .

**Example:** If  $P$  is normal with mean 0 and nonsingular covariance matrix  $\Sigma$ , then for any matrix  $A$  with  $\Sigma = A A^\top$  the density of  $P \circ A$  has product form.

**Step 2:** Let  $\rho_k$  denote the independent marginal densities and  $\phi_k$  the marginal distribution functions of the probability distribution  $P$ . With the transformations  $x_k = \phi_k(\xi_k)$ ,  $k \in \mathfrak{D}$ , one obtains

$$\int_{\mathbb{R}^d} f(\xi) \prod_{k=1}^d \rho_k(\xi_k) d\xi = \int_{[0,1]^d} f(\phi_1^{-1}(x_1), \dots, \phi_d^{-1}(x_d)) dx_1 \cdots dx_d$$

# ANOVA decomposition and effective dimension

We consider a multivariate function  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  and intend to compute the mean of  $f(\xi)$ , i.e.

$$\mathbb{E}[f(\xi)] = I_{d,\rho}(f) = \int_{\mathbb{R}^d} f(\xi_1, \dots, \xi_d) \rho(\xi_1, \dots, \xi_d) d\xi_1 \cdots d\xi_d,$$

where  $\xi$  is a  $d$ -dimensional random vector with density

$$\rho(\xi) = \prod_{k=1}^d \rho_k(\xi_k) \quad (\xi \in \mathbb{R}^d).$$

We are interested in a representation of  $f$  consisting of  $2^d$  terms

$$f(\xi) = f_0 + \sum_{i=1}^d f_i(\xi_i) + \sum_{\substack{i,j=1 \\ i < j}}^d f_{ij}(\xi_i, \xi_j) + \cdots + f_{12\dots d}(\xi_1, \dots, \xi_d).$$

The previous representation can be more compactly written as

$$(*) \quad f(\xi) = \sum_{u \subseteq \mathcal{D}} f_u(\xi^u),$$

where  $\mathcal{D} = \{1, \dots, d\}$  and  $\xi^u$  contains only the components  $\xi_j$  with  $j \in u$  and belongs to  $\mathbb{R}^{|u|}$ . Here,  $|u|$  denotes the cardinality of  $u$ .

Next we make use of the space  $L_{2,\rho}(\mathbb{R}^d)$  of all square integrable functions with inner product

$$\langle f, \tilde{f} \rangle_\rho = \int_{\mathbb{R}^d} f(\xi) \tilde{f}(\xi) \rho(\xi) d\xi.$$

A representation of the form (\*) of  $f \in L_{2,\rho}(\mathbb{R}^d)$  is called **ANOVA decomposition of  $f$**  if

$$\int_{\mathbb{R}} f_u(\xi^u) \rho_k(\xi_k) d\xi_k = 0 \quad (\text{for all } k \in u \text{ and } u \subseteq \mathfrak{D}).$$

The ANOVA terms  $f_u$ ,  $\emptyset \neq u \subseteq \mathfrak{D}$ , are orthogonal in  $L_{2,\rho}(\mathbb{R}^d)$ , i.e.

$$\langle f_u, f_v \rangle_\rho = \int_{\mathbb{R}^d} f_u(\xi) f_v(\xi) \rho(\xi) d\xi = 0 \quad \text{if and only if } u \neq v,$$

The ANOVA terms  $f_u$  allow a representation in terms of (so-called) **(ANOVA) projections**, i.e. for  $\xi^k = \Pi_k \xi = (\xi_1, \dots, \xi_{k-1}, \xi_{k+1}, \dots, \xi_d)$

$$(P_k f)(\xi^k) = \int_{-\infty}^{\infty} f(\xi_1, \dots, \xi_{k-1}, s, \xi_{k+1}, \dots, \xi_d) \rho_k(s) ds \quad (k \in \mathfrak{D}).$$

and

$$P_u f(\xi^u) = \left( \prod_{k \in u} P_k \right) f(\xi^u) \quad (\xi^u = \Pi_u \xi, u \subseteq \mathfrak{D}).$$

Then it holds (Kuo-Sloan-Wasilkowski-Woźniakowski 10):

$$f_u = \left( \prod_{j \in u} (I - P_j) \right) P_{-u}(f) = P_{-u}(f) + \sum_{v \subsetneq u} (-1)^{|u|-|v|} P_{-v}(f),$$

( $-u$  denotes the complement  $\mathfrak{D} \setminus u$ ).

We consider the variances of  $f$  and  $f_u$

$$\sigma^2(f) = \|f - I_{d,\rho}(f)\|_{2,\rho}^2 \quad \text{und} \quad \sigma_u^2(f) = \|f_u\|_{2,\rho}^2$$

and obtain

$$\sigma^2(f) = \|f\|_{L_2}^2 - (I_{d,\rho}(f))^2 = \sum_{\emptyset \neq u \subseteq \mathfrak{D}} \sigma_u^2(f).$$

The quotients

$$\frac{\sigma_u^2(f)}{\sigma^2(f)} \quad (u \subseteq \mathfrak{D})$$

are called **global sensitivity indices** for the importance of the group  $\xi_j$ ,  $j \in u$ , of variables of  $f$ . For small  $\varepsilon \in (0, 1)$  (e.g.  $\varepsilon = 0.01$ )

$$d_S(\varepsilon) = \min \left\{ s \in \mathfrak{D} : \sum_{|u| \leq s} \frac{\sigma_u^2(f)}{\sigma^2(f)} \geq 1 - \varepsilon \right\}$$

is called **effective (superposition) dimension** of  $f$ .

The following estimate is valid

$$(+)\quad \left\| f - \sum_{|u| \leq d_S(\varepsilon)} f_u \right\|_{2,\rho} \leq \sqrt{\varepsilon} \sigma(f),$$

i.e., the function  $f$  is approximated by a truncated ANOVA decomposition which contains all ANOVA terms  $f_u$  such that  $|u| \leq d_S(\varepsilon)$ .

If  $f$  is nonsmooth and the ANOVA terms  $f_u$ ,  $|u| \leq d_S(\varepsilon)$ , are smoother than  $f$ , the estimate (+) means an approximate smoothing of  $f$ .

Unfortunately, the effective superposition dimension is hardly computable in general, but an upper bound can be computed by finding the smallest  $s \in \mathcal{D}$  such that

$$\sum_{v \subseteq \{1, \dots, s\}} \sigma_v^2(f) \geq (1 - \varepsilon) \sigma^2(f).$$

This relies on a particular integral representation of the left-hand side, where the occurring integrals are computed approximately by means of Monte Carlo or Quasi-Monte Carlo methods based on large samples.

# ANOVA terms of mixed-integer two-stage integrands

## Example:

Let  $d = 3$ ,  $P$  denote a three-dimensional probability distribution with independent continuous marginal densities  $\rho_i$  and marginal distribution functions  $\varphi_i$ ,  $i = 1, 2, 3$ . We consider the convex polyhedral cone

$$\mathcal{K} = \{(t_1, t_2, t_3) \in \mathbb{R}^3 : 0 \leq t_3 \leq t_1, 0 \leq t_2 \leq t_3, 0 \leq t_1 \leq t_2\}$$

and the infimal function

$$\Phi(t) = \begin{cases} 1 & , t \in \text{int } \mathcal{K} \\ 0 & , \text{otherwise,} \end{cases}$$

which is piecewise constant and lower semicontinuous. The infimal value function is simple, but typical for pure integer optimization models.

Let the integrand  $f$  be defined by

$$f(\xi) = \Phi(\xi - Vx),$$

where we let for simplicity  $x = 0$ .

Then its  $k$ th first order ANOVA projection  $P_k f$  is

$$(P_k f)(\xi^k) = \int_{-\infty}^{+\infty} \Phi(\xi_s^k) \rho_k(s) ds,$$

where  $\xi^k \in \Pi_k \mathbb{R}^3$ ,  $k \in \{1, 2, 3\}$ , and

$$\Pi_1(\mathcal{K}) = \{(t_2, t_3) \in \mathbb{R}^2 : 0 \leq t_2 \leq t_3\}, \quad \Pi_2(\mathcal{K}) = \{(t_1, t_3) \in \mathbb{R}^2 : 0 \leq t_3 \leq t_1\}$$

$$\Pi_3(\mathcal{K}) = \{(t_1, t_2) \in \mathbb{R}^2 : 0 \leq t_1 \leq t_2\}.$$

We obtain

$$\begin{aligned}
 P_1 f(\xi^1) = P_1 f(\xi_2, \xi_3) &= \begin{cases} \int_{\xi_2}^{\xi_3} \rho_1(s) ds = \varphi_1(\xi_3) - \varphi_1(\xi_2) & , 0 \leq \xi_2 \leq \xi_3, \\ 0 & , \text{otherwise,} \end{cases} \\
 P_2 f(\xi^2) = P_2 f(\xi_1, \xi_3) &= \begin{cases} \int_{\xi_3}^{\xi_1} \rho_2(s) ds = \varphi_2(\xi_1) - \varphi_2(\xi_3) & , 0 \leq \xi_3 \leq \xi_1, \\ 0 & , \text{otherwise,} \end{cases} \\
 P_3 f(\xi^3) = P_3 f(\xi_1, \xi_2) &= \begin{cases} \int_{\xi_1}^{\xi_2} \rho_3(s) ds = \varphi_3(\xi_2) - \varphi_3(\xi_1) & , 0 \leq \xi_1 \leq \xi_2, \\ 0 & , \text{otherwise,} \end{cases}
 \end{aligned}$$

and, hence, all first order projections are **continuous and piecewise differentiable**. Next we consider the second order projections  $P_u f$ ,  $u \subset \{1, 2, 3\}$ ,  $|u| = 2$ . For example, one obtains that

$$P_{13} f(\xi_2) = \begin{cases} \int_0^{\xi_2} (\varphi_3(\xi_2) - \varphi_3(t)) \rho_1(t) dt & , \xi_2 \geq 0 \\ 0 & , \text{otherwise,} \end{cases}$$

is at least **continuously differentiable** on  $\Pi_{\{1,3\}}(\mathcal{K}) = \mathbb{R}$ . The same is true for the other second order projections. Of course, first and second order ANOVA projections gain further smoothness if the densities get smoother. Hence, the first order ANOVA terms of  $f$  belong at least to  $C^1(\mathbb{R})$ .

Note that **all facets of  $\mathcal{K}$  do not parallel any coordinate axis in  $\mathbb{R}^3$** .



We consider the objective function

$$f(\xi) = \langle c, x \rangle + \Phi(q(\xi), h(\xi) - Vx)$$

of our two-stage mixed-integer stochastic program for fixed  $x \in X$ . We know that  $f$  is linear-quadratic in  $\xi$  on the Borel sets  $\Xi_\nu(x) = \{\xi \in \mathbb{R}^d : q(\xi) \in U_\nu, h(\xi) \in Vx + B_\nu\}$ ,  $\nu \in \mathcal{N}$ , covering  $\mathbb{R}^d$  such that their closures are convex polyhedral.

### Assumptions:

**(B5)** The density  $\rho$  has fourth order absolute moments.

**(B6)**  $\rho(\xi) = \prod_{k=1}^d \rho_k(\xi_k)$  with  $\rho_k \in C^1(\mathbb{R})$ ,  $k \in \mathcal{D}$ .

**(B7)** All facets of the convex polyhedral sets  $\text{cl } \Xi_\nu(x)$  do not parallel any coordinate axis in  $\mathbb{R}^d$  for any fixed  $x \in X$  (**geometric condition**).

### Theorem:

Assume (B1)–(B7). Then the ANOVA terms  $f_u$ ,  $|u| \leq 2$ ,  $u \subset \mathcal{D}$ , of  $f$  have all mixed first Sobolev derivatives.

**Proposition:** If  $\rho$  is multivariate normal with nonsingular covariance matrix  $\Sigma$ , the **geometric condition (B7)** is satisfied almost everywhere with respect to the Haar measure over the topological group of  $d \times d$  real orthogonal matrices needed to transform  $\Sigma$  into diagonal form.

## RQMC convergence and error analysis

Assume  $f \in \mathbb{F}_d = \bigotimes_{i=1}^d W_{2,\gamma_i,\psi_i}^1(\mathbb{R})$ , where  $W_{2,\gamma_i,\psi_i}^1(\mathbb{R})$  is the Sobolev space of functions  $h \in L_{2,\rho_i}(\mathbb{R})$ , which are absolutely continuous with derivative  $h' \in L_{2,\psi_i}(\mathbb{R})$ , and norm

$$\|h\|_{\gamma_i,\psi_i}^2 = \left( \int_{\mathbb{R}} h(\xi)\rho_i(\xi)d\xi \right)^2 + \frac{1}{\gamma_i} \int_{\mathbb{R}} (h'(\xi)\psi_i(\xi))^2 d\xi.$$

The functions  $\psi_i$ ,  $i = 1, \dots, d$ , are selected such that the function

$$g = f(\varphi_1^{-1}(\cdot), \dots, \varphi_d^{-1}(\cdot))$$

belongs to  $\mathbb{G}_d$  and  $\mathbb{F}_d$  is a complete tensor product Sobolev space (Kuo-Sloan-Wasilkowski-Waterhouse 10, Nichols-Kuo 14).

The QMC error may be estimated as follows:

$$\begin{aligned} \left| \int_{\mathbb{R}^d} f(\xi)\rho(\xi)d\xi - n^{-1} \sum_{j=1}^n f(\xi^j) \right| &= \left| \int_{[0,1]^d} g(x)dx - n^{-1} \sum_{j=1}^n g(x^j) \right| \\ &\leq \sum_{0 < |u| \leq d} \left| \int_{[0,1]^{|u|}} g_u(x^u)dx^u - n^{-1} \sum_{j=1}^n g_u(x^j) \right|, \end{aligned}$$

where  $x^j = (x_1^j, \dots, x_d^j)$ ,  $x_i^j = \varphi_i^{-1}(\xi_i^j) \in (0, 1)^d$ ,  $i = 1, \dots, d$ ,  $j = 1, \dots, n$ , are the QMC points.

If the points  $x^j$ ,  $j = 1, \dots, n$ , are **randomly shifted lattice points**,  $n$  is prime and  $\delta \in (0, \frac{1}{2}]$ , we may continue

$$\left( \mathbb{E} \left| \int_{[0,1]^d} g(x) dx - n^{-1} \sum_{j=1}^n g(x^j) \right|^2 \right)^{\frac{1}{2}} \leq C(\delta) n^{-1+\delta} +$$

$$\sum_{|u| > d_S(\varepsilon)} \left( \mathbb{E} \left| \int_{[0,1]^{|u|}} g_u(x^u) dx^u - n^{-1} \sum_{j=1}^n g_u(x^j) \right|^2 \right)^{\frac{1}{2}} \\ \leq C(\delta) n^{-1+\delta} + O(\sqrt{\varepsilon})$$

if the ANOVA terms  $g_u$ ,  $|u| \leq d_S(\varepsilon)$ , belong to  $\mathbb{G}_d$  and the sequence  $(\gamma_j)$  is selected properly.

The condition  $g_u \in \mathbb{G}_d$  is satisfied if  $f_u \in \mathbb{F}_d$ .

## Numerical results

The optimization model contains the **electrical load**  $\xi_\delta$  and the **electricity price**  $\xi_c$  as stochastic parameters. Both are components of the random vector

$$\xi = (\xi_{\delta,1}, \xi_{c,1}, \dots, \xi_{\delta,T}, \xi_{c,T})^\top.$$

The time horizon consists of  $T$  intervals. At each time period  $t \in \{1, \dots, T\}$  the **load has to be covered**. During peak load periods load covering requires electricity trading based on bilateral contracts with fixed prices or day-ahead trading with stochastic prices. Peak/offpeak load periods typically require to **switch on/off (cycling) units**.

A **two-stage electricity production and trading model** is of the form

$$\min \left\{ \sum_{t=1}^T \langle c_t, x_t \rangle + \int_{\mathbb{R}^T} \Phi(q(\xi), h(\xi) - Vx) P(d\xi) : x \in X \right\}$$

$$\Phi(q, h) = \inf \left\{ \sum_{t=1}^T \langle q_t, y_t \rangle : Wy + Vx \geq h, y \in Y \right\},$$

where  $x_t$  denotes the outputs of the base load units with costs  $c_t$ . The set  $X$  contains capacity limits and eventual ramping constraints at  $t$ .

The vector  $y_t$  of second-stage decisions contains the 0-1 decisions and outputs of cycling units, and the amounts of trading. The constraint  $Wy + Vx \geq h(\xi)$  describes load covering at any  $t$  and minimum up/down times of the cycling units. The constraint  $y \in Y$  describes capacity limits, ramping constraints and integer requirements.  $P$  denotes the probability distribution of  $\xi$  on  $\mathbb{R}^{2T}$ .

We assume that the centered **stochastic load-price process**  $\{\bar{\xi}_t = (\bar{\xi}_{\delta,t}, \bar{\xi}_{c,t})\}_{t=1}^T$  may be modeled as **linear multivariate time series ARMA(p,q)**

$$\bar{\xi}_t + \sum_{i=1}^p A_i \bar{\xi}_{t-i} = \sum_{i=0}^q B_i \eta_{t-i}, \quad t = 1, \dots, T,$$

with independent standard normal innovations  $\eta_t$ ,  $t = 1, \dots, T$ , and suitable matrices  $A_i$  and  $B_i$  (Eichhorn-Römisch-Wegner 05).

Let  $m$  and  $\Sigma$  denote **mean and covariance matrix of  $\xi$** , respectively.

To generate RQMC samples for the load/price vector  $\xi$  with mean  $m = \mathbb{E}[\xi] \in \mathbb{R}^{2T}$  and covariance matrix  $\Sigma = \mathbb{E}[(\xi - m)(\xi - m)^\top]$  in our two-stage mixed-integer electricity portfolio optimization model, we first decompose  $\Sigma$  by a suitable matrix  $A$  such that  $\Sigma = A A^\top$ . In this way we obtain a **standard normal** random vector  $z = (z_1, \dots, z_{2T})^\top$  such that

$$\xi = Az + m.$$

If  $\phi$  denotes the standard normal distribution function, then the vector  $\eta = (\eta_1, \dots, \eta_{2T})^\top$  with  $z_i = \phi^{-1}(\eta_i)$ ,  $i = 1, \dots, 2T$ , is **uniformly distributed in  $[0, 1]^{2T}$** . We used the triangular Cholesky matrix  $A = L_{\text{Ch}}$  and the matrix  $A = U_{\text{PCA}}$  of the **principal component analysis (PCA) factorization**

$$U_{\text{PCA}} = (\sqrt{\lambda_1}u_1 \cdots \sqrt{\lambda_d}u_d)$$

with the **eigenvalues  $\lambda_1 \geq \dots \geq \lambda_d > 0$**  and **eigenvectors  $u_1, \dots, u_d$  of the covariance matrix  $\Sigma$** .

For our tests we used  $T = 100$  and, hence,  $d = 2T = 200$ .

By computing the upper bounds of the effective dimension using  $2^{15}$  randomly scrambled Sobol' points we obtained

$$d_S(0.01) \leq 2 \quad \text{with PCA and} \quad 2 < d_S(0.01) \leq 200 \quad \text{with CH.}$$

Hence, principal component analysis leads to a strong reduction of the effective dimension.

For the numerical tests  $n$  samples  $\eta^j \in [0, 1]^d$ ,  $j = 1, \dots, n$ , of Mersenne Twister MC and of the two RQMC methods were generated and inserted after the transformations  $z_i^j = \phi^{-1}(\eta_i^j)$ ,  $i = 1, \dots, 2T$ , and  $\xi^j = A z^j + m$ ,  $j = 1, \dots, n$ , into

$$\min \left\{ \sum_{t=1}^T \langle c_t, x_t \rangle + \frac{1}{n} \sum_{j=1}^n \Phi(q(\xi^j), h(\xi^j) - Vx) : x \in X \right\}.$$

For MC and randomly scrambled Sobol' points we used  $n = 128, 256, 512$  and for randomly shifted lattice rules  $n = 127, 257, 509$  (since prime numbers  $n$  are favorable for the latter). The Mersenne Twister was also used for the random scrambling and the random shifts.

The relative root mean square error (RSME) of the optimal value of the mixed-integer linear two-stage model is estimated by performing 10 runs of every experiment and repeat the process 30 times.

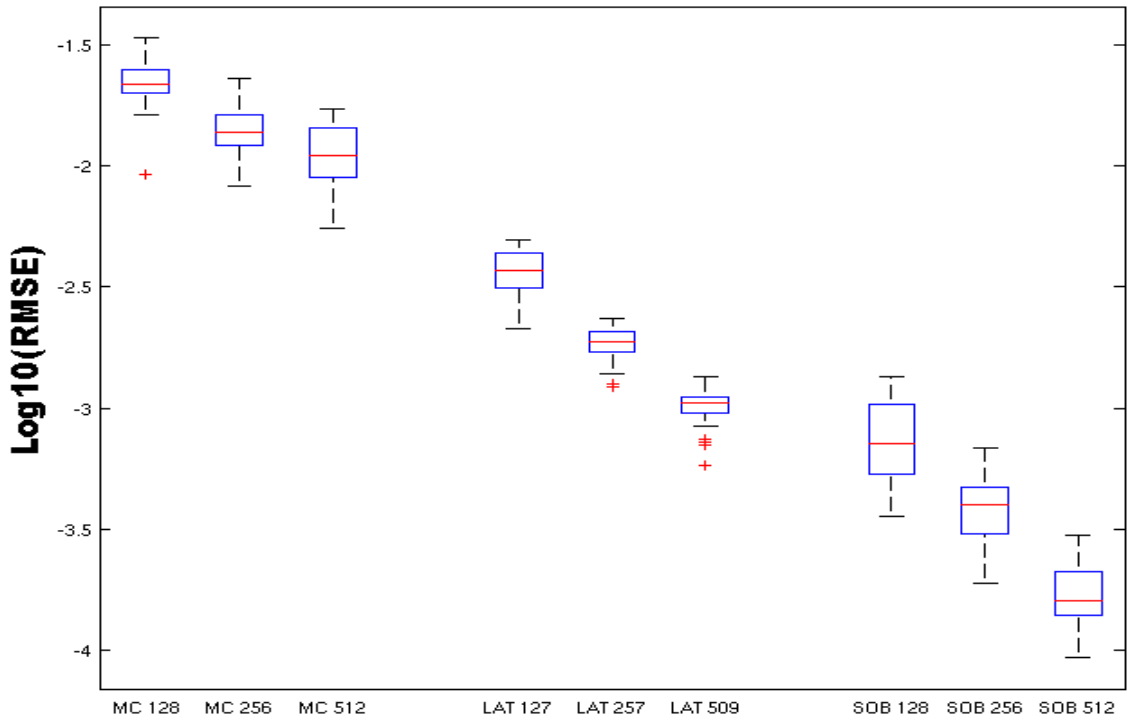
The lower and upper bounds of the boxes correspond to the first and third quartile and the line in between to the median. Outliers not belonging to boxes are marked by plus signs.

The average convergence rates of the three methods are [the theoretical rate  \$-0.5\$  for MC](#), [about  \$-0.9\$  for randomly shifted lattice rules](#) and  [\$-1.0\$  for randomly scrambled Sobol' points if PCA factorization is used](#).

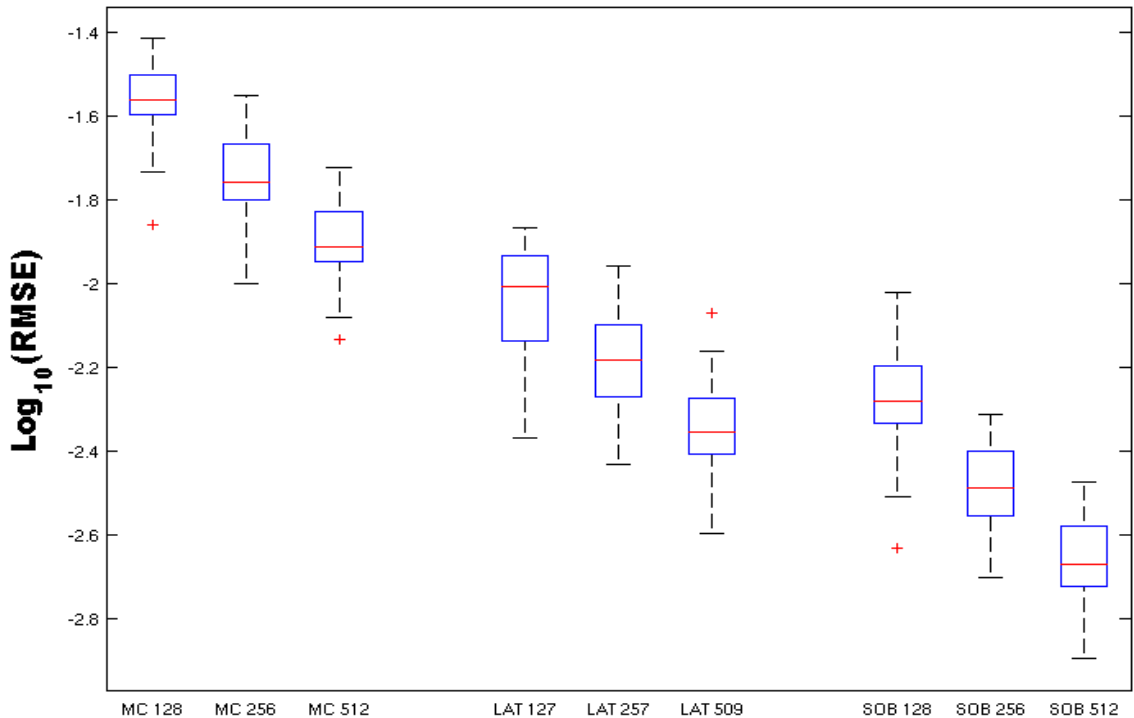
[An explanation for the much better behavior of both randomized QMC methods is the approximate smoothing of integrands achieved by the low effective dimension due to the use of PCA.](#)

[All three methods showed only average convergence rate  \$-0,5\$  if CH is used. However, it is also visible that both randomized QMC methods lead to smaller errors than MC.](#)





Shown are the  $\text{Log}_{10}$  of relative RMSE for the optimal values of the two-stage model by using the **PCA** factorization of the covariance matrix. Results for Mersenne Twister MC and randomly scrambled Sobol' QMC with 128, 256 and 512 points and randomly shifted lattice rules QMC with 127, 257 and 509 lattice points.



Shown are the  $\text{Log}_{10}$  of relative RMSE for the optimal values of the two-stage model by using the **CH** factorization of the covariance matrix. Results for Mersenne Twister MC and randomly scrambled Sobol' QMC with 128, 256 and 512 points and randomly shifted lattice rules QMC with 127, 257 and 509 lattice points.

## Conclusions

- Randomized Quasi-Monte Carlo methods are advantageous compared to MC methods also for integrands having kinks or even discontinuities at least in case of normal distributions and if the effective dimension of the integrand is low.
- Instead of  $10^4$  MC samples one only needs about  $10^2$  samples for randomly scrambled Sobol' point sets and randomly shifted lattice rules. The advantages consist in the improved accuracy for given sample size or in shorter running times for smaller sample sizes. The latter becomes crucial for high-dimensional models.

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