# Progress in high-dimensional numerical integration and its application to stochastic optimization

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Short course, Rutgers University, May 21-23, 2013

# Part III: QMC algorithms for solving stochastic optimization problems: Challenges and solutions

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## Introduction

**Aim:** Apply randomized Quasi-Monte Carlo methods, in particular, randomly shifted lattice rules to optimization models containing high-dimensional integrals.

#### **Example:** Option pricing (Wang-Sloan 11)

Consider the pricing of a path-dependent option with payoff  $g(S_{t_1}, \ldots, S_{t_d})$  where  $S_{t_j}$  are the prices of the underlying asset at times  $t_j$ ,  $j = 1, \ldots, d$ . Suppose the prices are considered at equally spaced times  $t_j = j\frac{T}{d}$ , where T is the expiration date, and the asset price follows a geometric Brownian motion

$$dS_t = rS_t dt + \sigma S_t dB_t \,,$$

where r is the risk-free interest rate,  $\sigma$  the volatility and  $B_t$  the standard Brownian motion (normal with zero mean and  $\mathbb{E}[B_tB_s] = \min\{t,s\}$ ).

The analytical solution of the (scalar linear) stochastic differential equation is

$$S_t = S_0 \exp\left(\left(r - \frac{\sigma^2}{2}\right)t + \sigma B_t\right).$$

The value of the option at t = 0 is  $\mathbb{E}[\exp(-rT)g(S_{t_1}, \ldots, S_{t_d})]$ .

Consider Asian call options based on the geometric or arithmetic average of the underlying asset. With the strike price K at time T their terminal payoffs are

$$g(S_{t_1},\ldots,S_{t_d}) = \max\left\{0,\prod_{t=1}^d S_{t_j}^{\frac{1}{d}} - K\right\} \quad \text{or} \quad = \max\left\{0,\frac{1}{d}\sum_{j=1}^d S_{t_j} - K\right\}.$$

If  $\Sigma$  denotes the covariance matrix of the normal random vector  $(B_{t_1}, \ldots, B_{t_d})^{\top}$ and A is a matrix satisfying  $\Sigma = A A^{\top}$ , the random vector  $(z_1, \ldots, z_d)^{\top}$  such that

$$(B_{t_1},\ldots,B_{t_d})^{\top} = A(z_1,\ldots,z_d)^{\top}$$

is standard normal with independent components. For the first case it holds

$$\prod_{t=1}^{d} S_{t_j}^{\frac{1}{d}} = \exp\left(m + \frac{\sigma}{T} \sum_{k=1}^{d} A_k z_k\right)$$

with  $A_k = \sum_{j=1}^d a_{jk}$ ,  $A = (a_{jk})$  and  $m = \log S_0 + \frac{T(d-1)}{2d}(r - \frac{\sigma^2}{2})$ . Hence, the value of the option at t = 0 is

$$\exp(-rT)\int_{\mathbb{R}^d} \max\left\{0, \exp\left(m + \frac{\sigma}{T}\sum_{k=1}^d A_k z_k\right) - K\right\} \rho_d(z) dz$$

with the *d*-dimensional standard normal density  $\rho_d$ .

# **Example:** (Optimization problem with random constraints)

We consider the linear optimization problem with random constraints

 $\min\{c^{\top}x : T(\xi)x = h(\xi), x \in X\},\$ 

where X is a polyhedron in  $\mathbb{R}^m$ ,  $T(\xi)$  a random matrix and  $h(\xi)$  a random vector. The model is inappropriate to find a deterministic decision !

Idea: Introduce a compensation or recourse variable  $y \ge 0$ , a recourse matrix W, a (possibly random) recourse cost vector  $q(\xi)$ , replace the constraint " $T(\xi)x = h(\xi)$ " by " $Wy = h(\xi) - T(\xi)x$ " and select a random recourse decision  $y(\xi)$  with minimal recourse costs " $q(\xi)^{\top}y(\xi)$ ". Adding the expected recourse costs to the original cost term  $c^{\top}x$  leads to the two-stage stochastic optimization model

$$\min\{c^{\top}x + \int_{\mathbb{R}^d} \inf\{q(\xi)^{\top}y : Wy = h(\xi) - T(\xi)x, y \ge 0\}\rho_d(\xi)d\xi : x \in X\},\$$

where  $\rho_d$  is the density of the underlying random vector  $\xi$  on  $\mathbb{R}^d$ .

**Challenge:** In both examples the integrands do not belong to the tensor product Sobolev space (after transformation to  $[0, 1]^d$ ).

## Two-stage linear stochastic optimization

We consider the linear two-stage stochastic program

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

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

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

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

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

Let pos  $W = W(\mathbb{R}^{\overline{m}})$ ,  $\mathcal{D} = \{ u \in \mathbb{R}^{\overline{m}} : \{ z \in \mathbb{R}^r : W^\top z \le u \} \neq \emptyset \}.$ 

#### **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  $(\overline{m} + r)$ -dimensional polyhedral cone  $\mathcal{D} \times \text{pos } W$  and there exist  $(r, \overline{m})$ -matrices  $C_j$  and  $(\overline{m} + r)$ -dimensional polyhedral cones  $\mathcal{K}_j$ ,  $j = 1, ..., \ell$ , such that

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

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

**Challenge:** The integrand  $f(x, \cdot)$  is not in the tensor product Sobolev space.

#### The 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 
$$D = \{1, \ldots, d\}$$
 and  $f \in L_{1,\rho}(\mathbb{R}^d)$  with  $\rho(\xi) = \prod_{j=1}^d \rho_j(\xi_j)$ , where  $f \in L_{p,\rho}(\mathbb{R}^d)$  iff  $\int_{\mathbb{R}^d} |f(\xi)|^p \rho(\xi) d\xi < \infty \quad (p \ge 1).$ 

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

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

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

## The dimension distribution and effective dimension of a function

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

$$\nu_{S}(s) := \sum_{|u|=s} \frac{\sigma_{u}^{2}(f)}{\sigma^{2}(f)} \qquad \left(\nu_{T}(s) = \sum_{\max\{j: j \in u\}=s} \frac{\sigma_{u}^{2}(f)}{\sigma^{2}(f)}\right) \ (s \in D).$$

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

$$d_{S}(\varepsilon) = \min\left\{s \in D : \sum_{|u| \le s} \sigma_{u}^{2}(f) \ge (1 - \varepsilon)\sigma^{2}(f)\right\} \le d_{T}(\varepsilon)$$
$$d_{T}(\varepsilon) = \min\left\{s \in D : \sum_{u \subseteq \{1, \dots, s\}} \sigma_{u}^{2}(f) \ge (1 - \varepsilon)\sigma^{2}(f)\right\}$$

It holds

$$\max\left\{\left\|f-\sum_{|u|\leq d_{S}(\varepsilon)}f_{u}\right\|_{2,\rho}, \left\|f-\sum_{u\subseteq\{1,\dots,d_{T}(\varepsilon)\}}f_{u}\right\|_{2,\rho}\right\}\leq \sqrt{\varepsilon}\sigma(f).$$

(Caflisch-Morokoff-Owen 97, Owen 03, Wang-Fang 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

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

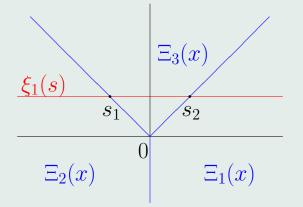
It holds  $\operatorname{int} \Xi_j(x) \neq \emptyset$ ,  $\operatorname{int} \Xi_j(x) \cap \operatorname{int} \Xi_i(x) = \emptyset$ ,  $i \neq j$ , and the sets  $\Xi_j(x)$ ,  $j = 1, \ldots, \ell$ , decompose  $\Xi$ . Furthermore, the intersection of two adjacent sets  $\Xi_i(x)$  and  $\Xi_j(x)$ ,  $i \neq j$ , is contained in some (d-1)-dimensional affine subspace.

(Griebel-Kuo-Sloan 13)

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

Then the kth projection  $P_k f$  has the explicit representation

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

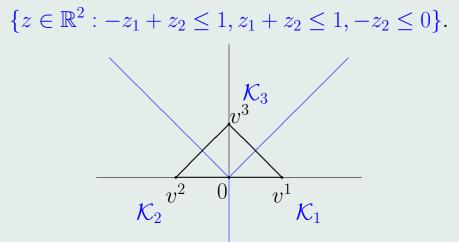
where  $s_0 = -\infty$ ,  $s_{p+1} = +\infty$  and  $p_{ij}(\cdot; x)$  are polynomials in  $\xi^k$  of degree 2-j, j = 0, 1, 2, with coefficients depending on x, and is continuously differentiable.  $P_k f$  is infinitely differentiable if the marginal density  $\rho_k$  belongs to  $C^{\infty}(\mathbb{R})$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

#### 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

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

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



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  $\pm_j(x) = Tx + \mathcal{K}_j$ , 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

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

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

As  $f_D$  is (Lipschitz) continuous and if the  $\xi^j$ , j = 1, ..., 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.

## Challenge: 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, 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  $\Sigma = Q^T D Q$  of  $\Sigma$  (with a diagonal matrix D containing the eigenvalues of  $\Sigma$ ).

**Challenge:** 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 choice of the matrix A in the decomposition  $\Sigma = A A^{\top}$  of thenonsingular covariance matrix  $\Sigma$ .

## 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  $A = (\sqrt{\lambda_1}u_1, \ldots, \sqrt{\lambda_d}u_d)$ , where  $\lambda_1 \ge \cdots \ge \lambda_d > 0$  are the eigenvalues of  $\Sigma$  in decreasing order and the corresponding orthonormal eigenvectors  $u_i$ ,  $i = 1, \ldots, d$ . 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).

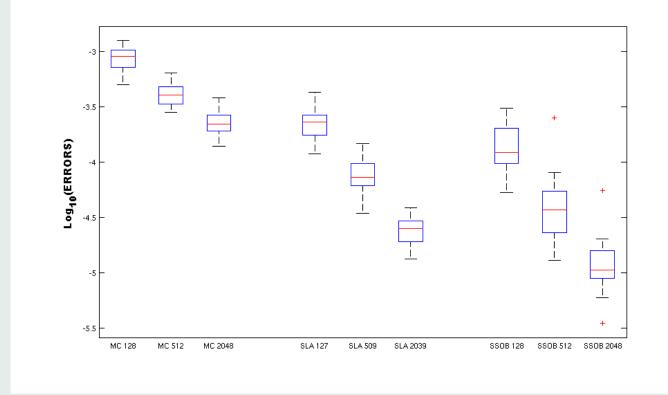
### Some computational experience

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

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

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  $\gamma_j = \frac{1}{i^3}$  and for MC the Mersenne-Twister. 10 runs were performed for the error estimates and 30 runs for plotting relative errors.

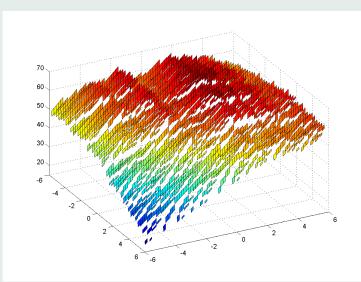
# Average rate of convergence for QMC: $O(n^{-0.9})$ and $O(n^{-0.8})$ . Instead of $n = 2^7$ SSobol samples one would need $n = 10^4$ MC samples to achieve a similar accuracy as SSobol.



 $\log_{10}$  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.
- The results are extendable and will be extended to mixed-integer two-stage models, to multi-stage situations, and to other models in stochastic optimization.



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

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