Quasi-Monte Carlo methods for linear two-stage stochastic programming problems

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Introduction

- Applied stochastic programming models in finance, production and energy often contain high-dimensional random vectors.
- 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.
- Two recently considered alternative approaches to scenario generation:
  - (a) Quasi-Monte Carlo methods (Koivu-Pennanen 05, Pennanen 09, Homem-de-Mello 08).
  - (b) Sparse grid quadrature rules (Chen-Mehrotra 08).
- Both are supported by encouraging complexity results for numerical integration.

Content

Complexity of numerical integration

We consider the approximate computation of

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

by a linear numerical integration or quadrature method of the form

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

with points $\xi^i \in [0,1]^d$ and weights $w_i \in \mathbb{R}$, $i = 1, \ldots, n$.
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 $\mathbb{B}_d = \{f \in \mathbb{F}_d : \|f\|_d \leq 1\}$ such that I_d and Q_n are linear bounded functionals on $\mathbb{F}_d$.

Worst-case error of Q_n over $\mathbb{B}_d$ and optimal error are given by:

$$\begin{aligned} e(Q_n) &= \sup_{f \in \mathbb{B}_d} |I_d(f) - Q_n(f)| \\ e(n, \mathbb{B}_d) &= \inf_{Q_n} e(Q_n) \,. \end{aligned}$$

(Novak 14)

It is known that due to the convexity and symmetry of $\mathbb{B}_d$ linear algorithms are optimal among nonlinear and adaptive ones (Bakhvalov 71, Novak 88).

The information complexity $n(\varepsilon, \mathbb{B}_d)$ is the minimal number of function values which is needed that the worst-case error is at most ε, i.e.,

$$n(\varepsilon, \mathbb{B}_d) = \min\{n : \exists Q_n \text{ such that } e(Q_n) \le \varepsilon\}$$

Of course, the behavior of $n(\varepsilon, \mathbb{B}_d)$ as function of (ε, d) depends heavily on $\mathbb{F}_d$.

Numerical integration is said to
be polynomially tractable if there exist constants $C > 0$ $q \ge 0$, $p > 0$ such that

$$n(\varepsilon, \mathbb{B}_d) \le C d^q \varepsilon^{-p},$$

be strongly polynomially tractable if there exist constants $C > 0$, $p > 0$ such that

$$n(\varepsilon, \mathbb{B}_d) \le C \varepsilon^{-p},$$

have the curse of dimension if there exist $c > 0$, $\varepsilon_0 > 0$ and $\gamma > 0$ such that

$$n(\varepsilon, \mathbb{B}_d) \ge c(1+\gamma)^d \text{ for all } \varepsilon \le \varepsilon_0 \text{ and for infinitely many } d \in \mathbb{N}.$$

Randomized algorithms:

A randomized quadrature algorithm is denoted by $(Q(\omega))_{\omega\in\Omega}$ and considered on a probabability space $(\Omega, \mathcal{F}, \mathbb{P})$.. We assume that $Q(\omega)$ is a quadrature algorithm for each ω and that it depends on ω in a measurable way. Let $n(f,\omega)$ denote the number of evaluations of $f \in \mathbb{F}_d$ needed to perform $Q(\omega)f$. The number

$$n(Q) = \sup_{f\in\mathbb{B}_d} \int_\Omega n(f,\omega)\mathbb{P}(d\omega)$$

is called the cardinality of the randomized algorithm Q and

$$e^{\mathrm{ran}}(Q) = \sup_{f\in\mathbb{B}_d} \left(\int_\Omega \|I_d f - Q(\omega)f\|^2 \, \mathbb{P}(d\omega)\right)^{\frac{1}{2}}$$

the error of Q. The minimal error of randomized algorithms is

$$e^{\mathrm{ran}}(n, \mathbb{B}_d) = \inf\{e^{\mathrm{ran}}(Q) : n(Q) \le n\}\,.$$

By construction it is clear that $e^{\mathrm{ran}}(n, \mathbb{B}_d) \le e(n, \mathbb{B}_d)$ holds.

Standard Monte Carlo (MC) method based on n i.i.d. samples: (Mathé 95)

$$e^{\mathrm{ran}}(Q) = (1+\sqrt{n})^{-1} \le n^{-\frac{1}{2}}$$

if $\mathbb{B}_d$ is the unit ball of $\mathbb{F}_d = L_p([0,1]^d)$ for $2 \le p < \infty$.

Example:

Consider the Banach space $\mathbb{F}_d = C^r([0,1]^d)$ $(r \in \mathbb{N})$ of r times continuously differentiable functions with the norm

$$\|f\|_{r,d} = \max_{|\alpha| \le r} \|D^\alpha f\|_\infty,$$

where $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ and $D^\alpha f$ denotes the mixed partial derivative of order $|\alpha| = \sum_{i=1}^d \alpha_i$, i.e.,

$$D^\alpha f(\xi) = \frac{\partial^{|\alpha|} f}{\partial \xi_1^{\alpha_1} \cdots \partial \xi_d^{\alpha_d}}(\xi)\,.$$

It is long known (Bakhvalov 59) that there exist constants $C_{r,d}$, $c_{r,d} > 0$ such that

$$c_{r,d}\, n^{-\frac{r}{d}} \le e(n, \mathbb{B}_d) \le C_{r,d}\, n^{-\frac{r}{d}}.$$

But, surprisingly it was shown only recently that the numerical integration on $C^r([0,1]^d)$ suffers from the curse of dimension (Hinrichs-Novak-Ullrich-Woźniakowski 14).

To obtain a convergence order for $e(n, \mathbb{B}_d)$ of essentially $O(n^{-r})$, differentiability requirements of higher order are necessary. At least the requirements have to increase with increasing dimension d.

For example, for the Sobolev space with dominating mixed smoothness

$$W_{2,\mathrm{mix}}^{(r,\dots,r)}([0,1]^d) = \{f : [0,1]^d \to \mathbb{R} : D^\alpha f \in L_2([0,1]^d) \text{ if } \|\alpha\|_\infty \le r\}$$

it is known that $e(n, \mathbb{B}_d) = O(n^{-r}(\log n)^{\frac{(d-1)}{2}})$ (Frolov 76, Bykovskii 85).

It is also known that $W_{2,\mathrm{mix}}^{(r,\dots,r)}([0,1]^d)$ is a tensor product space, i.e.,

$$W_{2,\mathrm{mix}}^{(r,\dots,r)}([0,1]^d) = \bigotimes_{j=1}^{d} W_2^r([0,1])$$

and a kernel reproducing Hilbert space H for several variants of inner products and corresponding kernels $K_d : [0,1]^d \times [0,1]^d \to \mathbb{R}$ (Thomas-Agnan 96) which satisfy the conditions (Aronszajn 50)

$$\begin{aligned} K_d(\cdot, x) &\in H && \text{for every } x \in [0,1]^d\,, \\ f(x) &= \langle f, K_d(\cdot, x)\rangle_H && \text{for all } f \in H,\ x \in [0,1]^d\,. \end{aligned}$$

and have product structure $K_d(x,y) = \prod_{i=1}^d K_1(x_i, y_i)$.

Although many problems in tensor product spaces suffer from the curse of dimension (Novak-Woźniakowski 08, 10, 12), the idea of introducing weights in inner products of mixed Sobolev spaces (Sloan-Woźniakowski 98) has led to a breakthrough.

We consider the linear space $W^1_{2,\gamma}([0,1])$ of all absolutely continuous functions on $[0,1]$ with derivatives belonging to $L_2([0,1])$ and the weighted inner product

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

and the kernel

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

where $B_1(x) = x - \frac{1}{2}$ and $B_2(x) = x^2 - x + \frac{1}{6}$.
Then the weighted tensor product mixed Sobolev space is

$$W^{(1,\dots,1)}_{2,\gamma,\mathrm{mix}}([0,1]^d) = \bigotimes_{j=1}^{d} W^1_{2,\gamma_j}([0,1])$$

with the kernel

$$K_{d,\gamma}(x,y) = \prod_{j=1}^{d} K_{1,\gamma_j}(x_j,y_j) = \sum_{u\subseteq\mathfrak{D}} \gamma_u \prod_{j\in u}\Big(\frac{1}{2}B_2(|x_j-y_j|) + B_1(x_j)B_1(y_j)\Big)$$

and inner product

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

where $\mathfrak{D} = \{1, \ldots, d\}$, the weights γ_i are positive and nonincreasing, and γ_u is given in product form by

$$\gamma_u = \prod_{i \in u} \gamma_i$$

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 for $j \in u$.

Theorem: (Sloan-Woźniakowski 98, Sloan-Wang-Woźniakowski 04)
Numerical integration is strongly polynomially tractable on $W_{2,\gamma,\mathrm{mix}}^{(1,\ldots,1)}([0,1]^d)$ if

$$\sum_{j=1}^{\infty} \gamma_j < \infty \,,$$

and there exist Quasi-Monte Carlo algorithms being strongly polynomially tractable.

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 ξ^i, $i = 1, \ldots, n$, 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 and Q_n are linear bounded functionals on $\mathbb{F}_d$.

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

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

QMC methods in 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 $K : [0,1]^d \times [0,1]^d \to \mathbb{R}$, i.e.,

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

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

$$e(Q_n) = \sup_{f\in\mathbb{B}_d} \left|I_d(f) - Q_n(f)\right| = \sup_{f\in\mathbb{B}_d} |\langle f, h_n\rangle| = \|h_n\|_d$$

according to Riesz' representation 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

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

(Hickernell 98, Sloan-Woźniakowski 98)

Digital nets and sequences

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. t is called the quality parameter of the net.

A sequence (ξ^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.

(Niederreiter 87, Dick-Pilichshammer 10)

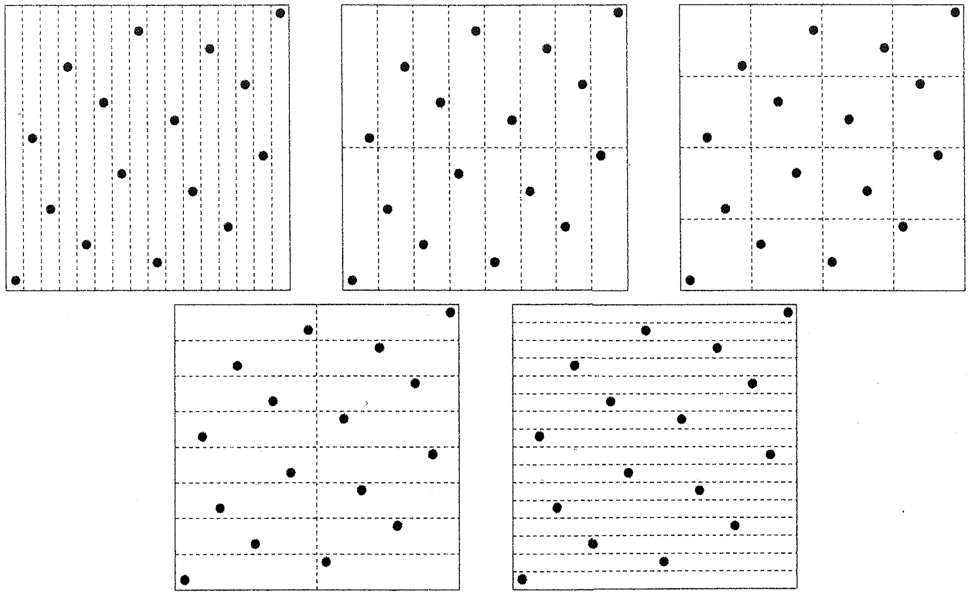


Fig. 5.2 A $(0, 4, 2)$-net in base 2; every 2-dimensional elementary interval in base 2 of area 2^{-4} contains exactly one point

Theorem: (Leobacher-Pillichshammer 14)

For the star-discrepancy of a (t,m,d)-net $\{\xi^1,\dots,\xi^n\}$, where $n=b^m$, in base b we have

$$D_n^*(\xi^1,\dots,\xi^n) = \sup_{\xi\in[0,1]^d}\Big|\prod_{j=1}^d \xi_j - \frac{1}{n}\sum_{i=1}^n \mathbf{1}_{[0,\xi)}(\xi^i)\Big| \le \frac{1}{b^{m-t}}\sum_{k=0}^{d-1}\binom{m-t}{k}(b-1)^k .$$

For the star-discrepancy of a (t,d)-sequence (ξ^i) in base b it holds

$$D_n^*(\xi^1,\dots,\xi^n) \le \frac{b^t(b-1)}{n}\sum_{m=0}^{r}\sum_{k=0}^{d-1}\binom{m-t}{k}(b-1)^k ,$$

where $r=\left\lfloor\frac{\log n}{\log b}\right\rfloor$.

Corollary:

For the star-discrepancy of a (t,d)-sequence (ξ^i) in base b one has

$$D_n^*(\xi^1,\dots,\xi^n) \le \frac{b^t(b-1)^d(d-1)}{d!(\log b)^d}\frac{(\log n)^d}{n} + O\Big(\frac{(\log n)^{d-1}}{n}\Big)$$

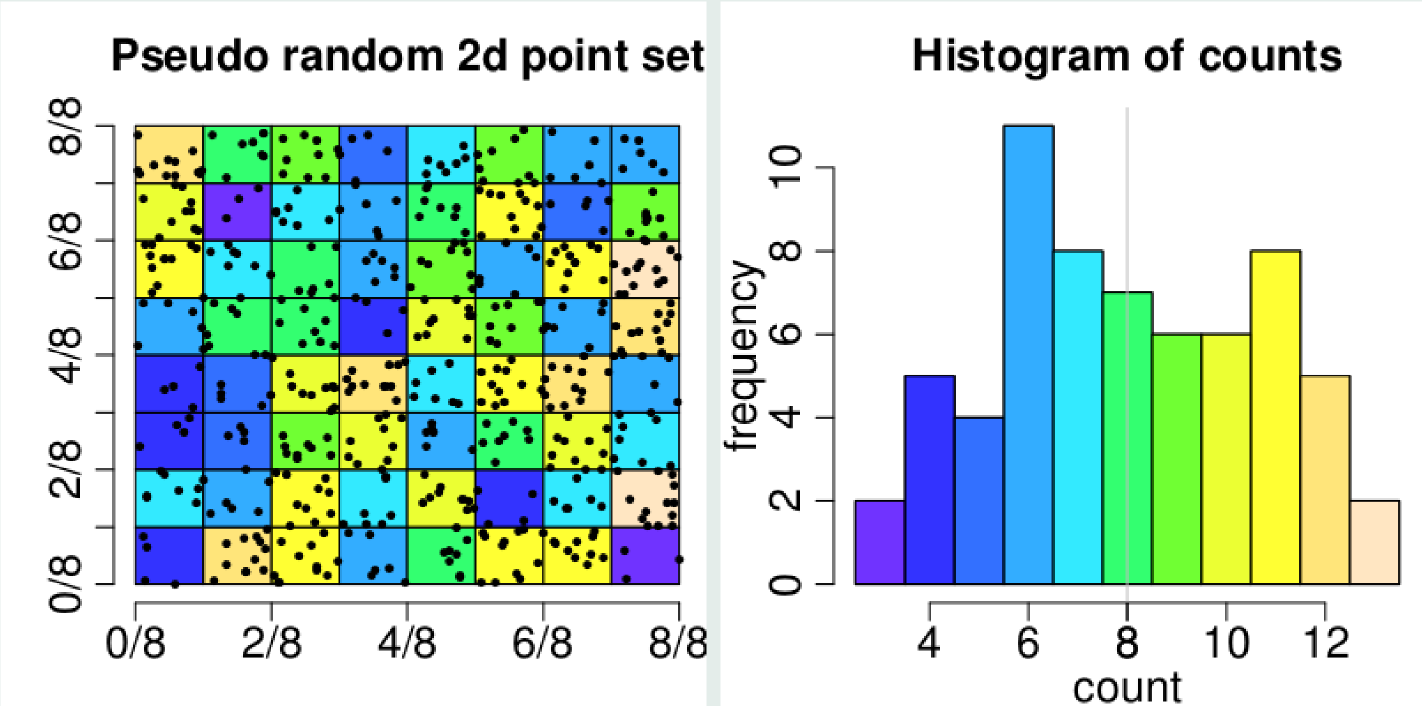
There exist specific construction methods for (t,m,d)-nets or (t,d)-sequences called digital methods.

Specific sequences:

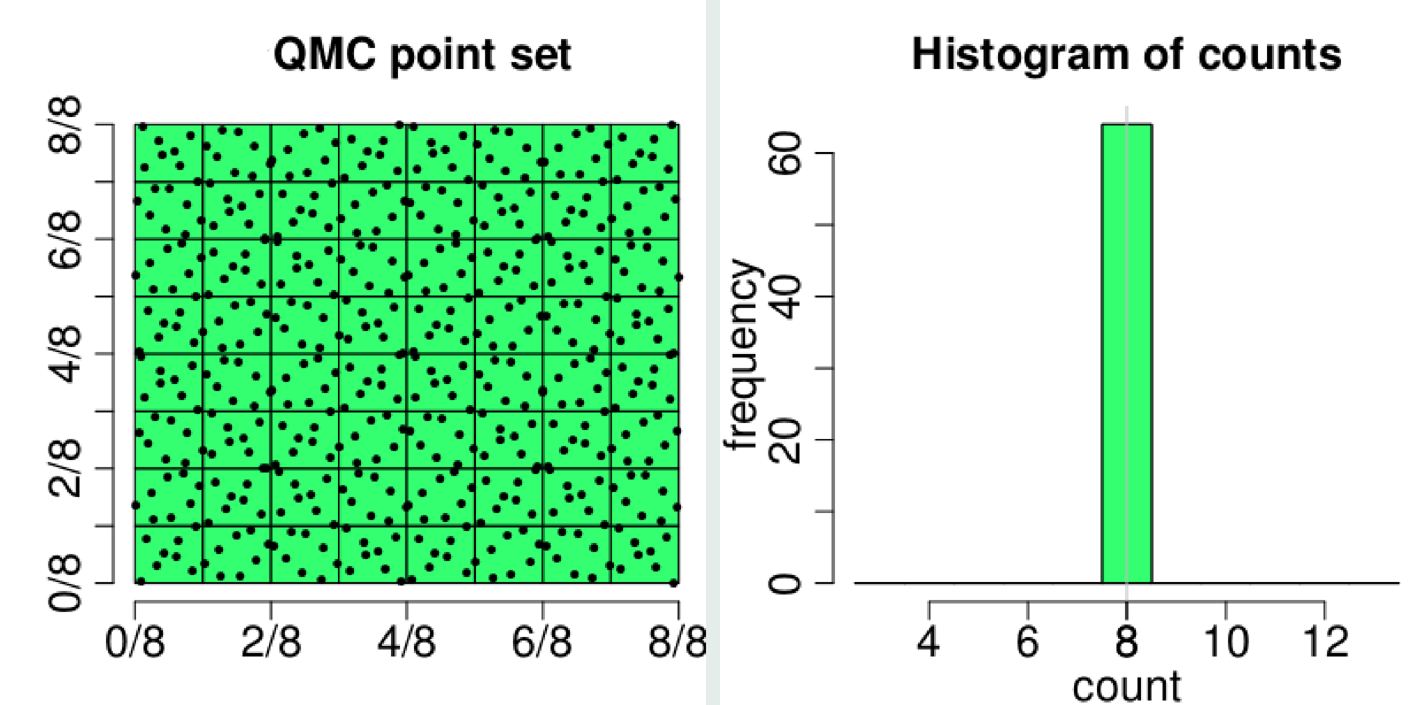
The Sobol' sequence (Sobol' 67) is a (t, d)-sequence in base $b = 2$, where t is a non-decreasing function of d;
the Faure sequence (Faure 82) is a $(0, d)$-sequence with $d \leq b$;
the classical Niederreiter sequences (Niederreiter 87);
the generalized Niederreiter sequences include both Sobol' and Faure constructions as special cases;
and the Niederreiter-Xing sequences.

(Dick-Pillichshammer 10, Dick-Kuo-Sloan 13).

$n = 2^9$ pseudo random numbers in $[0,1]^2$ generated by the Mersenne Twister



Sobol point set with $n = 2^9$ in $[0, 1]^2$



Lattice point sets and lattice rules

Let $g \in \mathbb{Z}^d$, $n \in \mathbb{N}$, $n \geq 2$ and the lattice point set $\mathcal{P}(g,n) = \{\xi^1, \dots \xi^n\}$

$$\xi^i = \left\{\frac{(i-1)}{n} g\right\} \in [0,1]^d, \quad i = 1, \dots, n\,,$$

with $\{z\}$ being defined as componentwise fractional part of $z \in \mathbb{R}_+$, i.e., $\{z\} = z - \lfloor z \rfloor \in [0,1)$. The vector g is called generating vector of the lattice point set. The idea is to choose g such that the star-discrepancy of the lattice point set has good convergence properties.

Proposition: (Leobacher-Pillichshammer 14)

It holds

$$D_n^\star(\xi^1, \dots, \xi^n) \leq \frac{d}{n} + \frac{1}{2} R_n(g)\,,$$

$$\text{where} \quad R_n(g) = \sum_{h \in C_d^\star(n) \cap \mathcal{L}(g,n)} \left(\prod_{j=1}^{d} \max\{1, |h_j|\} \right)^{-1} \quad \text{and}$$

$C_d^\star(n) = \left(\left(-\frac{n}{2}, \frac{n}{2}\right] \cap \mathbb{Z}\right)^d \setminus \{0\}\,, \quad \mathcal{L}(g,n) = \{h \in \mathbb{Z}^d \colon \langle h, g\rangle \equiv 0 \pmod{n}\}$.

The set $\mathcal{L}(g,n)$ is called dual lattice.

The idea is now to select $g \in \mathbb{Z}^d$ such that $R_n(g)$ gets small. The basic idea is to construct the generating vector component-by-component (CBC).

Algorithm: Let $n \in \mathbb{N}$.
(1) Choose $g_1 = 1$.
(2) For $s = 2, \ldots, d$, choose $g_s \in \{1, 2, \ldots, N-1\}$ to minimize $R_n((g_1, \ldots, g_{s-1}, z))$ as a function of $z \in \{1, 2, \ldots, N-1\}$.

Corollary:
Let $n \in \mathbb{N}$ be prime. If the generating vector g is constructed by the Algorithm above, then

$$D_n^\star(\xi^1, \ldots, \xi^d) \leq \frac{d}{n} + \frac{2^d}{n}(\log n + 1)^d \,.$$

A Quasi-Monte Carlo algorithm that uses a lattice point set as samples is called lattice rule.

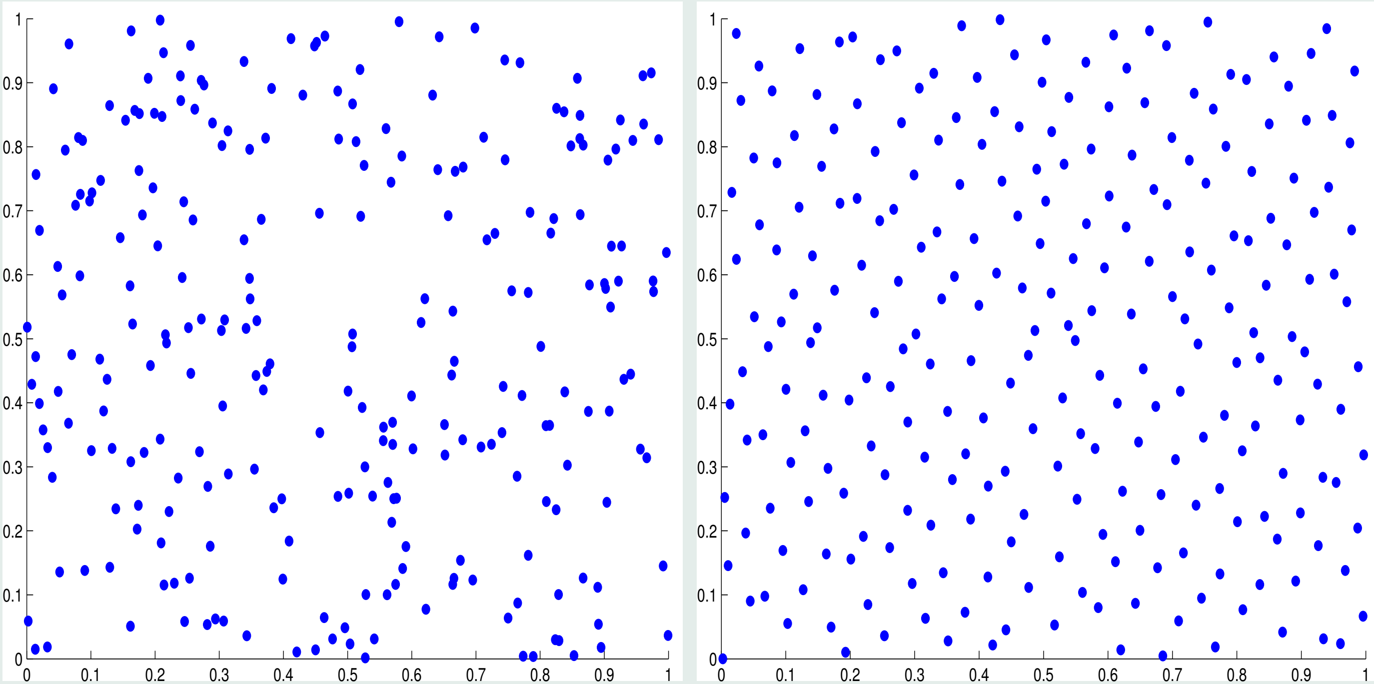
Randomized QMC methods

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 $\mathbb{Z}_b = \{0, 1, \ldots, b-1\}$ 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)

A randomly scrambled Sobol' sequence admits the following root mean-square quadrature error convergence rate for $f \in \mathcal{W}^{(1,\ldots,1)}_{2,\gamma,\mathrm{mix}}([0,1]^d)$ (Dick-Pillichshammer 10, Theorem 13.25)

$$\sqrt{\mathrm{Var}(Q_n(\omega)(f))} = \sqrt{\mathbb{E}[Q_n(\omega)(f) - I_d(f)]^2} \leq C(f)\, n^{-\frac{3}{2}} (\log n)^{\frac{d-1}{2}} \, .$$

Randomly shifted lattice rules

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

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

Theorem:
Let n be prime, $\mathbb{F}_d = \mathcal{W}^{(1,\ldots,1)}_{2,\gamma,\mathrm{mix}}([0,1]^d)$.
Then $g \in \mathbb{Z}^d$ can be CBC-constructed 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

$$e^{\mathrm{ran}}(Q_n) \leq C(\delta)\, n^{-1+\delta}\,,$$

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

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

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

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

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

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

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

Clearly, $P_k f$ is constant with respect to ξ_k. For $u \subseteq D$ we write

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

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:

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

where $f_\emptyset = I_d(f) = P_{\mathfrak{D}}(f)$ 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 ξ_j, $j \in \mathfrak{D} \backslash u$ and $j \in u \backslash v$, 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 $\{f_u\}_{u \subseteq \mathfrak{D}}$ 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

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

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

Owen's superposition (truncation) dimension distribution of f: Probability measure ν_S (ν_T) defined on the power set of D

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

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

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

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

It holds

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

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

Integrands of two-stage linear stochastic programs

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 Ξ, 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 ξ, Φ is the second-stage optimal value function

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

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

Assumptions:

(A1) $h(\xi) - T(\xi)x \in \operatorname{pos} W$ 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)
Φ is finite, polyhedral and continuous on the $(\overline{m}+r)$-dimensional convex polyhedral cone $\mathcal{D} \times \mathrm{pos}\, W$ and there exist $(r, \overline{m})$-matrices C_j and $(\overline{m}+r)$-dimensional convex polyhedral cones $\mathcal{K}_j$, $j = 1, \ldots, \ell$, such that

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

The function $\Phi(u, \cdot)$ is convex on $\mathrm{pos}\, W$ for each $u \in \mathcal{D}$, and $\Phi(\cdot, t)$ is concave on $\mathcal{D}$ for each $t \in \mathrm{pos}\, W$. 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.

Hence, the two-stage integrands are of the form

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

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

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 ρ_i, $i \in \mathfrak{D}$.

(A4) All common faces of adjacent convex polyhedral sets

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

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

Proposition:

(A1) implies that two-stage integrands

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

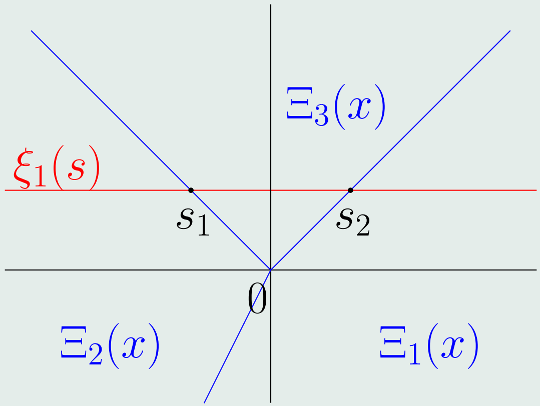
are continuous and piecewise linear-quadratic.

For each $x \in X$, $f(x, \cdot)$ is linear-quadratic on each convex polyhedral set $\Xi_j(x)$, $j = 1, \ldots, \ell$. 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 Ξ. 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 $\xi_i \in \mathbb{R}$, $i = 1, \ldots, d$, $i \neq k$, be given. We set $\xi^k = (\xi_1, \ldots, \xi_{k-1}, \xi_{k+1}, \ldots, \xi_d)$ and

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

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 kth coordinate axis.

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

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

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).

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 ξ^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 ρ_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

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

belongs to $W^{(1,\ldots,1)}_{2,\rho,\mathrm{mix}}(\mathbb{R}^d)$ if all marginal densities ρ_k, $k \in \mathfrak{D}$, belong to $C^1(\mathbb{R})$.

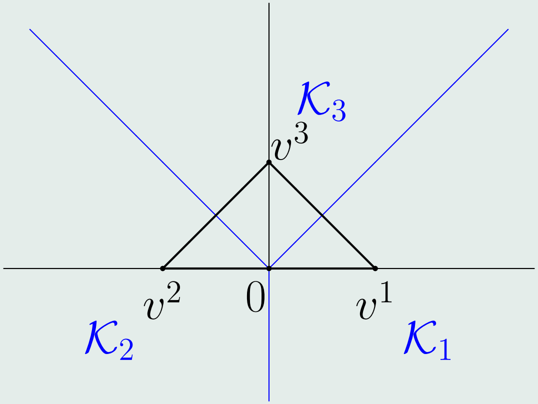
Remark:
The second order ANOVA approximation $f^{(2)}$ is a good approximation of f if the effective superposition dimension $d_S(\varepsilon)$ is at most 2. Then

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

and f belongs essentially to the tensor product Sobolev space $\mathcal{W}^{(1,\ldots,1)}_{2,\mathrm{mix}}(\mathbb{R}^d)$.
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 Φ 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

$$\Big\| \int_{\mathbb{R}^d} f(\xi)\rho(\xi)d\xi - \frac{1}{n}\sum_{j=1}^{n} f(\xi^j)\Big\|_{L_2} = \Big\| \int_{[0,1]^d} g(t)dt - \frac{1}{n}\sum_{j=1}^{n} g(t^j)\Big\|_{L_2}$$

$$\leq \sum_{0<|u|\leq d} \Big\| \int_{[0,1]^{|u|}} g_u(t^u)dt^u - \frac{1}{n}\sum_{j=1}^{n} g_u(t^j)\Big\|_{L_2}$$

$$\leq C(\delta)n^{-1+\delta} + \sum_{|u|=3}^{d} \Big\| \int_{[0,1]^d} g_u(t)dt - \frac{1}{n}\sum_{j=1}^{n} g_u(t^j)\Big\|_{L_2}$$

$$\leq C(\delta)n^{-1+\delta} + O(\sqrt{\varepsilon})$$

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

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

Since f_u, $|u| = 1, 2$, is first and mixed second order partially differentiable in the sense of Sobolev and φ^{-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 Σ and assume that Σ is transformed to a diagonal matrix by an orthogonal transformation.
Then for almost all covariance matrices Σ the second order ANOVA approximation $f^{(2)}$ of f belongs to the mixed Sobolev space $\mathcal{W}_{2,\rho,\mathrm{mix}}^{(1,\ldots,1)}(\mathbb{R}^d)$.

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 μ and nonsingular covariance matrix Σ. Let A be a matrix satisfying $\Sigma = A\,A^\top$. Then η 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 $A = (\sqrt{\lambda_1}u_1, \ldots, \sqrt{\lambda_d}u_d)$, where $\lambda_1 \geq \cdots \geq \lambda_d > 0$ are the eigenvalues of Σ 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. 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 ξ_δ and prices ξ_c as components of

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

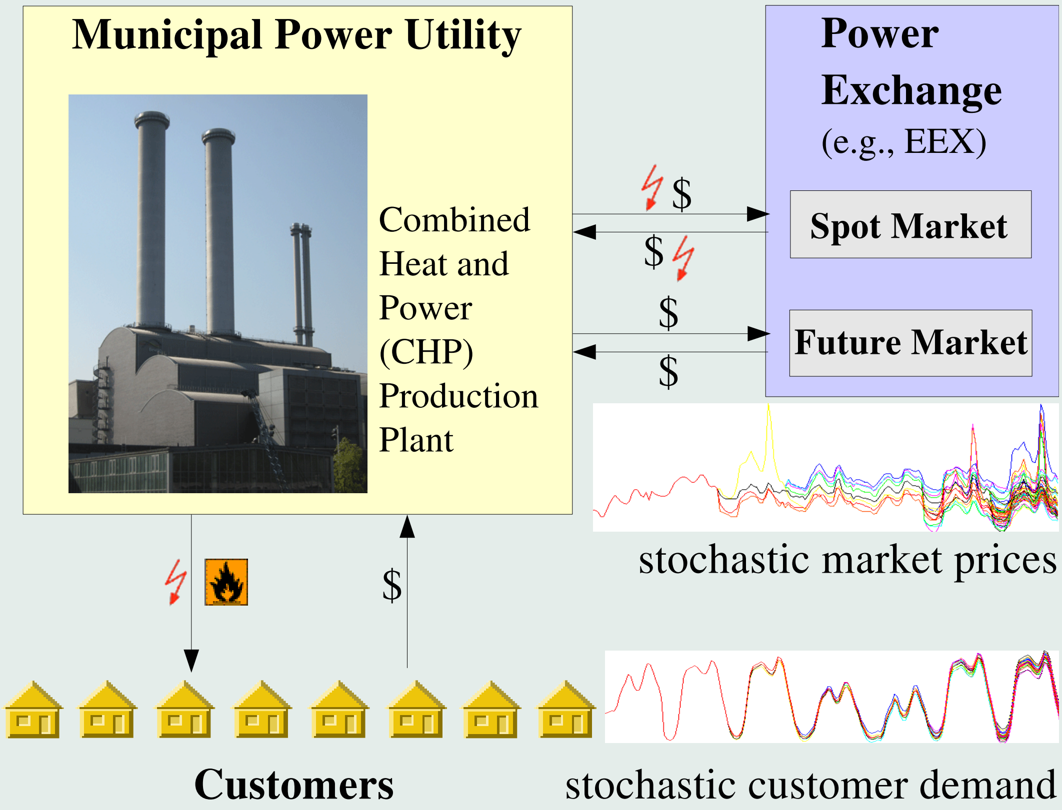
The company aims to satisfy stochastic demands $\xi_{\delta,t}$ in a time horizon $\{1, \dots, T\}$, but its production capacity based on their own units does eventually not suffice to cover the demand. Hence, it has to buy the necessary extra amounts on markets or from other providers. The model is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

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

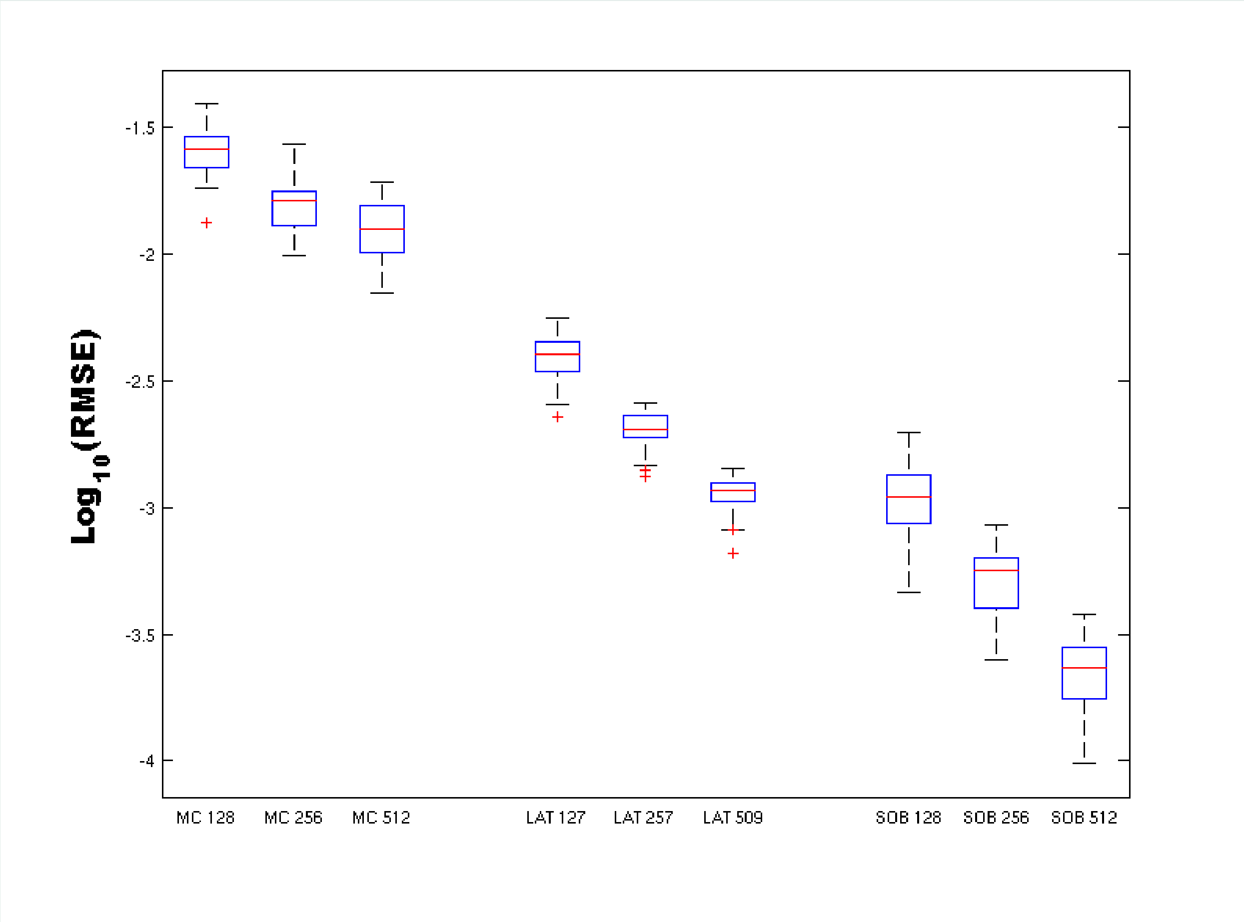
$$\begin{pmatrix} \bar{\xi}_{\delta,1} \\ \bar{\xi}_{c,1} \end{pmatrix} = B_1 \begin{pmatrix} \gamma_{1,1} \\ \gamma_{2,1} \end{pmatrix}, \quad \begin{pmatrix} \bar{\xi}_{\delta,t} \\ \bar{\xi}_{c,t} \end{pmatrix} = A \begin{pmatrix} \bar{\xi}_{\delta,t-1} \\ \bar{\xi}_{c,t-1} \end{pmatrix} + B_1 \begin{pmatrix}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


Municipal Power Utility
Combined Heat and Power (CHP) Production Plant
Power Exchange (e.g., EEX)
Spot Market
Future Market
$
$
$
$
$
stochastic market prices
Customers
stochastic customer demand

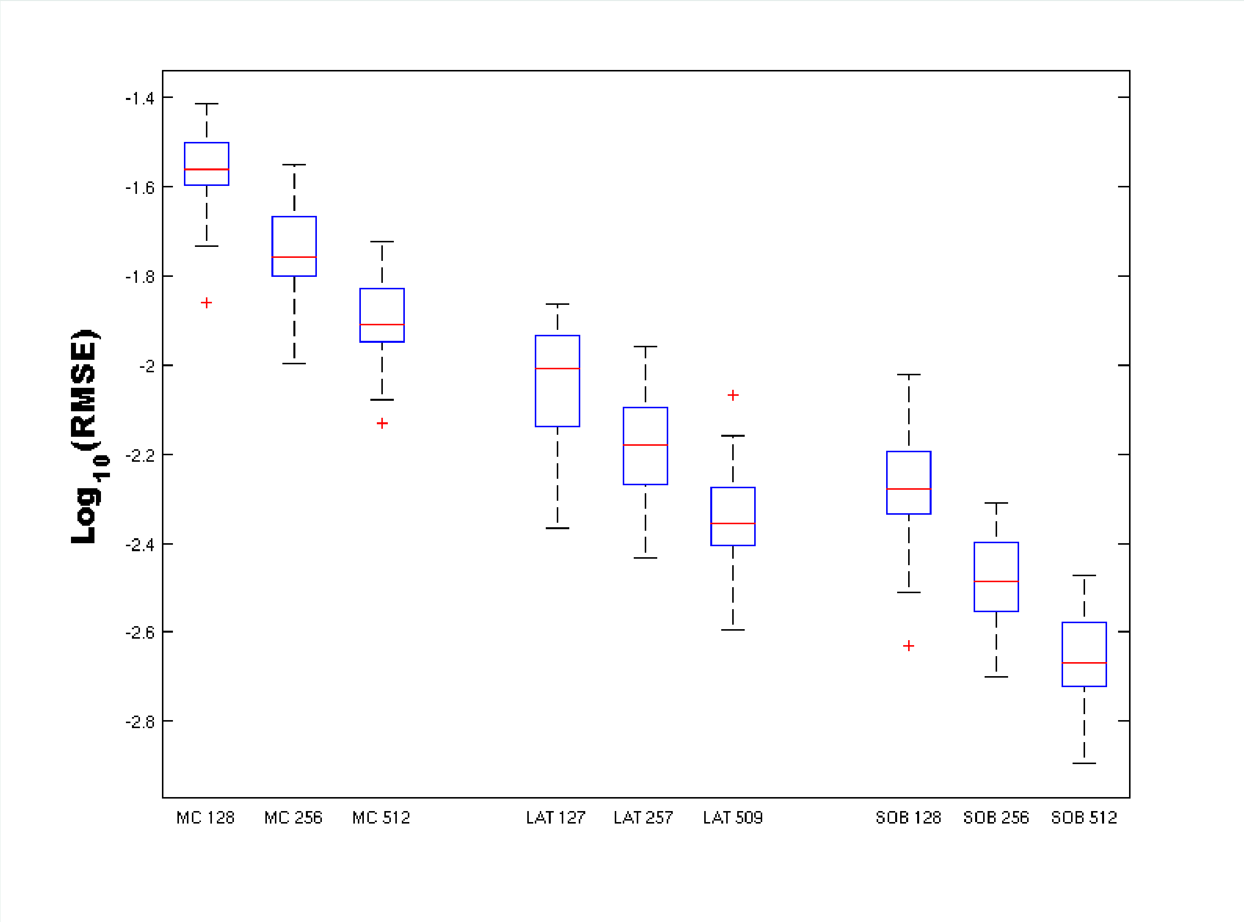
for $t = 2, \ldots, T$, where $\gamma_{1,t}, \gamma_{2,t} \sim$ N(0,1) and i.i.d. and $T = 100$.

We used PCA and CH for decomposing the covariance matrix of ξ. 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 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

Conclusions

- Our analysis provides a theoretical basis for applying modern randomized Quasi-Monte Carlo methods accompanied by dimension reduction techniques to two-stage stochastic programming problems.
- 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.
- The analysis also applies to sparse grid quadrature techniques.
- 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.

F. J. Hickernell: A generalized discrepancy and quadrature error bound, *Mathematics of Computation* 67 (1998), 299–322.

A. Hinrichs, E. Novak, M. Ullrich and H. Woźniakowski: The curse of dimensionality for numerical integration of smooth functions, *Mathematics of Computation* 83 (2014), 2853–2863.

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.

P. Mathé: The optimal error of Monte Carlo integration, *Journal of Complexity* 11 (1995), 394–415.

E. Novak: *Deterministic and Stochastic Error Bounds in Numerical Analysis*, Lecture Notes in Mathematics Vol. 1349, Springer, Berlin, 1988.

E. Novak: Some results on the complexity of numerical integration, arXiv:1409.6714v1 [math.NA], 2014.

E. Novak and H. Woźniakowski: *Tractability of Multivariate Problems, Volume I, II and III*, EMS Tracts in Mathematics, Eur. Math. Soc. Publ. House, Zürich 2008, 2010 and 2012.

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.

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.