

# Quasi-Monte Carlo approximations in stochastic optimization

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# Introduction

- Computational methods for solving stochastic programs require (first) a discretization of the underlying probability distribution induced by a numerical integration scheme and (second) an efficient solver for the finite-dimensional program.
- Discretization means scenario or sample generation.
- Standard approach: Variants of Monte Carlo (MC) methods.
- Recent alternative approaches to scenario generation:
  - (a) Optimal quantization of probability distributions  
(Pflug-Pichler 2011).
  - (b) Quasi-Monte Carlo (QMC) methods  
(Koivu-Pennanen 05, Homem-de-Mello 08).
  - (c) Sparse grid quadrature rules  
(Chen-Mehrotra 08).
  - (d) Moment matching methods  
(Høyland-Wallace 01, Gülpinar-Rustem-Settergren 04)

- Known convergence rates in terms of scenario or sample size  $n$ :

MC:  $\hat{e}_n(f) = O(n^{-\frac{1}{2}})$  if  $f \in L_2$ ,

(a):  $e_n(f) = O(n^{-\frac{1}{d}})$  if  $f \in \text{Lip}$ ,

(b): classical:  $e_n(f) = O(n^{-1}(\log n)^d)$  if  $f \in \text{BV}$ ,

recently:  $\hat{e}_n(f) \leq C(\delta)n^{-1+\delta}$  ( $\delta \in (0, \frac{1}{2}]$ ) if  $f \in W^{(1, \dots, 1)}$ ,

where  $C(\delta)$  does not depend on  $d$ ,

(c):  $e_n(f) = O(n^{-r}(\log n)^{(d-1)(r+1)})$  if  $f \in W^{(r, \dots, r)}$ ,

where  $d$  is the dimension of the random vector and  $e_n(f)$  the quadrature error for integrand  $f$  and sample size  $n$ , i.e.,

$$e_n(f) = \left| \int_{[0,1]^d} f(\xi) d\xi - \frac{1}{n} \sum_{i=1}^n f(\xi^i) \right|$$

and  $\hat{e}_n(f)$  denotes mean (square) quadrature error.

- Monte Carlo methods and (a) may be justified by available stability results for stochastic programs, but there is almost no reasonable justification in cases (b), (c) and (d).
- In applications of stochastic programming  $d$  is often large.

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## Quasi-Monte Carlo methods

We consider the approximate computation of

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

by a QMC algorithm

$$Q_{n,d}(f) = \frac{1}{n} \sum_{i=1}^n f(\xi^i)$$

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  $\mathbb{B}_d$ .

Worst-case error of  $Q_{n,d}$  over  $\mathbb{B}_d$ :

$$e(Q_{n,d}) = \sup_{f \in \mathbb{B}_d} |I_d(f) - Q_{n,d}(f)|$$

## Classical convergence results:

**Theorem:** (Proinov 88)

If the real function  $f$  is continuous on  $[0, 1]^d$ , then there exists  $C > 0$  such that

$$|Q_{n,d}(f) - I_d(f)| \leq C\omega_f(D_n^*(\xi^1, \dots, \xi^n)^{\frac{1}{d}}),$$

where  $\omega_f(\delta) = \sup\{|f(\xi) - f(\tilde{\xi})| : \|\xi - \tilde{\xi}\| \leq \delta, \xi, \tilde{\xi} \in [0, 1]^d\}$  is the modulus of continuity of  $f$  and

$$D_n^*(\xi^1, \dots, \xi^n) := \sup_{x \in [0,1]^d} |\text{disc}(x)|, \quad \text{disc}(x) = \lambda^d([0, x]) - \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{[0,x]}(\xi^i),$$

is the **star-discrepancy** of  $\xi^1, \dots, \xi^n$  ( $\lambda^d$  denotes Lebesgue's measure on  $\mathbb{R}^d$ ).

**Theorem:** (Koksma-Hlawka 61)

If  $V_{\text{HK}}(f)$  is the variation of  $f$  in the sense of Hardy and Krause, it holds

$$|I_d(f) - Q_{n,d}(f)| \leq V_{\text{HK}}(f) D_n^*(\xi^1, \dots, \xi^n)$$

for any  $n \in \mathbb{N}$  and any  $\xi^1, \dots, \xi^n \in [0, 1]^d$ .

## Extended Koksma-Hlawka inequality:

$$|I_d(f) - Q_{n,d}(f)| \leq \|\text{disc}(\cdot)\|_{p,p'} \|f\|_{q,q'},$$

where  $1 \leq p, p', q, q' \leq \infty$ ,  $\frac{1}{p} + \frac{1}{q} = 1$ ,  $\frac{1}{p'} + \frac{1}{q'} = 1$ , and

$$\|\text{disc}(\cdot)\|_{p,p'} = \left( \sum_{u \subseteq D} \left( \int_{[0,1]^{|u|}} |\text{disc}(x_u, 1)|^{p'} dx_u \right)^{\frac{p}{p'}} \right)^{\frac{1}{p}}$$

and

$$\|f\|_{q,q'} = \left( \sum_{u \subseteq D} \left( \int_{[0,1]^{|u|}} \left| \frac{\partial^{|u|} f}{\partial x_u}(x_u, 1) \right|^{q'} dx_u \right)^{\frac{q}{q'}} \right)^{\frac{1}{q}}$$

with the obvious modifications if one or more of  $p, p', q, q'$  are infinite.

In particular, the [classical Koksma-Hlawka inequality](#) essentially corresponds to  $p = p' = \infty$  if  $f$  belongs to the tensor product Sobolev space  $\mathcal{W}_{2,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$  which is defined next.

By  $(x_u, 1)$  we mean the  $d$ -dimensional vector with the same components as  $x$  for indices in  $u$  and the rest of the components replaced by 1.

## The case of kernel reproducing Hilbert spaces

We assume that  $\mathbb{F}_d$  is a **kernel reproducing Hilbert space** with inner product  $\langle \cdot, \cdot \rangle$  and kernel  $K : [0, 1]^d \times [0, 1]^d \rightarrow \mathbb{R}$ , i.e.,

$$K(\cdot, y) \in \mathbb{F}_d \text{ and } \langle f(\cdot), K(\cdot, y) \rangle = f(y) \quad (\forall y \in [0, 1]^d, f \in \mathbb{F}_d).$$

If  $I_d$  is a linear bounded functional on  $\mathbb{F}_d$ , the quadrature error  $e_n(Q_{n,d})$  allows the representation

$$e_n(Q_{n,d}) = \sup_{f \in \mathbb{B}_d} |I_d(f) - Q_{n,d}(f)| = \sup_{f \in \mathbb{B}_d} |\langle f, h_n \rangle| = \|h_n\|_d$$

according to Riesz' theorem for linear bounded functionals.

The **representer**  $h_n \in \mathbb{F}_d$  of the quadrature error is of the form

$$h_n(x) = \int_{[0,1]^d} K(x, y) dy - \frac{1}{n} \sum_{i=1}^n K(x, \xi^i) \quad (\forall x \in [0, 1]^d),$$

and it holds

$$e_n^2(Q_{n,d}) = \int_{[0,1]^{2d}} K(x, y) dx dy - \frac{2}{n} \sum_{i=1}^n \int_{[0,1]^d} K(\xi^i, y) dy + \frac{1}{n^2} \sum_{i,j=1}^n K(\xi^i, \xi^j)$$



## Example: Weighted tensor product Sobolev space

$$\mathbb{F}_d = \mathcal{W}_{2,\text{mix}}^{(1,\dots,1)}([0, 1]^d) = \bigotimes_{i=1}^d W_2^1([0, 1])$$

equipped with the weighted norm  $\|f\|_\gamma^2 = \langle f, f \rangle_\gamma$  and inner product

$$\langle f, g \rangle_\gamma = \sum_{u \subseteq \{1, \dots, d\}} \gamma_u^{-1} \int_{[0,1]^{|u|}} \frac{\partial^{|u|} f}{\partial x_u}(x_u, 1) \frac{\partial^{|u|} g}{\partial x_u}(x_u, 1) dx_u,$$

where  $\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_d > 0$ ,  $\gamma_u = \prod_{j \in u} \gamma_j$ , is a kernel reproducing Hilbert space with the kernel

$$K_{d,\gamma}(x, y) = \prod_{j=1}^d (1 + \gamma_j \mu(x_j, y_j)) \quad (x, y \in [0, 1]^d),$$

where

$$\mu(t, s) = \begin{cases} \min\{|t - 1|, |s - 1|\} & , (t - 1)(s - 1) > 0, \\ 0 & , \text{else.} \end{cases}$$

Note that  $f \in \mathbb{F}_d$  iff  $\frac{\partial^{|u|} f}{\partial x_u}(\cdot, 1) \in L_2([0, 1]^{|u|})$  for all  $u \subseteq D$ .

**Theorem:** (Sloan-Woźniakowski 98)

Let  $\mathbb{F}_d = \mathcal{W}_{2,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$ . Then the worst-case error

$$e^2(Q_{n,d}) = \sup_{\|f\|_\gamma \leq 1} |I_d(f) - Q_{n,d}(f)| = \sum_{\emptyset \neq u \subseteq D} \prod_{j \in u} \gamma_j \int_{[0,1]^{|u|}} \text{disc}^2(x_u, 1) dx_u$$

is called **weighted  $L_2$ -discrepancy** of  $\xi^1, \dots, \xi^n$ .

Note that any  $f \in \mathbb{F}_d$  is of bounded variation  $V_{\text{HK}}(f)$  in the sense of Hardy and Krause and it holds

$$V(f) = \sum_{\emptyset \neq u \subseteq D} \int_{[0,1]^{|u|}} \left| \frac{\partial^{|u|} f}{\partial x_u}(x_u, 1) \right| dx_u.$$

**Problem:** Integrands in two-stage stochastic programming do not belong to  $\mathbb{F}_d$  (piecewise linear functions are not of bounded variation (Owen 05)).

# First general QMC construction: Digital nets (Sobol 69, Niederreiter 87)

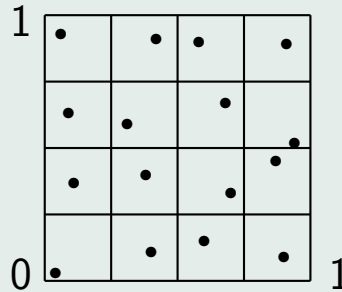
Elementary subintervals  $E$  in base  $b$ :

$$E = \prod_{j=1}^d \left[ \frac{a_j}{b^{d_j}}, \frac{a_j + 1}{b^{d_j}} \right),$$

where  $a_i, d_i \in \mathbb{Z}_+, 0 \leq a_i < b^{d_i}, i = 1, \dots, d$ .

Let  $m, t \in \mathbb{Z}_+, m > t$ . A set of  $b^m$  points in  $[0, 1)^d$  is a  $(t, m, d)$ -net in base  $b$  if every elementary subinterval  $E$  in base  $b$  with  $\lambda^d(E) = b^{t-m}$  contains  $b^t$  points.

Illustration of a  $(0, 4, 2)$ -net with  $b = 2$



A sequence  $(\xi^i)$  in  $[0, 1)^d$  is a  $(t, d)$ -sequence in base  $b$  if, for all integers  $k \in \mathbb{Z}_+$  and  $m > t$ , the set

$$\{\xi^i : kb^m \leq i < (k+1)b^m\}$$

is a  $(t, m, d)$ -net in base  $b$ .

There exist  $(t, d)$ -sequences  $(\xi^i)$  in  $[0, 1]^d$  such that

$$D_n^*(\xi^1, \dots, \xi^n) = O(n^{-1}(\log n)^{d-1}) \leq C(\delta, d) n^{-1+\delta} \quad (\forall \delta > 0).$$

**Specific sequences:** Faure, Sobol', Niederreiter and Niederreiter-Xing sequences (Lemieux 09, Dick-Pillichshammer 10).

**Recent development:** Scrambled  $(t, m, d)$ -nets, where the digits are randomly permuted (Owen 95).

**Second general QMC construction: Lattices** (Korobov 59, Sloan-Joe 94)

**Lattice rules:** Let  $g \in \mathbb{Z}^d$  and consider the lattice points

$$\{\xi^i = \left\{ \frac{i}{n} g \right\} : i = 1, \dots, n\},$$

where  $\{z\}$  is defined as *componentwise fractional part* of  $z \in \mathbb{R}_+$ , i.e.,  $\{z\} = z - \lfloor z \rfloor \in [0, 1)$ .

The generator  $g$  is chosen such that the lattice rule has good convergence properties. Such lattice rules may achieve better convergence rates  $O(n^{-k+\delta})$ ,  $k \in \mathbb{N}$ , for integrands in  $C^k$ .

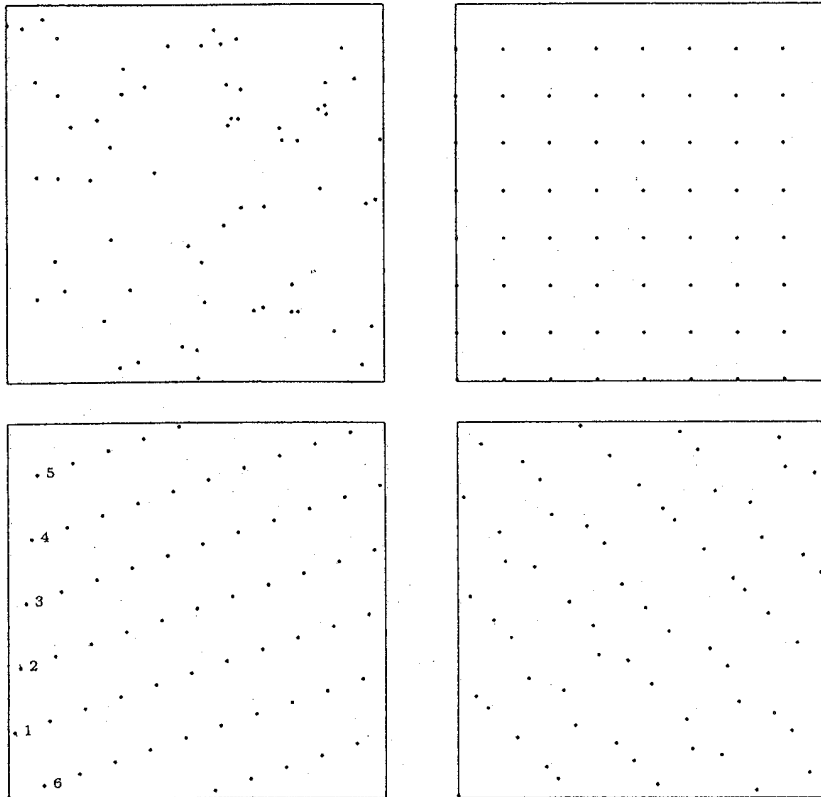


Fig. 5.3 Four different point sets with  $n = 64$ : random (top left), rectangular grid (top right), Korobov lattice (bottom left), and Sobol' (bottom right).

## Recent development: Randomized lattice rules.

Randomly shifted lattice points:

If  $\Delta$  is a sample from uniform distribution in  $[0, 1]^d$ . put

$$Q_{n,d}(f) = \frac{1}{n} \sum_{i=1}^n f\left(\frac{i}{n}g + \Delta\right).$$

### Theorem:

Let  $n$  be prime,  $\mathbb{F}_d = \mathcal{W}_{2,\text{mix}}^{(1,\dots,1)}([0, 1]^d)$  and  $g \in \mathbb{Z}^d$  be constructed componentwise. Then there exists for any  $\delta \in (0, \frac{1}{2}]$  a constant  $C(\delta) > 0$  such that the mean quadrature error attains the optimal convergence rate

$$\hat{e}(Q_{n,d}) \leq C(\delta)n^{-1+\delta},$$

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

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

## ANOVA decomposition of multivariate functions

**Idea:** Decompositions of  $f$  may be used, where most of the terms are smooth, but hopefully only some of them relevant.

Let  $D = \{1, \dots, d\}$  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**  $P_k$ ,  $k \in D$ , 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  $u \subseteq D$  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  $f$ :

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

where  $f_\emptyset = I_d(f) = P_D(f)$  and recursively

$$f_u = P_{-u}(f) - \sum_{v \subset u} f_v$$

or (due to 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  $\xi_j$ ,  $j \in D \setminus u$  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  $\{f_u\}_{u \subseteq D}$  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

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



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

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

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

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

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

It holds

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

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

## Proposition:

(A1) and (A2) imply that the two-stage stochastic program represents a **convex minimization problem with respect to the first stage decision  $x$  with polyhedral constraints.**

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

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

$$\bigcup_{j=1}^{\ell} \mathcal{K}_j = \mathcal{D} \times \text{pos } W \quad \text{and} \quad \text{int } \mathcal{K}_i \cap \text{int } \mathcal{K}_j = \emptyset, \quad i \neq j,$$
$$\Phi(u, t) = \langle C_j u, t \rangle, \quad \text{for each } (u, t) \in \mathcal{K}_j, \quad j = 1, \dots, \ell.$$

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.

## Error estimates for optimal values and solution sets

With  $v(P)$  and  $S(P)$  denoting the optimal value and solution set of

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

it holds

$$\begin{aligned} |v(P) - v(Q)| &\leq L \sup_{x \in X} \left| \int_{\Xi} f(x, \xi) P(d\xi) - \int_{\Xi} f(x, \xi) Q(d\xi) \right| \\ \emptyset \neq S(Q) &\subseteq S(P) + \Psi_P \left( L \sup_{x \in X} \left| \int_{\Xi} f(x, \xi) (P - Q)(d\xi) \right| \right), \end{aligned}$$

where  $L > 0$  is some constant,  $P$  the original probability distribution and  $Q$  its perturbation, and  $\Psi_P$  the **conditioning function** given by

$$\Psi_P(\eta) := \eta + \psi_P^{-1}(2\eta) \quad (\eta \in \mathbb{R}_+),$$

where the **growth function**  $\psi_P$  is

$$\psi_P(\tau) := \min \left\{ \int_{\Xi} f_0(x, \xi) P(d\xi) - v(P) : d(x, S(P)) \geq \tau, x \in X \right\}$$

with inverse  $\psi_P^{-1}(t) := \sup \{ \tau \in \mathbb{R}_+ : \psi_P(\tau) \leq t \}$ . (Römisch 03)

# ANOVA decomposition of two-stage integrands

## Assumptions:

(A1), (A2) and

(A3)  $P$  has a density of the form  $\rho(\xi) = \prod_{j=1}^d \rho_j(\xi_j)$  ( $\xi \in \mathbb{R}^d$ ) with continuous marginal densities  $\rho_j$ ,  $j \in D$ .

## Proposition:

(A1) implies that the function  $f(x, \cdot)$ , where

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

is the two-stage integrand, is **continuous and piecewise linear-quadratic**.

For each  $x \in X$ ,  $f(x, \cdot)$  is linear-quadratic on each polyhedral set

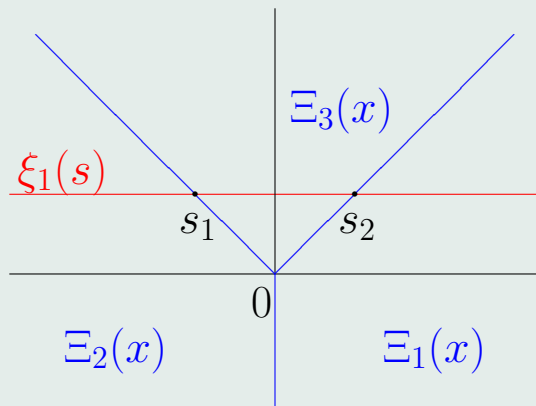
$$\Xi_j(x) = \{\xi \in \Xi : (q(\xi), h(\xi) - T(\xi)x) \in \mathcal{K}_j\} \quad (j = 1, \dots, \ell).$$

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  $k \in D$ , 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  $k \in D$ ,  $x \in X$ . Assume (A1)–(A3) and that all  $(d - 1)$ -dimensional affine subspaces containing nontrivial intersections of adjacent sets  $\Xi_i(x)$  and  $\Xi_j(x)$  do not parallel the  $k$ th coordinate axis.

Then the  $k$ th projection  $P_k f$  has the explicit representation

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

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.

$P_k f$  is infinitely differentiable if the marginal density  $\rho_k$  belongs to  $C^\infty(\mathbb{R})$ .

## Theorem:

Let  $x \in X$ , assume (A1)–(A3) and that the following **geometric condition (GC)** be satisfied: All  $(d - 1)$ -dimensional affine subspaces containing nontrivial intersections of adjacent sets  $\Xi_i(x)$  and  $\Xi_j(x)$  do not parallel any coordinate axis.

Then the **ANOVA approximation**

$$f_{d-1} := \sum_{|u| \leq d-1} f_u \quad \text{i.e.} \quad f = f_{d-1} + f_D$$

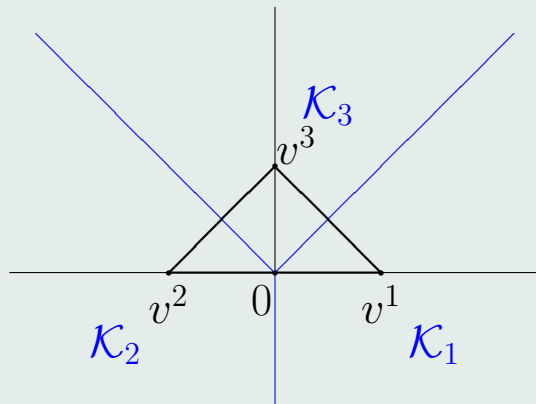
of  $f$  is infinitely differentiable if all densities  $\rho_k$ ,  $k \in D$ , belong to  $C_b^\infty(\mathbb{R})$ .

Here, the subscript  $b$  means that all derivatives of functions belonging to that space are bounded on  $\mathbb{R}$ .



**Example:** Let  $\bar{m} = 3$ ,  $d = 2$ ,  $P$  denote the two-dimensional standard normal distribution,  $h(\xi) = \xi$ ,  $q$  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  $C^\infty$ , but  $P_2 f$  is not differentiable.

## QMC quadrature error estimates

If the assumptions of the theorem are satisfied, the two-stage integrand  $f = f_x$  (for fixed  $x \in X$ ) allows the representation  $f = f_{d-1} + f_D$  with  $f_{d-1}$  belonging to  $\mathbb{F}_d$ . This implies

$$\begin{aligned} \left| \int_{[0,1]^d} f(\xi) d\xi - \frac{1}{n} \sum_{j=1}^n f(\xi^j) \right| &\leq e(Q_{n,d}) \|f_{d-1}\|_\gamma + \left| \int_{[0,1]^d} f_D(\xi) d\xi - \frac{1}{n} \sum_{j=1}^n f_D(\xi^j) \right| \\ &\leq e(Q_{n,d}) \|f_{d-1}\|_\gamma + \|f_D\|_{L_2} + \left( \frac{1}{n} \sum_{j=1}^n |f_D(\xi^j)|^2 \right)^{\frac{1}{2}} \end{aligned}$$

where  $\|\cdot\|_\gamma$  is the weighted tensor product Sobolev space norm.

As  $f_D$  is (Lipschitz) continuous and if the  $\xi^j$ ,  $j = 1, \dots, n$  are properly selected, the last term in the above estimate may be assumed to be bounded by  $2\|f_D\|_{L_2}$ .

Hence, if the **effective superposition dimension** satisfies  $d_S(\varepsilon) \leq d - 1$ , i.e.,  $\|f_D\|_{L_2} \leq \sqrt{\varepsilon}\sigma(f)$  holds for some small  $\varepsilon > 0$ , the first term  $e(Q_{n,d}) \|f_{d-1}\|_\gamma$  dominates and the **convergence rate of  $e(Q_{n,d})$  becomes most important**.

**Question:** How important is the geometric condition (GC) ?

**Partial answer:** If  $P$  is normal with nonsingular covariance matrix, (GC) is satisfied for almost all covariance matrices. Namely, it holds

**Proposition:** Let  $x \in X$ , (A1), (A2) be satisfied,  $\text{dom } \Phi = \mathbb{R}^r$  and  $P$  be a normal distribution with nonsingular covariance matrix  $\Sigma$ . Then the infinite differentiability of the ANOVA approximation  $f_{d-1}$  of  $f$  is a generic property, i.e., it holds in a residual set (countable intersection of open dense subsets) in the metric space of orthogonal  $(d, d)$ -matrices  $Q$  (endowed with the norm topology) appearing in the spectral decomposition  $\Sigma = Q^\top D Q$  of  $\Sigma$  (with a diagonal matrix  $D$  containing the eigenvalues of  $\Sigma$ ).

**Question:** For which two-stage stochastic programs is  $\|f_D\|_{L_2, \rho}$  small, i.e., the effective superposition dimension  $d_S(\varepsilon)$  of  $f$  is less than  $d - 1$  or even much less?

**Partial answer:** In case of a (log)normal probability distribution  $P$  the effective dimension depends on the mode of decomposition of the covariance matrix into a diagonal one.

## 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.

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.

A **problem-dependent principle** may be based on the following **equivalence principle** (Papageorgiou 02, Wang-Sloan 11).

**Proposition:** Let  $A$  be a fixed  $d \times d$  matrix such that  $A A^\top = \Sigma$ . Then it holds  $\Sigma = B B^\top$  if and only if  $B$  is of the form  $B = A Q$  with some orthogonal  $d \times d$  matrix  $Q$ .

**Idea:** Determine  $Q$  for given  $A$  such that the effective truncation dimension is **minimized** (Wang-Sloan 11).

## Some computational experience

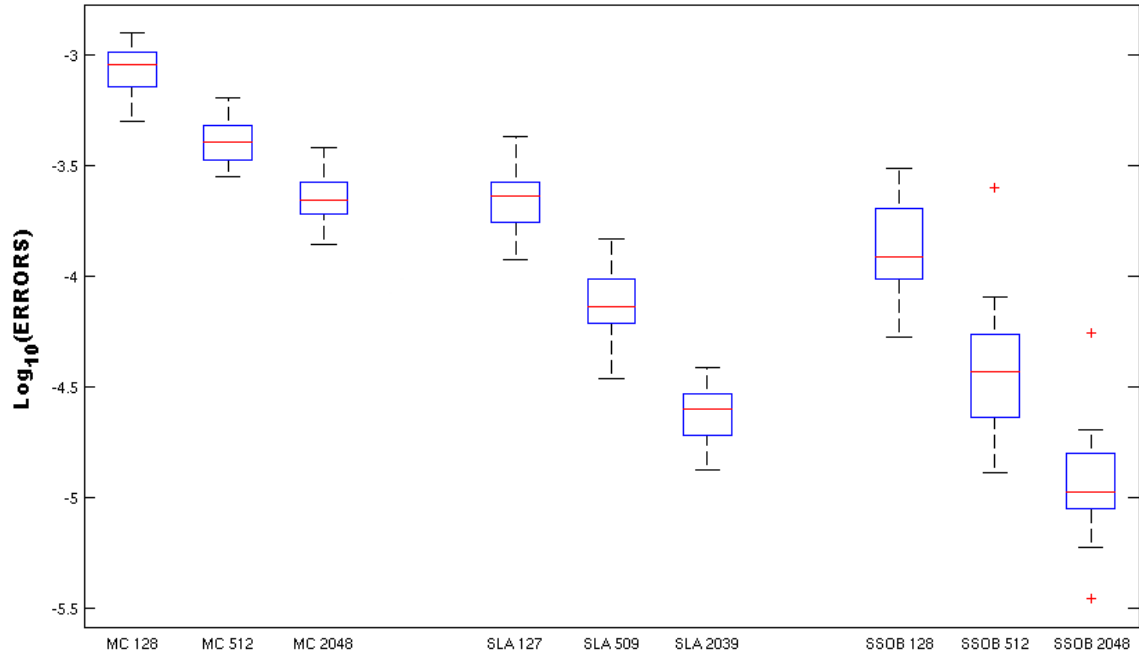
We considered a two-stage production planning problem for maximizing the expected revenue while satisfying a fixed demand in a time horizon with  $d = T = 100$  time periods and stochastic prices for the second-stage decisions. It is assumed that the probability distribution of the prices  $\xi$  is log-normal. The model is of the form

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

The use of PCA for decomposing the covariance matrix has led to effective truncation dimension  $d_T(0.01) = 2$ . As QMC methods we used a randomly scrambled Sobol sequence (SSobol) (Owen, Hickernell) with  $n = 2^7, 2^9, 2^{11}$  and a randomly shifted lattice rule (Sloan-Kuo-Joe) with  $n = 127, 509, 2039$ , weights  $\gamma_j = \frac{1}{j^2}$  and for MC the Mersenne-Twister. 10 runs were performed for the error estimates and 30 runs for plotting relative errors.

Average rate of convergence for QMC:  $O(n^{-0.9})$  and  $O(n^{-0.8})$ .

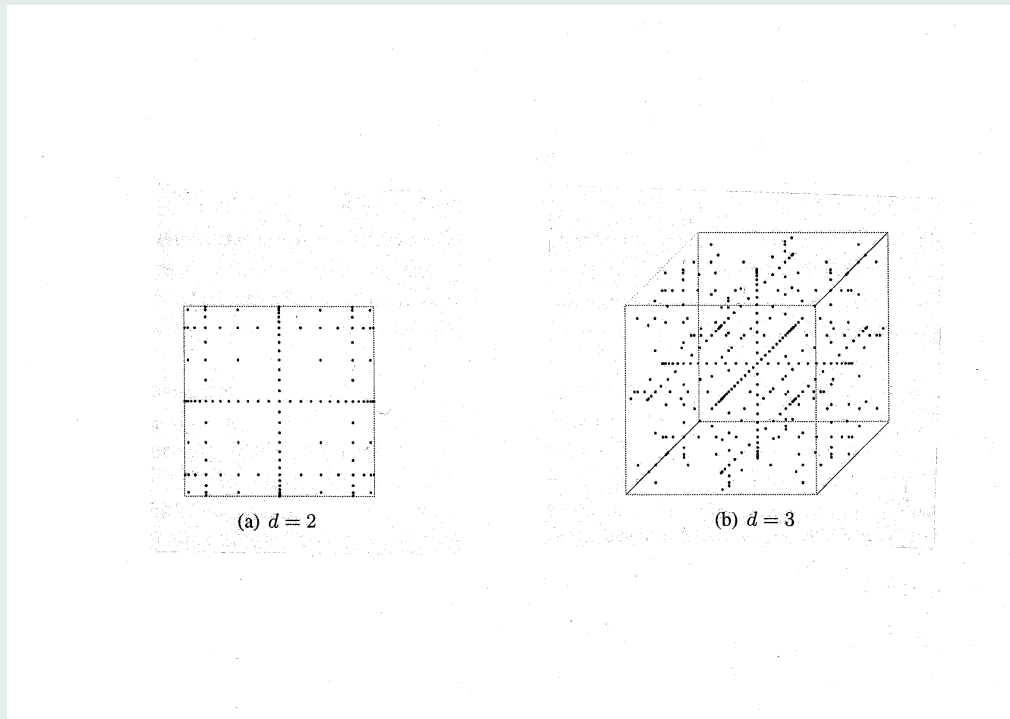
Instead of  $n = 2^7$  SSobol samples one would need  $n = 10^4$  MC samples to achieve a similar accuracy as SSobol.



$\log_{10}$  of the relative errors of MC, SLA (randomly shifted lattice rule) and SSOB (scrambled Sobol' points)

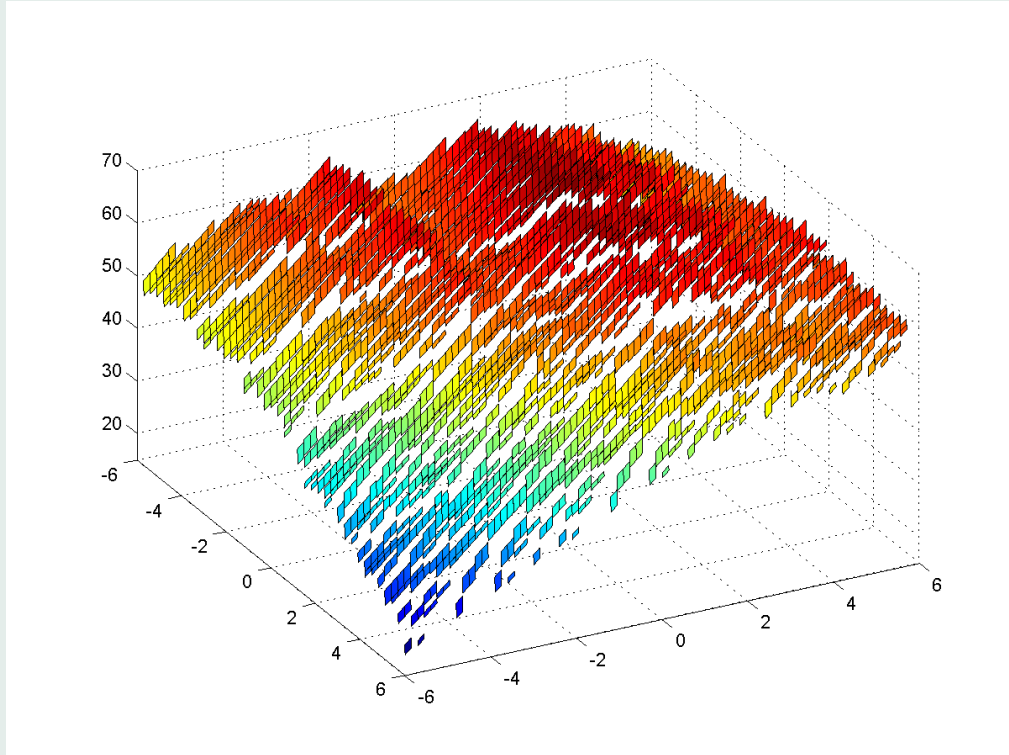
## Conclusions

- Our analysis provides a theoretical basis for applying QMC methods accompanied by dimension reduction techniques to two-stage stochastic programs.
- The analysis also applies to sparse grid quadrature techniques.



Sparse grids in the unit cube  $[0, 1]^d$

- The results are extendable and will be extended to [mixed-integer two-stage models](#), to [multi-stage situations](#), and to [models with stochastic dominance constraints](#).



Second-stage optimal value function of an integer program (van der Vlerk)



# References

- R. E. Caflisch, W. Morokoff and A. Owen: Valuation of mortgage backed securities using Brownian bridges to reduce effective dimension, *Journal of Computational Finance* 1 (1997), 27–46.
- M. Chen and S. Mehrotra: Epi-convergent scenario generation method for stochastic problems via sparse grid, *Stochastic Programming E-Print Series* 7-2008 ([www.speps.org](http://www.speps.org)).
- J. Dick, F. Pillichshammer: *Digital Nets and Sequences*, Cambridge University Press, Cambridge 2010.
- M. Griebel, F. Y. Kuo and I. H. Sloan: The smoothing effect of integration in  $\mathbb{R}^d$  and the ANOVA decomposition, *Mathematics of Computation* 82 (2013), 383-400.
- H. Heitsch, H. Leövey and W. Römisch, *Are Quasi-Monte Carlo algorithms efficient for two-stage stochastic programs?*, *Stochastic Programming E-Print Series* 5-2012 ([www.speps.org](http://www.speps.org)) and submitted.
- F. J. Hickernell: A generalized discrepancy and quadrature error bound, *Mathematics of Computation* 67 (1998), 299-322.
- T. Homem-de-Mello: On rates of convergence for stochastic optimization problems under non-i.i.d. sampling, *SIAM Journal on Optimization* 19 (2008), 524-551.
- 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.
- F. Y. Kuo, I. H. Sloan, G. W. Wasilkowski, B. J. Waterhouse: Randomly shifted lattice rules with the optimal rate of convergence for unbounded integrands, *Journal of Complexity* 26 (2010), 135–160.

- A. B. Owen: Randomly permuted  $(t, m, s)$ -nets and  $(t, s)$ -sequences, in: *Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing*, 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.
- A. B. Owen: Multidimensional variation for Quasi-Monte Carlo, in J. Fan, G. Li (Eds.), *International Conference on Statistics*, World Scientific Publ., 2005, 49–74.
- T. Pennanen, M. Koivu: Epi-convergent discretizations of stochastic programs via integration quadratures, *Numerische Mathematik* 100 (2005), 141–163.
- G. Ch. Pflug, A. Pichler: Approximations of probability distributions and stochastic optimization problems, in: *Stochastic Optimization Methods in Finance and Energy* (M.I. Bertocchi, G. Consigli, M.A.H. Dempster, eds.), Springer, 2011.
- W. Römisch: Stability of stochastic programming problems, in: *Stochastic Programming* (A. Ruszczyński, A. Shapiro eds.), *Handbooks in Operations Research and Management Science*, Volume 10, Elsevier, Amsterdam 2003, 483–554.
- 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.
- 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: Low discrepancy sequences in high dimensions: How well are their projections distributed? *Journal of Computational and Applied Mathematics* 213 (2008), 366–386.
- 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.