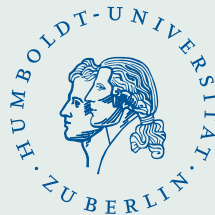


# Sparse grid and Quasi-Monte Carlo quadratures can be efficient for linear two-stage stochastic programs

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# Introduction

- Applied stochastic programming models in finance, production and energy often contain **random vectors of high dimension  $d$** .
- **Computational methods for solving stochastic programs** require a **discretization** of the underlying probability distribution **induced by a numerical integration scheme for computing expectations**.
- Discretization means **scenario or sample generation**.
- **Standard approach**: Variants of **Monte Carlo (MC) methods**, but the convergence rate  $O(\frac{1}{\sqrt{n}})$  for sample size  $n$  is impossibly slow and the dimensions of the Monte Carlo approximations grow by the factor  $n d$ .
- Two recently considered **alternative approaches to scenario generation**:
  - (a) **Quasi-Monte Carlo methods**  
(Koivu-Pennanen 05, Pennanen 09, Homem-de-Mello 08, Leövey-Römisch 15).
  - (b) **Sparse grid quadrature rules** (Chen-Mehrotra 08).

## Quadrature rules with sparse grids

We consider the unit cube  $[0, 1]^d$  in  $\mathbb{R}^d$ . Let a sequence of nested grids in  $[0, 1]$  be given, i.e.,

$$\Xi^i = \{\xi_1^i, \dots, \xi_{m_i}^i\} \subset \Xi^{i+1} \subset [0, 1] \quad (i \in \mathbb{N}),$$

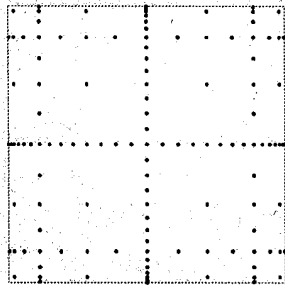
for example, the **dyadic grid**

$$\Xi^i = \left\{ \frac{j}{2^i} : j = 0, 1, \dots, 2^i \right\} \quad (i \in \mathbb{N}).$$

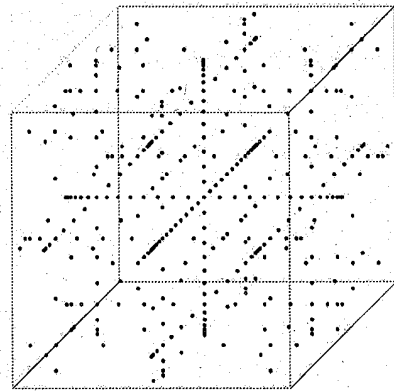
Then the point set in  $[0, 1]^d$  suggested by Smolyak (Smolyak 63) is

$$H(q, d) := \bigcup_{\sum_{j=1}^d i_j = q} \Xi^{i_1} \times \dots \times \Xi^{i_d} \quad (q \in \mathbb{N})$$

and called a **sparse grid in  $[0, 1]^d$** . Let  $n = n(q, d)$  denote the number of points in  $H(q, d)$ . In case of dyadic grids in  $[0, 1]$  the set  $H(q, d)$  consists of all  $d$ -dimensional dyadic grids with product of mesh sizes given by  $\frac{1}{2^q}$ .



(a)  $d = 2$



(b)  $d = 3$

The corresponding **tensor product quadrature rule** for  $n \geq d$  on  $[0, 1]^d$  (with the Lebesgue measure  $\lambda^d$ ) is of the form

$$Q_{n(q,d),d}(f) = \sum_{q-d+1 \leq |\mathbf{i}| \leq q} (-1)^{q-|\mathbf{i}|} \binom{d-1}{q-|\mathbf{i}|} \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} f(\xi_{j_1}^{i_1}, \dots, \xi_{j_d}^{i_d}) \prod_{l=1}^d a_{j_l}^{i_l},$$

where  $|\mathbf{i}| = \sum_{l=1}^d i_l$ ,  $n(q, d)$  is the number of quadrature knots and the coefficients  $a_j^{i_l}$  ( $j = 1, \dots, m_{i_l}$ ,  $l = 1, \dots, d$ ) are weights of  $d$  one-dimensional quadrature rules

$$\int_0^1 f(\xi) d\xi \approx Q^l(f) = \sum_{j=1}^{m_{i_l}} a_j^{i_l} f(\xi_j^{i_l}) \quad (l = 1, \dots, d).$$

The product weights are denoted by  $w_k$ ,  $k = 1, \dots, n(q, d)$ , and with the bijective mapping

$$\{\xi^k : k = 1, \dots, n(q, d)\} \leftrightarrow \{(\xi_{j_1}^{i_1}, \dots, \xi_{j_d}^{i_d}) : j_l = 1, \dots, m_{i_l}, q-d+1 \leq |\mathbf{i}| \leq q\}$$

the tensor product quadrature rule  $Q_{n(q,d),d}(f)$  may be rewritten as

$$Q_{n(q,d),d}(f) = \sum_{k=1}^{n(q,d)} w_k f(\xi^k).$$

Even if the one-dimensional weights are positive, **some of the weights  $w_k$  become negative**. Hence, an interpretation as discrete probability measure is not possible!

**Example:** Consider the classical **Clenshaw-Curtis rule  $Q^i$**  with  $m_1 = 1$ ,  $m_i = 2^{i-1} + 1$ ,  $i = 2, \dots, d$ ,  $\xi_1^1 = 0$  and

$$\xi_j^i = \frac{1}{2} \left( 1 - \cos \frac{\pi(j-1)}{m_i-1} \right) \quad (j = 1, \dots, m_i, i = 2, \dots, d)$$

and the weights  $a_j^i$ ,  $j = 1, \dots, m_i$ , be defined such that  $Q^i$  is exact for all univariate polynomials of degree at most  $m_i$ ,  $i = 1, \dots, d$  (Novak-Ritter 96).

**Proposition:**  $\|Q_{n(q,d),d}\|_\infty \leq c_d (\log n(q,d))^{d-1}$  for some  $c_d > 0$  and fixed  $d$ .

To present a convergence result for sparse grid quadratures we consider the **Sobolev space with dominating mixed smoothness**

$$W_{2,\text{mix}}^{(r,\dots,r)}([0,1]^d) = \left\{ f : [0,1]^d \rightarrow \mathbb{R} : \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}} \in L_2([0,1]^d), \|\alpha\|_\infty \leq r \right\}.$$

It is a **tensor product space** and a **kernel reproducing Hilbert space** for several variants of inner products.

For example, in case  $r = 1$ , one may consider the weighted kernel  $K_{d,\gamma}$

$$K_{d,\gamma}(x, y) = \prod_{i=1}^d K_{1,\gamma_i}(x_i, y_i) \quad (x, y \in [0, 1]^d).$$

For the linear space  $W_{2,\gamma}^1([0, 1])$  of all absolutely continuous functions on  $[0, 1]$  with derivatives belonging to  $L_2([0, 1])$  a weighted inner product is

$$\langle f, g \rangle_\gamma = \int_0^1 f(x)g(x)dx + \frac{1}{\gamma} \int_0^1 f'(x)g'(x)dx$$

with the corresponding kernel (Thomas-Agnan 96)

$$K_{1,\gamma}(x, y) = 1 + \gamma \left( \frac{1}{2} B_2(|x - y|) + B_1(x)B_1(y) \right),$$

where  $B_1(x) = x - \frac{1}{2}$  and  $B_2(x) = x^2 - x + \frac{1}{6}$  are Bernoulli polynomials.

**Theorem:** (Gerstner-Griebel 98, Novak-Ritter 96)

If  $f$  belongs to  $\mathcal{W}_{2,\gamma,\text{mix}}^{(r,\dots,r)}([0, 1]^d)$ , it holds

$$\left| \int_{[0,1]^d} f(\xi) d\xi - \sum_{k=1}^n w_k f(\xi^k) \right| \leq C_{r,d} \|f\|_{d,\gamma} n^{-r} (\log n)^{(d-1)(r+1)}.$$

## Quasi-Monte Carlo methods

We consider the approximate computation of

$$I_d(f) = \int_{[0,1]^d} f(\xi) d\xi$$

by a Quasi-Monte Carlo (QMC) algorithm

$$Q_n(f) = \frac{1}{n} \sum_{i=1}^n f(\xi^i)$$

with (non-random) points  $\xi^i$ ,  $i = 1, \dots, n$ , from  $[0, 1]^d$ .

We assume that  $f$  belongs to a linear normed space  $\mathbb{F}_d$  of functions on  $[0, 1]^d$  with norm  $\|\cdot\|_d$  and unit ball  $\mathbb{B}_d$  such that  $I_d$  is a linear bounded functional on  $\mathbb{F}_d$ .

**Worst-case error** of  $Q_n$  over  $\mathbb{B}_d$ :

$$e(Q_n) = \sup_{f \in \mathbb{B}_d} |I_d(f) - Q_n(f)|$$

If  $\mathbb{F}_d$  is a kernel reproducing Hilbert space, there exists  $h_n \in \mathbb{F}_d$  such that

$$e(Q_n) = \|h_n\|_d.$$



There are two **main groups** of QMC methods:

(Dick-Pillichshammer 10, Dick-Kuo-Sloan 13, Leobacher-Pillichshammer 14)

(1) **Digital nets and sequences**,

(2) **Lattice rules**.

Specific digital sequences:

**Sobol' sequence** (Sobol' 67);

**Faure sequence** (Faure 82);

**classical Niederreiter sequences** (Niederreiter 87);

**generalized Niederreiter sequences** (Niederreiter 05)

include both Sobol' and Faure constructions as special cases;

**Niederreiter-Xing sequences** (Niederreiter-Xing 95–02).

Specific rank-1 lattices:

$$\left\{ \frac{(i-1)}{n} g \right\}, \quad i = 1, \dots, n,$$

where  $g \in \mathbb{Z}^d$  is the **generator** of the lattice and the braces  $\{\cdot\}$  mean taking componentwise the fractional part.

## Randomized QMC methods

A randomized version of a QMC point set has the properties that

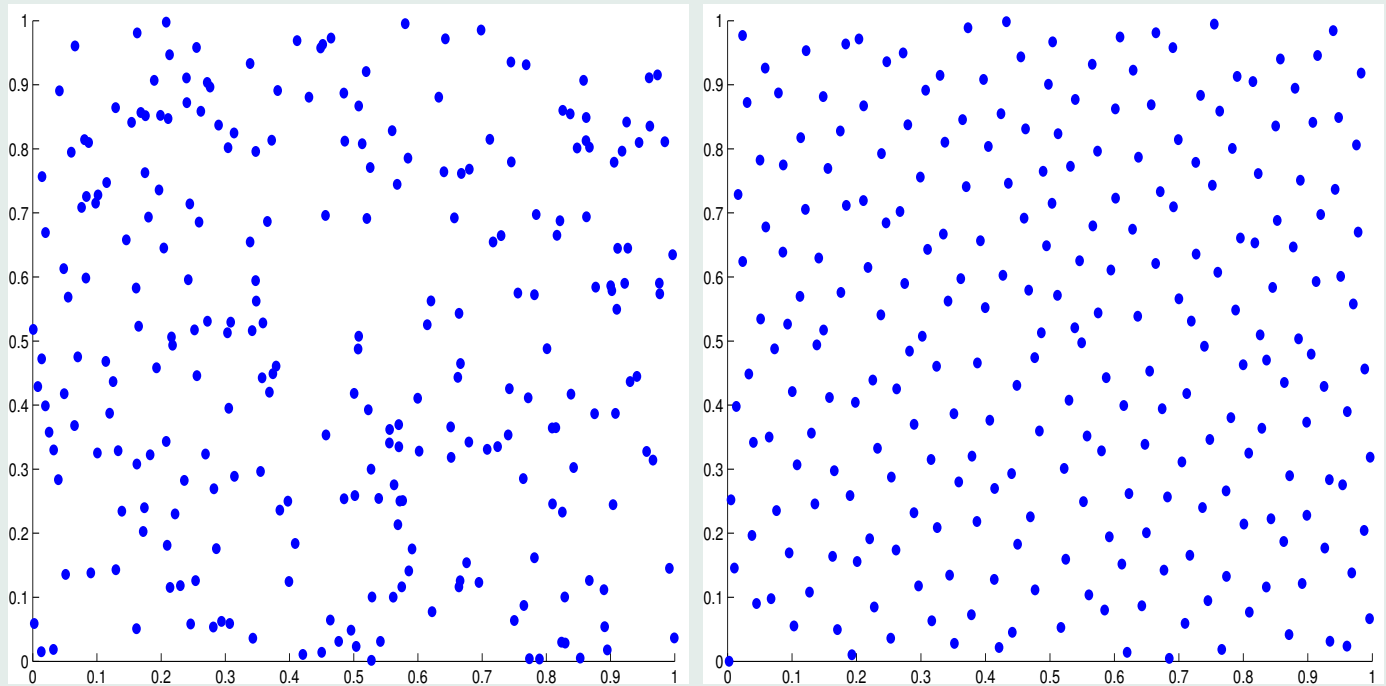
- (i) each point in the randomized point set has a uniform distribution over  $[0, 1)^d$  (**uniformity**),
- (ii) the QMC properties are preserved under the randomization with probability one (**equidistribution**).

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

**Examples** of such techniques are

- (a) **random shifts** of lattice rules,
- (b) **scrambling**, i.e., random permutations of the integers  $\mathbb{Z}_b = \{0, 1, \dots, b-1\}$  applied to the digits in  $b$ -adic representations,
- (c) **affine matrix 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  $\mathbb{Z}_b$ .

The two properties (i) and (ii) allow for error estimates and may lead to improved convergence properties compared to the original QMC method.



Comparison of  $n = 2^7$  Monte Carlo Mersenne Twister points and randomly binary shifted Sobol' points in dimension  $d = 500$ , projection (8,9)

**Randomly scrambled Sobol' sequences** admit the following **root mean-square quadrature error convergence rate** for  $f \in \mathbb{F}_d = \mathcal{W}_{2,\gamma,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$

$$\sup_{f \in \mathbb{B}_d} \sqrt{\mathbb{E}[Q_n(\omega)(f) - I_d(f)]^2} \leq C_d n^{-\frac{3}{2}} (\log n)^{\frac{d-1}{2}}.$$

(Dick-Pillichshammer 10, Theorem 13.25)

## Randomly shifted lattice rules

If  $\Delta$  is a random vector having uniform distribution on  $[0, 1]^d$ , put

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

### Theorem:

Let  $n$  be prime,  $\mathbb{F}_d = \mathcal{W}_{2, \gamma, \text{mix}}^{(1, \dots, 1)}([0, 1]^d)$ .

Then  $g \in \mathbb{Z}^d$  can be constructed component-by-component such that for any  $\delta \in (0, \frac{1}{2}]$  there exists a constant  $C(\delta) > 0$  such that the **root mean-square worst-case quadrature error attains the optimal convergence rate**

$$\sup_{f \in \mathbb{B}_d} \sqrt{\mathbb{E}[Q_n(\omega)(f) - I_d(f)]^2} \leq C(\delta) n^{-1+\delta},$$

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

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

# ANOVA decomposition of multivariate functions and effective dimension

**Idea:** Use decompositions of  $f$ , where most of the terms are smooth, but hopefully only some of them relevant.

Let  $\mathfrak{D} = \{1, \dots, d\}$  and  $f \in L_{1,\rho}(\mathbb{R}^d)$  with  $\rho(\xi) = \prod_{j=1}^d \rho_j(\xi_j)$ , where

$$f \in L_{p,\rho}(\mathbb{R}^d) \quad \text{iff} \quad \int_{\mathbb{R}^d} |f(\xi)|^p \rho(\xi) d\xi < \infty \quad (p \geq 1).$$

Let the projection  $P_k$ ,  $k \in \mathfrak{D}$ , be defined by

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

Clearly,  $P_k f$  is constant with respect to  $\xi_k$ . For  $u \subseteq \mathfrak{D}$  we write

$$P_u f = \left( \prod_{k \in u} P_k \right) (f),$$

where the product means composition, and note that the ordering within the product is not important because of Fubini's theorem. The function  $P_u f$  is constant with respect to all  $x_k$ ,  $k \in u$ .

ANOVA-decomposition of  $f$ :

$$f = \sum_{u \subseteq \mathcal{D}} f_u,$$

where  $f_\emptyset = I_d(f) = P_{\mathcal{D}}(f)$  and recursively (Kuo-Sloan-Wasilkowski-Woźniakowski 10)

$$f_u = \sum_{v \subseteq u} (-1)^{|u|-|v|} P_{-v} f = P_{-u}(f) + \sum_{v \subset u} (-1)^{|u|-|v|} P_{u-v}(P_{-u}(f)),$$

where  $P_{-u}$  and  $P_{u-v}$  mean integration with respect to  $\xi_j$ ,  $j \in \mathcal{D} \setminus u$  and  $j \in u \setminus v$ , respectively. The second representation motivates that  $f_u$  is essentially as smooth as  $P_{-u}(f)$ .

If  $f$  belongs to  $L_{2,\rho}(\mathbb{R}^d)$ , its ANOVA terms  $\{f_u\}_{u \subseteq \mathcal{D}}$  are orthogonal in  $L_{2,\rho}(\mathbb{R}^d)$ .

We set  $\sigma^2(f) = \|f - I_d(f)\|_{L_2}^2$  and  $\sigma_u^2(f) = \|f_u\|_{L_2}^2$ , and have

$$\sigma^2(f) = \|f\|_{L_2}^2 - (I_d(f))^2 = \sum_{\emptyset \neq u \subseteq \mathcal{D}} \sigma_u^2(f).$$

The normalized ratios  $\frac{\sigma_u^2(f)}{\sigma^2(f)}$  serve as indicators for the importance of  $\xi^u$  in  $f$ .

Owen's **superposition (truncation) dimension distribution** of  $f$ : Probability measure  $\nu_S$  ( $\nu_T$ ) defined on the power set of  $D$

$$\nu_S(s) := \sum_{|u|=s} \frac{\sigma_u^2(f)}{\sigma^2(f)} \quad \left( \nu_T(s) = \sum_{\max\{j:j \in u\}=s} \frac{\sigma_u^2(f)}{\sigma^2(f)} \right) \quad (s \in \mathfrak{D}).$$

**Effective superposition (truncation) dimension**  $d_S(\varepsilon)$  ( $d_T(\varepsilon)$ ) of  $f$  is the  $(1 - \varepsilon)$ -quantile of  $\nu_S$  ( $\nu_T$ ):

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

$$d_T(\varepsilon) = \min \left\{ s \in \mathfrak{D} : \sum_{u \subseteq \{1, \dots, s\}} \sigma_u^2(f) \geq (1 - \varepsilon) \sigma^2(f) \right\}$$

It holds

$$\max \left\{ \left\| f - \sum_{|u| \leq d_S(\varepsilon)} f_u \right\|_{2, \rho}, \left\| f - \sum_{u \subseteq \{1, \dots, d_T(\varepsilon)\}} f_u \right\|_{2, \rho} \right\} \leq \sqrt{\varepsilon} \sigma(f).$$

## Integrands of two-stage linear stochastic programs

We consider the linear two-stage stochastic program

$$\min \left\{ \int_{\Xi} f(x, \xi) P(d\xi) : x \in X \right\},$$

where  $f$  is extended real-valued defined on  $\mathbb{R}^m \times \mathbb{R}^d$  given by

$$f(x, \xi) = \langle c, x \rangle + \Phi(q(\xi), h(\xi) - T(\xi)x), \quad (x, \xi) \in X \times \Xi,$$

$c \in \mathbb{R}^m$ ,  $X \subseteq \mathbb{R}^m$  and  $\Xi \subseteq \mathbb{R}^d$  are convex polyhedral,  $W$  is an  $(r, \bar{m})$ -matrix,  $P$  is a Borel probability measure on  $\Xi$ , and the vectors  $q(\xi) \in \mathbb{R}^{\bar{m}}$ ,  $h(\xi) \in \mathbb{R}^r$  and the  $(r, m)$ -matrix  $T(\xi)$  are affine functions of  $\xi$ ,  $\Phi$  is the second-stage optimal value function

$$\Phi(u, t) = \inf \{ \langle u, y \rangle : Wy = t, y \geq 0 \} \quad ((u, t) \in \mathbb{R}^{\bar{m}} \times \mathbb{R}^r),$$

Let  $\text{pos } W = W(\mathbb{R}_+^{\bar{m}})$ ,  $\mathcal{D} = \{u \in \mathbb{R}^{\bar{m}} : \{z \in \mathbb{R}^r : W^\top z \leq u\} \neq \emptyset\}$ .

### Assumptions:

**(A1)**  $h(\xi) - T(\xi)x \in \text{pos } W$  and  $q(\xi) \in \mathcal{D}$  for all  $(x, \xi) \in X \times \Xi$ .

**(A2)**  $\int_{\Xi} \|\xi\|^2 P(d\xi) < \infty$ .



**Lemma:** (Walkup-Wets 69, Nožička-Guddat-Hollatz-Bank 74)

$\Phi$  is finite, polyhedral and continuous on the  $(\bar{m} + r)$ -dimensional convex polyhedral cone  $\mathcal{D} \times \text{pos } W$  and there exist  $(r, \bar{m})$ -matrices  $C_j$  and  $(\bar{m} + r)$ -dimensional convex polyhedral cones  $\mathcal{K}_j$ ,  $j = 1, \dots, \ell$ , such that

$$\bigcup_{j=1}^{\ell} \mathcal{K}_j = \mathcal{D} \times \text{pos } W \quad \text{and} \quad \text{int } \mathcal{K}_i \cap \text{int } \mathcal{K}_j = \emptyset, \quad i \neq j,$$

$$\Phi(u, t) = \langle C_j u, t \rangle, \quad \text{for each } (u, t) \in \mathcal{K}_j, \quad j = 1, \dots, \ell,$$

$$\Phi(u, t) = \max_{j=1, \dots, \ell} \langle C_j u, t \rangle.$$

The function  $\Phi(u, \cdot)$  is convex on  $\text{pos } W$  for each  $u \in \mathcal{D}$ , and  $\Phi(\cdot, t)$  is concave on  $\mathcal{D}$  for each  $t \in \text{pos } W$ . The intersection  $\mathcal{K}_i \cap \mathcal{K}_j$ ,  $i \neq j$ , is either equal to  $\{0\}$  or contained in a  $(\bar{m} + r - 1)$ -dimensional subspace of  $\mathbb{R}^{\bar{m} + r}$  if the two cones are adjacent.

Hence, the two-stage integrands are of the form

$$f(x, \xi) = \langle c, x \rangle + \max_{j=1, \dots, \ell} \langle C_j q(\xi), h(\xi) - T(\xi)x \rangle \quad ((x, \xi) \in X \times \Xi).$$

$$f(x, \xi) = \langle c, x \rangle + \langle C_j q(\xi), h(\xi) - T(\xi)x \rangle \quad \text{if } (q(\xi), h(\xi) - T(\xi)x) \in \mathcal{K}_j.$$

# ANOVA decomposition of two-stage integrands

**Assumptions: (A1), (A2)** and

**(A3)**  $P$  has a density of the form  $\rho(\xi) = \prod_{i=1}^d \rho_i(\xi_i)$  ( $\xi \in \mathbb{R}^d$ ) with continuous marginal densities  $\rho_i$ ,  $i \in \mathcal{D}$ .

**(A4)** All common faces of adjacent convex polyhedral sets

$$\Xi_j(x) = \{\xi \in \Xi : (q(\xi), h(\xi) - T(\xi)x) \in \mathcal{K}_j\} \quad (j = 1, \dots, \ell)$$

do not parallel any coordinate axis for all  $x \in X$  (*geometric condition*).

**Proposition:**

(A1) implies that two-stage integrands

$$f_x(\xi) := f(x, \xi) = \langle c, x \rangle + \Phi(q(\xi), h(\xi) - T(\xi)x) \quad (x \in X, \xi \in \Xi)$$

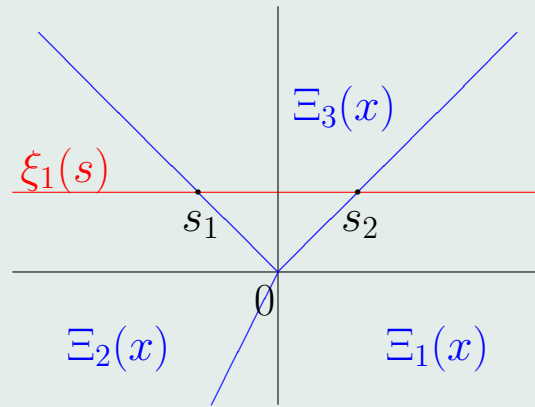
are **continuous and piecewise linear-quadratic**.

For each  $x \in X$ ,  $f(x, \cdot)$  is linear-quadratic on each convex polyhedral set  $\Xi_j(x)$ ,  $j = 1, \dots, \ell$ . It holds  $\text{int } \Xi_j(x) \neq \emptyset$ ,  $\text{int } \Xi_j(x) \cap \text{int } \Xi_i(x) = \emptyset$ ,  $i \neq j$ , and the sets  $\Xi_j(x)$ ,  $j = 1, \dots, \ell$ , decompose  $\Xi$ . Furthermore, the intersection of two adjacent sets  $\Xi_i(x)$  and  $\Xi_j(x)$ ,  $i \neq j$ , is contained in some  $(d - 1)$ -dimensional affine subspace.

To compute projections  $P_k f$  for  $k \in \mathfrak{D}$ , let  $\xi_i \in \mathbb{R}$ ,  $i = 1, \dots, d$ ,  $i \neq k$ , be given. We set  $\xi^k = (\xi_1, \dots, \xi_{k-1}, \xi_{k+1}, \dots, \xi_d)$  and

$$\xi_k(s) = (\xi_1, \dots, \xi_{k-1}, s, \xi_{k+1}, \dots, \xi_d) \in \mathbb{R}^d \quad (s \in \mathbb{R}).$$

We fix  $x \in X$  and consider the one-dimensional affine subspace  $\{\xi_k(s) : s \in \mathbb{R}\}$ :



Example with  $d = 2 = p$ , where the polyhedral sets are cones

It meets the nontrivial intersections of two adjacent polyhedral sets  $\Xi_i(x)$  and  $\Xi_j(x)$ ,  $i \neq j$ , at finitely many points  $s_i$ ,  $i = 1, \dots, p$  if all  $(d - 1)$ -dimensional subspaces containing the intersections do not parallel the  $k$ th coordinate axis.

The  $s_i = s_i(\xi^k)$ ,  $i = 1, \dots, p$ , are affine functions of  $\xi^k$ . It holds

$$s_i = - \sum_{l=1, l \neq k}^p \frac{g_{il}}{g_{ik}} \xi_l + a_i \quad (i = 1, \dots, p)$$

for some  $a_i \in \mathbb{R}$  and  $g_i \in \mathbb{R}^d$  belonging to an intersection of polyhedral sets.

### Proposition:

Let  $k \in \mathfrak{D}$ ,  $x \in X$  and assume (A1)–(A4).

For every  $\xi$  the  $k$ th projection  $P_k f$  at  $\xi$  has the explicit representation

$$P_k f(\xi^k) = \sum_{i=1}^{p(\xi;x)+1} \sum_{j=0}^2 p_{ij}(\xi; x) \int_{s_{i-1}(\xi;x)}^{s_i(\xi;x)} s^j \rho_k(s) ds,$$

where  $s_0 = -\infty$ ,  $s_{p+1} = +\infty$  and  $p_{ij}(\cdot; x)$  are polynomials in  $\xi^k$  of degree  $2 - j$ ,  $j = 0, 1, 2$ , with coefficients depending on  $x$ , and is continuously differentiable on  $\mathbb{R}^d$ .  $P_k f$  is  $s$ -times continuously differentiable almost everywhere on  $\mathbb{R}^d$  if the marginal density  $\rho_k$  belongs to  $C^{s-1}(\mathbb{R})$ .

## Theorem:

Let  $x \in X$ , assume (A1)–(A4) and  $f = f(x, \cdot)$  be the two-stage integrand. Then the second order ANOVA approximation of  $f$

$$f^{(2)} := \sum_{|u| \leq 2} f_u \quad \text{where} \quad f = f^{(2)} + \sum_{|u|=3}^d f_u$$

belongs to  $W_{2,\rho,\text{mix}}^{(1,\dots,1)}(\mathbb{R}^d)$  if all marginal densities  $\rho_k$ ,  $k \in \mathfrak{D}$ , belong to  $C^1(\mathbb{R})$ .

## Remark:

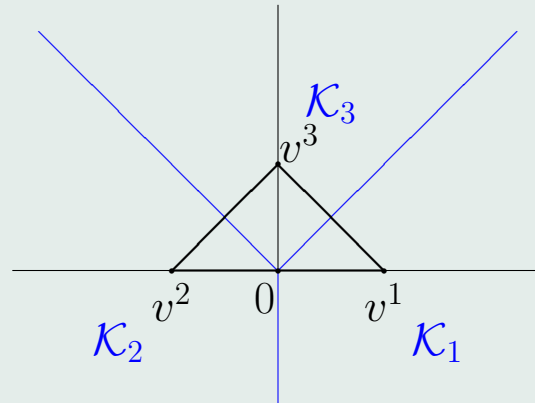
The second order ANOVA approximation  $f^{(2)}$  is a good approximation of  $f$  if the effective superposition dimension  $d_S(\varepsilon)$  is at most 2. Then

$$\left\| \sum_{|u|=3}^d f_u \right\|_{2,\rho}^2 = \sum_{|u|=3}^d \|f_u\|_{2,\rho}^2 \leq \varepsilon \sigma^2(f)$$

and  $f$  belongs essentially to the tensor product Sobolev space  $\mathcal{W}_{2,\text{mix}}^{(1,\dots,1)}(\mathbb{R}^d)$ . Hence, a favorable behavior of randomly shifted lattice rules may be expected.

**Example:** Let  $\bar{m} = 3$ ,  $d = 2$ ,  $P$  satisfy (A2) and (A3),  $h(\xi) = \xi$ ,  $q$  and  $T$  be fixed and  $W$  be given such that (A1) is satisfied and the dual feasible set is

$$\{z \in \mathbb{R}^2 : -z_1 + z_2 \leq 1, z_1 + z_2 \leq 1, -z_2 \leq 0\}.$$



Dual feasible set, its vertices  $v^j$  and the normal cones  $\mathcal{K}_j$  to its vertices

The function  $\Phi$  and the integrand are of the form

$$\Phi(t) = \max_{i=1,2,3} \langle v^i, t \rangle = \max\{t_1, -t_1, t_2\} = \max\{|t_1|, t_2\}$$

$$f(\xi) = \langle c, x \rangle + \Phi(\xi - Tx) = \langle c, x \rangle + \max\{|\xi_1 - [Tx]_1|, \xi_2 - [Tx]_2\}$$

and the convex polyhedral sets are  $\Xi_j(x) = Tx + \mathcal{K}_j$ ,  $j = 1, 2, 3$ .

The ANOVA projection  $P_1 f$  is in  $C^1$ , but  $P_2 f$  is not differentiable.

## Quasi-Monte Carlo error estimates

If the assumptions of the theorem are satisfied, one may argue for **randomly shifted lattice rules** as follows

$$\begin{aligned} & \left\| \int_{\mathbb{R}^d} f(\xi) \rho(\xi) d\xi - \frac{1}{n} \sum_{j=1}^n f(\xi^j) \right\|_{L_2} = \left\| \int_{[0,1]^d} g(t) dt - \frac{1}{n} \sum_{j=1}^n g(t^j) \right\|_{L_2} \\ & \leq \sum_{0 < |u| \leq d} \left\| \int_{[0,1]^{|u|}} g_u(t^u) dt^u - \frac{1}{n} \sum_{j=1}^n g_u(t^j) \right\|_{L_2} \\ & \leq C(\delta) n^{-1+\delta} + \sum_{|u|=3}^d \left\| \int_{[0,1]^d} g_u(t) dt - \frac{1}{n} \sum_{j=1}^n g_u(t^j) \right\|_{L_2} \\ & \leq C(\delta) n^{-1+\delta} + O(\sqrt{\varepsilon}) \end{aligned}$$

if the effective superposition dimension of  $f$  satisfies  $d_S(\varepsilon) \leq 2$  and the transformed functions  $g_u$ ,  $|u| = 1, 2$ , belong to the weighted tensor product Sobolev space on  $[0, 1]^d$ . The functions  $g$  and  $g_u$  are defined by

$$g = f \circ \varphi^{-1} \quad \text{on } (0, 1)^d \quad \text{and} \quad g_u = f_u \circ \varphi_u^{-1} \quad \text{on } (0, 1)^{|u|},$$

where

$$\varphi := (\varphi_1, \dots, \varphi_d), \quad \varphi_i(t) := \int_{-\infty}^t \rho_i(s) ds \quad (i \in \mathfrak{D}).$$

Since  $f_u$ ,  $|u| = 1, 2$ , is first and mixed second order partially differentiable in the sense of Sobolev and  $\varphi^{-1}$  can be assumed to be smooth,  $g_u$ ,  $|u| = 1, 2$ , is also first and mixed second order partially differentiable in the sense of Sobolev.

However, in general, the mixed derivatives of  $g_u$  are **not quadratically integrable**. Hence the Sobolev spaces have to be modified by introducing weight functions. (Kuo-Sloan-Wasilkowski-Waterhouse 10).

Here, we assume for simplicity that the mixed derivatives of  $g_u$ ,  $|u| = 1, 2$ , belong to the mixed Sobolev spaces.

Since the constants involved in our estimates may be chosen to be uniform with respect to the first-stage decision  $x$  varying in a compact set  $X$ , **the final estimate carries over to the  $L_2$ -distance of the optimal values of the original and approximate two-stage program.**



**Question:** How restrictive is the geometric condition (A4) ?

**Partial answer:** If  $P$  is normal with nonsingular covariance matrix, (A4) is a generic property. Namely, it holds

**Proposition:** Let  $x \in X$ , (A1) be satisfied,  $P$  be a normal distribution with nonsingular covariance matrix  $\Sigma$  and assume that  $\Sigma$  is transformed to a diagonal matrix by an orthogonal transformation.

Then for almost all covariance matrices  $\Sigma$  the second order ANOVA approximation  $f^{(2)}$  of  $f$  belongs to the mixed Sobolev space  $\mathcal{W}_{2,\gamma,\text{mix}}^{(1,\dots,1)}(\mathbb{R}^d)$ .

**Question:** For which two-stage stochastic programs is the effective superposition dimension  $d_S(\varepsilon)$  of  $f$  is less than or equal to 2?

**Partial answer:** In case of a (log)normal probability distribution  $P$  the effective dimension depends on the mode of decomposition of the covariance matrix in order to transform the random vector to one with independent components.

## Dimension reduction in case of (log)normal distributions

Let  $P$  be the normal distribution with mean  $\mu$  and nonsingular covariance matrix  $\Sigma$ . Let  $A$  be a matrix satisfying  $\Sigma = A A^\top$ . Then  $\eta$  defined by  $\xi = A\eta + \mu$  is standard normal.

The (lower triangular) **standard Cholesky matrix**  $A = L_C$  performing the factorization  $\Sigma = L_C L_C^\top$  seems to assign the same importance to every variable and, hence, **is not suitable to reduce the effective dimension**.

A **universal principle** is **principal component analysis (PCA)**. Here, one uses  $A = (\sqrt{\lambda_1}u_1, \dots, \sqrt{\lambda_d}u_d)$ , where  $\lambda_1 \geq \dots \geq \lambda_d > 0$  are the eigenvalues of  $\Sigma$  in decreasing order and the corresponding orthonormal eigenvectors  $u_i$ ,  $i = 1, \dots, d$ . (Wang-Fang 03, Wang-Sloan 05) report an **enormous reduction of the effective truncation dimension** in financial models if PCA is used. Our numerical results confirm this observation.

However, there is **no consistent dimension reduction effect** for any such matrix  $A$  (Papageorgiou 02, Wang-Sloan 11).

## Computational experience

We consider a **stochastic production planning problem** which consists in minimizing the expected costs of a company during a certain time horizon. The model contains **stochastic demands**  $\xi_\delta$  and **prices**  $\xi_c$  as components of

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

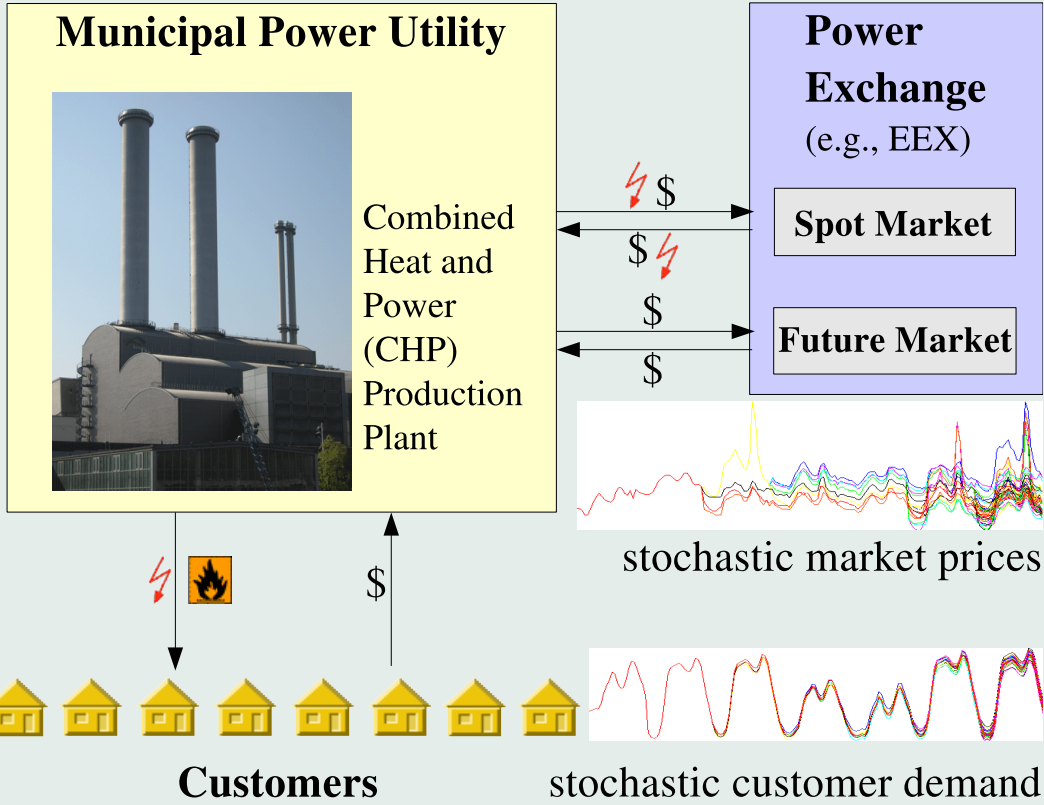
The company aims to satisfy stochastic demands  $\xi_{\delta,t}$  in a time horizon  $\{1, \dots, T\}$ , but its production capacity based on their own units does eventually not suffice to cover the demand. Hence, it has to buy the necessary extra amounts on markets or from other providers. The model is of the form

$$\max \left\{ \sum_{t=1}^T \left( c_t^\top x_t + \int_{\mathbb{R}^T} q_t(\xi)^\top y_t P(d\xi) \right) : Wy + Vx = h(\xi), y \geq 0, x \in X \right\}$$

We assume that the stochastic demands and prices  $\xi_{\delta,t}, \xi_{c,t}$  may be modeled as a **multivariate ARMA(1,1) process**, i.e.,

$$\begin{pmatrix} \xi_{\delta,t} \\ \xi_{c,t} \end{pmatrix} = \begin{pmatrix} \bar{\xi}_{\delta,t} \\ \bar{\xi}_{c,t} \end{pmatrix} + \begin{pmatrix} E_{1,t} \\ E_{2,t} \end{pmatrix}, \quad \text{for } t = 1, \dots, T, \text{ and}$$

$$\begin{pmatrix} \bar{\xi}_{\delta,1} \\ \bar{\xi}_{c,1} \end{pmatrix} = B_1 \begin{pmatrix} \gamma_{1,1} \\ \gamma_{2,1} \end{pmatrix}, \quad \begin{pmatrix} \bar{\xi}_{\delta,t} \\ \bar{\xi}_{c,t} \end{pmatrix} = A \begin{pmatrix} \bar{\xi}_{\delta,t-1} \\ \bar{\xi}_{c,t-1} \end{pmatrix} + B_1 \begin{pmatrix} \gamma_{1,t} \\ \gamma_{2,t} \end{pmatrix} + B_2 \begin{pmatrix} \gamma_{1,t-1} \\ \gamma_{2,t-1} \end{pmatrix}$$



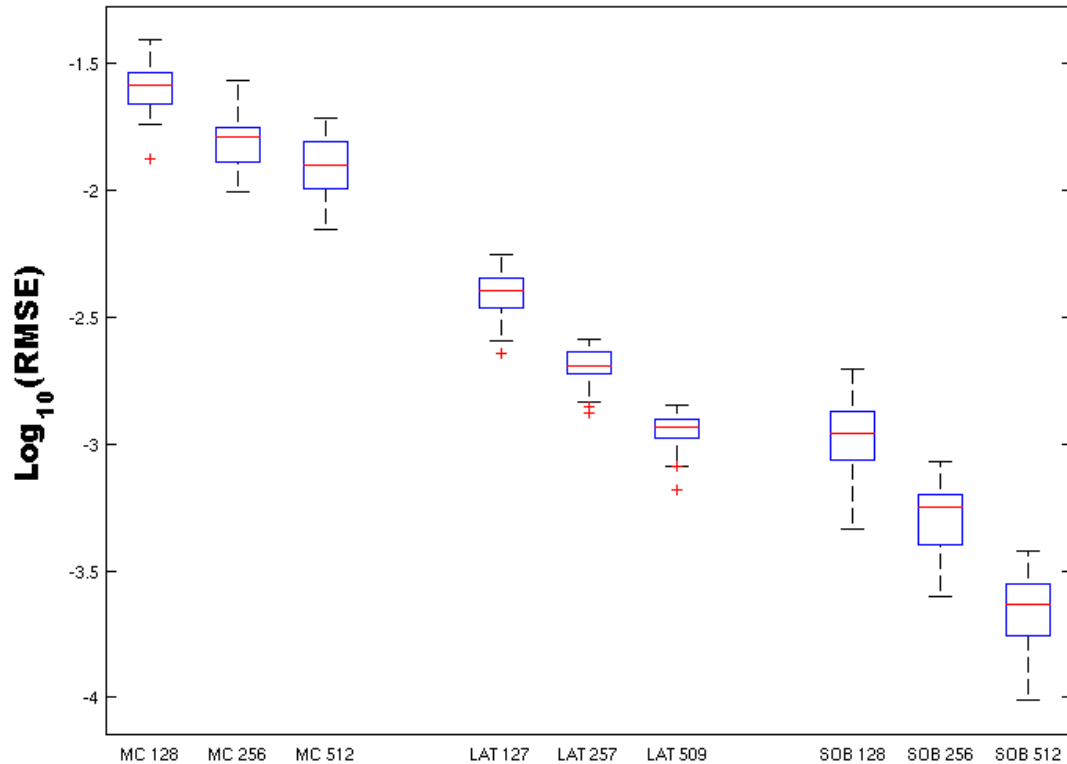
for  $t = 2, \dots, T$ , where  $\gamma_{1,t}, \gamma_{2,t} \sim \mathcal{N}(0,1)$  and i.i.d. and  $T = 100$ .

We used **PCA** and CH for decomposing the covariance matrix of  $\xi$ . PCA has led to **effective truncation dimension**  $d_T(0.01) = 2$  while for CH  $d_T(0.01) = 200$ . As QMC methods we used a **randomly scrambled Sobol sequence (SOB)** and a **randomly shifted lattice rule (LAT)** with weights  $\gamma_j = \frac{1}{j^3}$  and for MC the Mersenne-Twister.

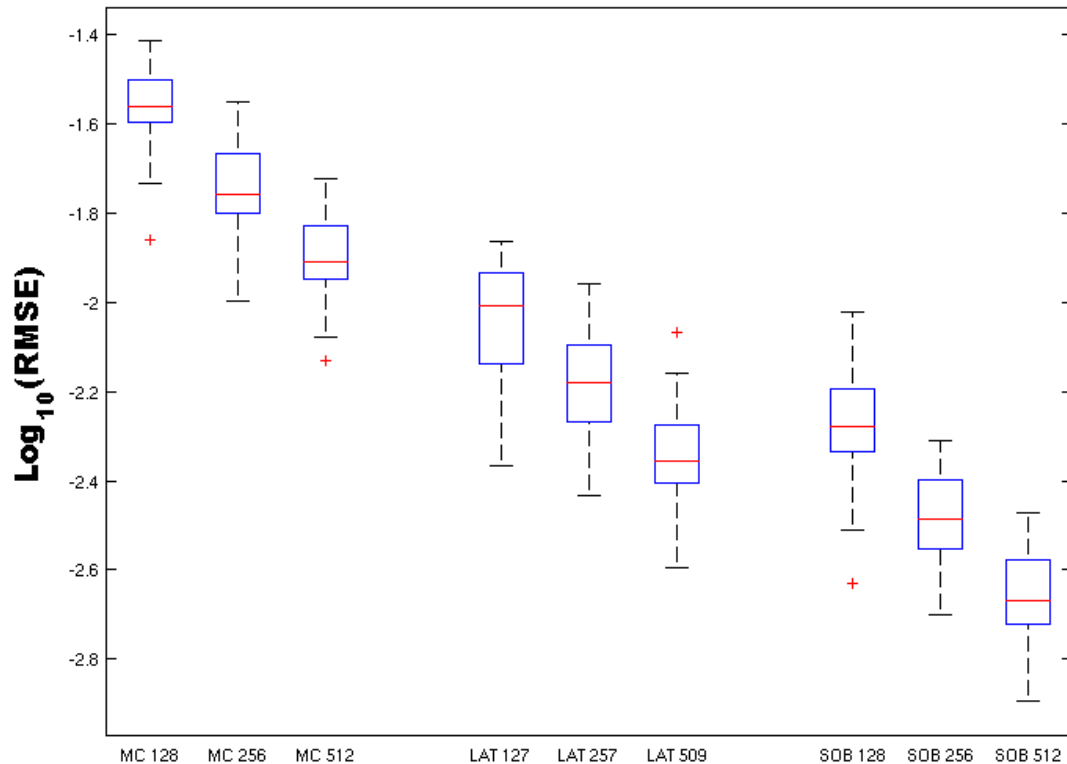
We used  $n = 128, 256, 512$  for the Mersenne Twister and for Sobol' points. For randomly shifted lattices we used  $n = 127, 257, 509$ . The random shifts were generated using the Mersenne Twister. We estimated the relative root mean square errors (RMSE) of the optimal costs by taking 10 runs for each experiment, and repeated the process 30 times for the box plots in the figures.

The average of the **estimated rates of convergence under PCA** was approximately  $-0.9$  for **randomly shifted lattice rules**, and  $-1.0$  for the **randomly scrambled Sobol' points**. This is clearly superior compared to the MC rate  $-0.5$ .

The box-plots show the first quartile as lower bound of the box, the third quartile as upper bound and the median as line between the bounds, Outliers are marked as plus signs and the rest of the results lie between the brackets.



$\log_{10}$  of the relative errors of optimal values obtained with MC, LAT (randomly shifted lattice rule) and SOB (scrambled Sobol' points) using principal component analysis PCA



$\log_{10}$  of the relative errors of optimal values obtained with MC, LAT (randomly shifted lattice rule) and SOB (scrambled Sobol' points) using Cholesky CH

## Conclusions

- Our analysis provides a theoretical basis for applying sparse grid quadratures and modern randomized Quasi-Monte Carlo methods accompanied by dimension reduction techniques to two-stage stochastic programs.
- The analysis confirms our numerical experience that modern randomized QMC methods are often superior compared to Monte Carlo and never worse. They allow for a distinct reduction of sample sizes from  $n$  to almost  $\sqrt{n}$ .
- Of course, the implementation effort increases for QMC compared to MC.
- The analysis appears to be extendable to mixed-integer two-stage models and to multi-stage situations. This is supported by our numerical experience, too.



## References:

- J. Dick, F. Y. Kuo and I. H. Sloan: High-dimensional integration – the Quasi-Monte Carlo way, *Acta Numerica* 22 (2013), 133–288.
- J. Dick, F. Pillichshammer: *Digital Nets and Sequences*, Cambridge University Press, Cambridge 2010.
- T. Gerstner, M. Griebel: Numerical integration using sparse grids, *Numerical Algorithms* 18 (1998), 209–232.
- M. Holtz: *Sparse Grid Quadrature in High Dimensions with Applications in Finance and Insurance*, Springer, Heidelberg, 2010.
- F. Y. Kuo: Component-by-component constructions achieve the optimal rate of convergence in weighted Korobov and Sobolev spaces, *Journal of Complexity* 19 (2003), 301–320.
- F. Y. Kuo, I. H. Sloan, G. W. Wasilkowski, H. Woźniakowski: On decomposition of multivariate functions, *Mathematics of Computation* 79 (2010), 953–966.
- P. L’Ecuyer and Ch. Lemieux: Recent advances in randomized quasi-Monte Carlo methods, in *Modeling Uncertainty* (M. Dror, P. L’Ecuyer, F. Szidarovski eds.), Kluwer, Boston, 2002, 419–474.
- G. Leobacher and F. Pillichshammer: *Introduction to Quasi-Monte Carlo Integration and Applications*, Birkhäuser, Heidelberg, 2014.
- [H. Leövey and W. Römisch: Quasi-Monte Carlo methods for linear two-stage stochastic programming problems, \*Mathematical Programming\* 151 \(2015\), 315–345.](#)
- E. Novak, K. Ritter: High dimensional integration of smooth functions over cubes, *Numerische Mathematik* 75 (1996), 79–97.
- D. Nuyens and R. Cools: Fast algorithms for component-by-component constructions of rank-1 lattice rules in shift-invariant reproducing kernel Hilbert spaces, *Mathematics of Computation* 75 (2006), 903–922.

- A. B. Owen: Randomly permuted  $(t, m, s)$ -nets and  $(t, s)$ -sequences, in: *Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing* (H. Niederreiter and P. J.-S. Shiue eds.), Lecture Notes in Statistics, Vol. 106, Springer, New York, 1995, 299–317.
- A. B. Owen: The dimension distribution and quadrature test functions, *Statistica Sinica* 13 (2003), 1–17.
- I. H. Sloan and H. Woźniakowski: When are Quasi Monte Carlo algorithms efficient for high-dimensional integration, *Journal of Complexity* 14 (1998), 1–33.
- I. H. Sloan, F. Y. Kuo and S. Joe: Constructing randomly shifted lattice rules in weighted Sobolev spaces, *SIAM Journal Numerical Analysis* 40 (2002), 1650–1665.
- S. A. Smolyak: Quadrature and interpolation formulas for tensor products of certain classes of functions, *Soviet Math. Dokl.* 4 (1963), 240–243.
- I. M. Sobol': The distribution of points in a cube and the approximate evaluation of integrals, *U.S.S.R. Comput. Math. and Math. Phys.* 7 (1967), 86–112.
- C. Thomas-Agnan: Computing a family of reproducing kernels for statistical applications, *Numerical Algorithms* 13 (1996), 21–32.
- X. Wang and K.-T. Fang: The effective dimension and Quasi-Monte Carlo integration, *Journal of Complexity* 19 (2003), 101–124.
- X. Wang and I. H. Sloan: Quasi-Monte Carlo methods in financial engineering: An equivalence principle and dimension reduction, *Operations Research* 59 (2011), 80–95.
- G. W. Wasilkowski and H. Woźniakowski: Explicit cost bounds of algorithms for multivariate tensor product problems, *Journal of Complexity* 11 (1995), 1–56.