Lattice Rules for Quasi-Monte Carlo

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Monte Carlo integration

Want to estimate

$$\mu = \mu(f) = \int_{[0,1)^s} f(\mathbf{u}) \, d\mathbf{u} = \mathbb{E}[f(\mathbf{U})]$$

where $f : [0,1)^s \to \mathbb{R}$ and **U** is a uniform r.v. over $[0,1)^s$. Standard (or crude) Monte Carlo:

- Generate *n* independent copies of **U**, say U_1, \ldots, U_n ;
- estimate μ by $\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n f(\mathbf{U}_i)$.

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 by $\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n f(\mathbf{U}_i)$.

Almost sure convergence as $n \to \infty$ (strong law of large numbers). For confidence interval of level $1 - \alpha$, can use central limit theorem:

$$\mathbb{P}\left[\mu \in \left(\hat{\mu}_n - \frac{c_\alpha S_n}{\sqrt{n}}, \ \hat{\mu}_n + \frac{c_\alpha S_n}{\sqrt{n}}\right)\right] \approx 1 - \alpha,$$

where S_n^2 is any consistent estimator of $\sigma^2 = \operatorname{Var}[f(\mathbf{U})]$.

Quasi-Monte Carlo (QMC)

Replace the independent random points \mathbf{U}_i by a set of deterministic points $P_n = {\mathbf{u}_0, \dots, \mathbf{u}_{n-1}}$ that cover $[0, 1)^s$ more evenly.

Estimate

$$\mu = \int_{[0,1)^s} f(\mathbf{u}) \mathrm{d}\mathbf{u}$$
 by $Q_n = \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{u}_i).$

Integration error $E_n = Q_n - \mu$.

 P_n is called a highly-uniform point set or low-discrepancy point set if some measure of discrepancy between the empirical distribution of P_n and the uniform distribution converges to 0 faster than $O(n^{-1/2})$ (the typical rate for independent random points).

Main construction methods: lattice rules and digital nets.

Simple case: one dimension (s = 1)

Obvious solutions:

$$P_n = \mathbb{Z}_n/n = \{0, 1/n, \dots, (n-1)/n\}$$
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for which $E_n = \mathcal{O}(n^{-2})$ if f'' is bounded.

Simplistic solution for s > 1: rectangular grid $P_n = \{(i_1/d, ..., i_s/d) \text{ such that } 0 \le i_j < d \ \forall j\} \text{ where } n = d^s.$



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Midpoint rule in s dimensions. Quickly becomes impractical when s increases. Moreover, each one-dimensional projection has only d distinct points, each two-dimensional projections has only d^2 distinct points, etc.

Lattice rules

[Korobov 1959; Sloan and Joe 1994; etc.] Integration lattice:

$$oldsymbol{L}_{oldsymbol{s}} = \left\{ oldsymbol{v} = \sum_{j=1}^{s} z_j oldsymbol{v}_j ext{ such that each } z_j \in \mathbb{Z}
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where $\mathbf{v}_1, \ldots, \mathbf{v}_s \in \mathbb{R}^s$ are linearly independent over \mathbb{R} and where L_s contains \mathbb{Z}^s . Lattice rule: Take $P_n = {\mathbf{u}_0, \ldots, \mathbf{u}_{n-1}} = L_s \cap [0, 1)^s$.

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Lattice rule of rank 1: $\mathbf{u}_i = i\mathbf{v}_1 \mod 1$ for $i = 0, \dots, n-1$, where $n\mathbf{v}_1 = \mathbf{a} = (a_1, \dots, a_s) \in \{0, 1, \dots, n-1\}^s$.

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For any $\mathfrak{u} \subset \{1, \ldots, s\}$, the projection $L_s(\mathfrak{u})$ of L_s is also a lattice.

Fully projection-regular: Each $P_n(\mathfrak{u}) = L_s(\mathfrak{u}) \cap [0,1)^{|\mathfrak{u}|}$ contains *n* distinct points. For a rule of rank 1: true iff $gcd(n, a_j) = 1$ for all *j*.



Here, each one-dimensional projection is $\{0, 1/n, \dots, (n-1)/n\}$.



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Another example: s = 2, n = 1021, $v_1 = (1, 90)/n$

$$P_n = \{ \mathbf{u}_i = i\mathbf{v}_1 \mod 1 : i = 0, \dots, n-1 \} \\ = \{ (i/1021, (90i/1021) \mod 1) : i = 0, \dots, 1020 \}.$$



A bad lattice: s = 2, n = 101, $\mathbf{v}_1 = (1, 51)/n$



Good uniformity for one-dimensional projections, but not in two dim.

Sequence of imbedded lattices

Sequence of lattices $L^1_s \subset L^2_s \subset L^3_s \subset \ldots$

 $L_s^{\xi} \cap [0,1)^s$ contains n_{ξ} points: $n_{\xi-1}$ divides n_{ξ} for all ξ .

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Simple case: lattices of rank 1, $n_{\xi} = 2^{\xi}$, $\mathbf{a}_{\xi} \mod n_{\xi-1} = \mathbf{a}_{\xi-1}$.

Then, $a_{\xi,j} = a_{\xi-1,j}$ or $a_{\xi,j} = a_{\xi-1,j} + n_{\xi-1}$.

[Cranley and Patterson 1976, Joe 1990, Hickernell et al. 2001, Kuo et al. 2006]

Error in terms of Fourier expansion of f

$$f(\mathbf{u}) = \sum_{\mathbf{h} \in \mathbb{Z}^s} \hat{f}(\mathbf{h}) \exp(2\pi \mathrm{i} \, \mathbf{h} \cdot \mathbf{u}),$$

with Fourier coefficients

$$\hat{f}(\mathbf{h}) = \int_{[0,1)^s} f(\mathbf{u}) \exp(-2\pi \mathrm{i} \, \mathbf{h} \cdot \mathbf{u}) d\mathbf{u}.$$

If this series converges absolutely, then

$$E_n = Q_n - \mu = \sum_{\mathbf{0}
eq \mathbf{h} \in L_s^*} \hat{f}(\mathbf{h})$$

where $L_s^* = {\mathbf{h} \in \mathbb{R}^s : \mathbf{h}^t \mathbf{v} \in \mathbb{Z} \text{ for all } \mathbf{v} \in L_s} \subseteq \mathbb{Z}^s$ is the dual lattice.

Let $\alpha > 0$ be an even integer. If f has square-integrable mixed partial derivatives up to order $\alpha/2 > 0$, and the periodic continuation of its derivatives up to order $\alpha/2 - 1$ is continuous across the unit cube boundaries, then

$$|\widehat{f}(\mathbf{h})| = \mathcal{O}((\mathsf{max}(1,h_1)\cdots\mathsf{max}(1,h_s))^{-lpha/2}).$$

Moreover, there are rank-1 integration lattices for which

$$\mathcal{P}_{\alpha/2} := \sum_{\mathbf{0} \neq \mathbf{h} \in L_s^*} (\max(1, h_1) \cdots \max(1, h_s))^{-\alpha/2} = \mathcal{O}(n^{-\alpha/2+\epsilon}),$$

and they are easy to find via CBC construction. This criterion was proposed long ago as a figure of merit, usually with $\alpha = 2$. This is the error for a worst-case f for which $|\hat{f}(\mathbf{h})| = (\max(1, |h_1|) \cdots \max(1, |h_s|))^{-\alpha/2}$.

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12

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Unfortunately, this bound becomes rapidly useless (in many ways) when s increases. But it can be generalized in various directions: put different weights $w(\mathbf{h})$ on vectors \mathbf{h} , or on subsets of coordinates; truncate the series if α is not even; etc. Notions of tractability... Also hard to estimate the error.

Randomized quasi-Monte Carlo (RQMC)

$$\hat{\mu}_{n,\text{rqmc}} = \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{U}_i),$$

with $P_n = { \mathbf{U}_0, \dots, \mathbf{U}_{n-1} } \subset (0,1)^s$ an RQMC point set:

(i) each point U_i has the uniform distribution over (0, 1)^s;
(ii) P_n as a whole is a low-discrepancy point set.

$$\mathbb{E}[\hat{\mu}_{n,\mathrm{rqmc}}] = \mu$$
 (unbiased).

$$\operatorname{Var}[\hat{\mu}_{n,\operatorname{rqmc}}] = \frac{\operatorname{Var}[f(\mathsf{U}_i)]}{n} + \frac{2}{n^2} \sum_{i < j} \operatorname{Cov}[f(\mathsf{U}_i), f(\mathsf{U}_j)].$$

We want to make the last sum as negative as possible.

Weaker attempts to do the same: antithetic variates (n = 2), Latin hypercube sampling (LHS), stratification, ...

Variance estimation:

Can compute *m* independent realizations X_1, \ldots, X_m of $\hat{\mu}_{n,\text{rqmc}}$, then estimate μ and $\text{Var}[\hat{\mu}_{n,\text{rqmc}}]$ by their sample mean \overline{X}_m and sample variance S_m^2 . Could be used to compute a confidence interval.

Temptation: assume that \bar{X}_m has the normal distribution.

Beware: often wrong unless $m \to \infty$.

CLT for fixed *m* and $n \rightarrow \infty$ holds for nets with Owen nested scrambling, but not for randomly-shifted lattice rules.









A small lattice shifted by the red vector, modulo 1.



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Can generate the shift uniformly in the parallelotope determined by basis vectors,



Can generate the shift uniformly in the parallelotope determined by basis vectors,



Can generate the shift uniformly in the parallelotope determined by basis vectors, or in any shifted copy of it.



Perhaps less obvious: Can generate it in any of the colored shapes below.



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Generating the shift uniformly in one tile

Proposition. Let $R \subset [0,1)^s$ such that

$$\{R_i = (R + \mathbf{u}_i) \mod 1, i = 0, \dots, n-1\}$$

is a partition of $[0,1)^s$ in *n* regions of volume 1/n.

Then, sampling the random shift **U** uniformly in any given R_i is equivalent to sampling it uniformly in $[0, 1)^s$.

The error function

$$g_n(\mathbf{U}) = \hat{\mu}_{n,\mathrm{rqmc}} - \mu$$

over any R_i is the same as over R.

Error function $g_n(\mathbf{u})$ for $f(u_1, u_2) = (u_1 - 1/2)(u_2 - 1/2)$.



 u_1
Error function $g_n(\mathbf{u})$ for $f(u_1, u_2) = (u_1 - 1/2) + (u_2 - 1/2)$.



 u_1

Error function $g_n(\mathbf{u})$ for $f(u_1, u_2) = u_1 u_2 (u_1 - 1/2) (u_2 - 1/2)$.



 u_x

Variance for randomly-shifted lattice

Suppose f has Fourier expansion

$$f(\mathsf{u}) = \sum_{\mathsf{h} \in \mathbb{Z}^s} \hat{f}(\mathsf{h}) e^{2\pi \mathrm{i} \mathsf{h}^{\mathrm{t}} \mathsf{u}}.$$

For a randomly shifted lattice, the exact variance is (always)

$$\operatorname{Var}[\hat{\mu}_{n,\mathrm{rqmc}}] = \sum_{\mathbf{0}
eq \mathbf{h} \in L_s^*} |\hat{f}(\mathbf{h})|^2,$$

where L_s^* is the dual lattice.

From the viewpoint of variance reduction, an optimal lattice for given f minimizes the square "discrepancy" $D^2(P_n) = \operatorname{Var}[\hat{\mu}_{n,\operatorname{rqmc}}]$.

$$\operatorname{Var}[\hat{\mu}_{n,\operatorname{rqmc}}] = \sum_{\mathbf{0} \neq \mathbf{h} \in L_s^*} |\hat{f}(\mathbf{h})|^2.$$

Let $\alpha > 0$ be an even integer. If f has square-integrable mixed partial derivatives up to order $\alpha/2 > 0$, and the periodic continuation of its derivatives up to order $\alpha/2 - 1$ is continuous across the unit cube boundaries, then

$$|\widehat{f}(\mathbf{h})|^2 = \mathcal{O}((\max(1,h_1)\cdots\max(1,h_s))^{-lpha}).$$

Moreover, there is a vector $\mathbf{v}_1 = \mathbf{v}_1(n)$ such that

$$\mathcal{P}_{lpha} := \sum_{\mathbf{0}
eq \mathbf{h} \in L_s^*} (\max(1, h_1) \cdots \max(1, h_s))^{-lpha} = \mathcal{O}(n^{-lpha + \epsilon}).$$

This \mathcal{P}_{α} is the variance for a worst-case f having

$$|\widehat{f}(\mathbf{h})|^2 = (\max(1,|h_1|)\cdots\max(1,|h_s|))^{-lpha}.$$

A larger α means a smoother f and a faster convergence rate.

If α is an even integer, this worst-case f is

$$f^*(\mathbf{u}) = \sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \prod_{j \in \mathfrak{u}} \frac{(2\pi)^{\alpha/2}}{(\alpha/2)!} B_{\alpha/2}(u_j).$$

where $B_{\alpha/2}$ is the Bernoulli polynomial of degree $\alpha/2$. In particular, $B_1(u) = u - 1/2$ and $B_2(u) = u^2 - u + 1/6$. Easy to compute P_{α} and to search for good lattices in this case!

However: This worst-case function is not necessarily representative of what happens in applications. Also, the hidden factor in \mathcal{O} increases quickly with *s*, so this result is not very useful for large *s*.

To get a bound that is uniform in s, the Fourier coefficients must decrease rapidly with the dimension and "size" of vectors **h**; that is, f must be "smoother" in high-dimensional projections. This is typically what happens in applications for which RQMC is effective!

A very general weighted \mathcal{P}_{α}

 \mathcal{P}_{α} can be generalized by giving different weights $w(\mathbf{h})$ to the vectors \mathbf{h} :

$$ilde{\mathcal{P}}_lpha := \sum_{oldsymbol{0}
eq oldsymbol{h} \in \mathcal{L}_s^*} w(oldsymbol{h})(\max(1,|h_1|)\cdots\max(1,|h_s|))^{-lpha}.$$

But how do we choose these weights? There are too many!

The optimal weights to minimize the variance are:

$$w(\mathbf{h}) = (\max(1,|h_1|)\cdots\max(1,|h_s|))^{lpha}|\hat{f}(\mathbf{h})|^2.$$

ANOVA decomposition

The Fourier expansion has too many terms to handle.

As a cruder expansion, we can write $f(\mathbf{u}) = f(u_1, \dots, u_s)$ as:

$$f(\mathbf{u}) = \sum_{\mathbf{u} \subseteq \{1,...,s\}} f_{\mathbf{u}}(\mathbf{u}) = \mu + \sum_{i=1}^{s} f_{\{i\}}(u_i) + \sum_{i,j=1}^{s} f_{\{i,j\}}(u_i, u_j) + \cdots$$

where

$$f_{\mathfrak{u}}(\mathbf{u}) = \int_{[0,1)^{|\overline{\mathfrak{u}}|}} f(\mathbf{u}) \, \mathrm{d}\mathbf{u}_{\overline{\mathfrak{u}}} - \sum_{\mathfrak{v} \subset \mathfrak{u}} f_{\mathfrak{v}}(\mathbf{u}_{\mathfrak{v}}),$$

and the Monte Carlo variance decomposes as

$$\sigma^2 = \sum_{\mathfrak{u} \subseteq \{1, \dots, s\}} \sigma_{\mathfrak{u}}^2, \quad \text{ where } \sigma_{\mathfrak{u}}^2 = \operatorname{Var}[f_{\mathfrak{u}}(\mathsf{U})].$$

The $\sigma_{\mathfrak{u}}^2$'s can be estimated (perhaps very roughly) by MC or RQMC. Intuition: Make sure the projections $P_n(\mathfrak{u})$ are very uniform for subsets \mathfrak{u} with large $\sigma_{\mathfrak{u}}^2$. Weighted $\mathcal{P}_{\gamma,\alpha}$ with projection-dependent weights $\gamma_{\mathfrak{u}}$ Denote $\mathfrak{u}(\mathbf{h}) = \mathfrak{u}(h_1, \ldots, h_s)$ the set of indices j for which $h_j \neq 0$.

$$\mathcal{P}_{\gamma, lpha} = \sum_{\mathbf{0}
eq \mathbf{h} \in L_s^*} \gamma_{\mathfrak{u}(\mathbf{h})}(\max(1, |h_1|) \cdots \max(1, |h_s|))^{-lpha}$$

For $\alpha/2$ integer > 0, with $\mathbf{u}_i = (u_{i,1}, \dots, u_{i,s}) = i\mathbf{v}_1 \mod 1$,

$$\mathcal{P}_{\gamma,\alpha} = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1,\ldots,s\}} \frac{1}{n} \sum_{i=0}^{n-1} \gamma_{\mathfrak{u}} \left[\frac{-(-4\pi^2)^{\alpha/2}}{(\alpha)!} \right]^{|\mathfrak{u}|} \prod_{j \in \mathfrak{u}} B_{\alpha}(u_{i,j}),$$

and the corresponding variation is

$$V_{\gamma}^{2}(f) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1,...,s\}} \frac{1}{\gamma_{\mathfrak{u}}(4\pi^{2})^{\alpha|\mathfrak{u}|/2}} \int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{\alpha|\mathfrak{u}|/2}}{\partial \mathfrak{u}^{\alpha/2}} f_{\mathfrak{u}}(\mathfrak{u}) \right|^{2} d\mathfrak{u},$$

for $f:[0,1)^s \to \mathbb{R}$ smooth enough. Then,

$$\operatorname{Var}[\hat{\mu}_{n,\mathrm{rqmc}}] = \sum_{\mathfrak{u} \subseteq \{1,...,s\}} \operatorname{Var}[\hat{\mu}_{n,\mathrm{rqmc}}(f_{\mathfrak{u}})] \leq V_{\gamma}^2(f) \mathcal{P}_{\gamma,lpha} \; .$$

Weighted $\mathcal{P}_{\gamma,\alpha}$:

$$\mathcal{P}_{\boldsymbol{\gamma},\boldsymbol{\alpha}} = \sum_{\mathbf{0}\neq\mathbf{h}\in L_s^*} \gamma_{\mathfrak{u}(\mathbf{h})}(\max(1,h_1),\ldots,\max(1,h_s))^{-\alpha}$$

Variance for a worst-case function whose square Fourier coefficients are

$$|\hat{f}(\mathbf{h})|^2 = \gamma_{\mathfrak{u}(\mathbf{h})}(\max(1,h_1),\ldots,\max(1,h_s))^{-lpha}.$$

This is the RQMC variance for the function

$$f^*(\mathbf{u}) = \sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \sqrt{\gamma_{\mathfrak{u}}} \prod_{j \in \mathfrak{u}} \frac{(2\pi)^{\alpha/2}}{(\alpha/2)!} B_{\alpha/2}(u_j).$$

We also have for this f:

$$\sigma_{\mathfrak{u}}^{2} = \gamma_{\mathfrak{u}} \left[\operatorname{Var}[B_{\alpha/2}(U)] \frac{(4\pi^{2})^{\alpha/2}}{((\alpha/2)!)^{2}} \right]^{|\mathfrak{u}|} = \gamma_{\mathfrak{u}} \left[|B_{\alpha}(0)| \frac{(4\pi^{2})^{\alpha/2}}{(\alpha)!} \right]^{|\mathfrak{u}|}.$$

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For $\alpha = 2$, we should take $\gamma_{\mathfrak{u}} = (3/\pi^2)^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2 \approx (0.30396)^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2$. For $\alpha = 4$, we should take $\gamma_{\mathfrak{u}} = [45/\pi^4]^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2 \approx (0.46197)^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2$. For $\alpha \to \infty$, we have $\gamma_{\mathfrak{u}} \to (0.5)^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2$.

The ratios weight / variance should decrease exponentially with $|\mathfrak{u}|$.

Heuristics for choosing the weights

For f^* , we should take $\gamma_{\mathfrak{u}} = \rho^{|\mathfrak{u}|} \sigma_{\mathfrak{u}}^2$ for some constant ρ .

But there are still $2^s - 1$ subsets \mathfrak{u} to consider!

One could define a simple parametric model for the square variations and then estimate the parameters by matching the ANOVA variances σ_u^2 [Wang and Sloan 2006, L. and Munger 2012].

For example, product weights: $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$ for some constants $\gamma_j \ge 0$.

Order-dependent weights: $\gamma_{\mathfrak{u}}$ depends only on $|\mathfrak{u}|$. Example: $\gamma_{\mathfrak{u}} = 1$ for $|\mathfrak{u}| \leq d$ and $\gamma_{\mathfrak{u}} = 0$ otherwise. Wang (2007) suggests this with d = 2. Mixture: POD weights (Kuo et al. 2011).

Note that all one-dimensional projections (before random shift) are the same. So the weights $\gamma_{\mathfrak{u}}$ for $|\mathfrak{u}| = 1$ are irrelevant.

Weighted $\mathcal{R}_{\gamma,\alpha}$

When α is not even, one can take

$$\mathcal{R}_{\gamma,\alpha}(P_n) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1,...,s\}} \gamma_{\mathfrak{u}} \frac{1}{n} \sum_{i=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{h=-\lfloor (n-1)/2 \rfloor}^{\lfloor n/2 \rfloor} \max(1,|h|)^{-\alpha} e^{2\pi \mathrm{i} h u_{i,j}} - 1 \right)$$

Upper bounds on $\mathcal{P}_{\gamma,\alpha}$ can be computed in terms of $\mathcal{R}_{\gamma,\alpha}$.

Can be computed for any $\alpha > 0$ (finite sum). For example, can take $\alpha = 1$. We can compute it using FFT. .

Figure of merit based on the spectral test Compute the shortest vector $\ell_{\mathfrak{u}}(P_n)$ in dual lattice for each projection \mathfrak{u} and normalize by an upper bound $\ell_{|u|}^*(n)$ (with Euclidean length):

$$\mathcal{D}_{\mathfrak{u}}(P_n) = rac{\ell^*_{|\mathfrak{u}|}(n)}{\ell_{\mathfrak{u}}(P_n)} \geq 1.$$

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L. and Lemieux (2000), etc., maximize

$$M_{t_1,...,t_d} = \min\left[\min_{2 \le r \le t_1} \frac{\ell_{\{1,...,r\}}(P_n)}{\ell_r^*(n)}, \min_{\substack{2 \le r \le d \\ 1 = j_1 < \cdots < j_r \le t_r}} \frac{\ell_u(P_n)}{\ell_r^*(n)}\right].$$

Computing time of $\ell_{\mu}(P_n)$ is almost independent of n, but exponential in $|\mu|$. Poor lattices can be eliminated quickly.

Can use a different norm, compute shortest vector in primal lattice, etc.

Korobov lattices. Search over all admissible *a*, for $\mathbf{a} = (1, a, a^2, ..., ...)$. Random Korobov. Try *r* random values of *a*.

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Component by component (CBC) construction. (Sloan, Kuo, etc.). Let $a_1 = 1$; For j = 2, 3, ..., s, find $z \in \{1, ..., n-1\}$, gcd(z, n) = 1, such that $(a_1, a_2, ..., a_j = z)$ minimizes $\mathcal{D}(P_n(\{1, ..., j\}))$.

Fast CBC construction for $\mathcal{P}_{\gamma,\alpha}$: use FFT. (Nuyens, Cools).

Korobov lattices. Search over all admissible *a*, for $\mathbf{a} = (1, a, a^2, ..., ...)$. Random Korobov. Try *r* random values of *a*.

Rank 1, exhaustive search.

Pure random search. Try admissible vectors **a** at random.

Component by component (CBC) construction. (Sloan, Kuo, etc.). Let $a_1 = 1$;

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Fast CBC construction for $\mathcal{P}_{\gamma,\alpha}$: use FFT. (Nuyens, Cools).

Randomized CBC construction.

Let $a_1 = 1$; For $j = 2, \ldots, s$, try r random $z \in \{1, \ldots, n-1\}$, gcd(z, n) = 1, and retain $(a_1, a_2, \ldots, a_j = z)$ that minimizes $\mathcal{D}(P_n(\{1, \ldots, j\}))$.

Can add filters to eliminate poor lattices more quickly.

Embedded lattices $P_{n_1} \subset P_{n_2} \subset \ldots \land P_{n_m}$ with $n_1 < n_2 < \cdots < n_m$, for some m > 0. Usually: $n_k = b^{c+k}$ for integers $c \ge 0$ and $b \ge 2$, typically with b = 2, $\mathbf{a}_k = \mathbf{a}_{k+1} \mod n_k$ for all k < m, and the same random shift.

We need a measure that accounts for the quality of all m lattices. We standardize the merit at all levels k so they have a comparable scale:

 $\mathcal{E}_q(P_n) = \mathcal{D}_q(P_n)/D_q^*(n),$

where $D_q^*(n)$ is a normalization factor, e.g., a bound on $\mathcal{D}_q(P_n)$ or a bound on its average over all (a_1, \ldots, a_s) under consideration. For $\mathcal{P}_{\gamma,\alpha}$, bounds by Sinescu and L. (2012) and Dick et al. (2008).

For CBC, we do this for each coordinate j = 1, ..., s (replace s by j).

Then we can take as a global measure (with sum or max):

$$\left[\bar{\mathcal{E}}_{q,m}(P_{n_1},\ldots,P_{n_m})\right]^q = \sum_{k=1}^m w_k \left[\mathcal{E}_q(P_{n_k})\right]^q.$$

Construction: Nuyens (2012) provides Matlab code for fast-CBC construction of lattice rules based on $\mathcal{P}_{\gamma,\alpha}$, with product and order-dependent weights.

Precomputed tables for fixed criteria: Maisonneuve (1972), Sloan and Joe (1994), L. and Lemieux (2000), Kuo (2012), etc.

Software for **using** (randomized) lattice rules in simulations is also available in many places (e.g., in SSJ).

Lattice Builder

Implemented as C++ library, modular, object-oriented, accessible from a program via API. Various choices of figures of merit, arbitrary weights, construction methods, etc. Easily extensible.

For better run-time efficiency, uses static polymorphism, via templates, rather than dynamic polymorphism. Several other techniques to reduce computations and improve speed.

Offers a pre-compiled program with Unix-like command line interface. Also graphical interface.

Available for download on GitHub, with source code, documentation, and precompiled executable codes for Linux or Windows, in 32-bit and 64-bit versions.

Coming very soon: Construction of polynomial lattice rules as well.

Show graphical interface

Baker's (or tent) transformation To make the periodic continuation of *f* continuous.

If $f(0) \neq f(1)$, define \tilde{f} by $\tilde{f}(1-u) = \tilde{f}(u) = f(2u)$ for $0 \leq u \leq 1/2$. This \tilde{f} has the same integral as f and $\tilde{f}(0) = \tilde{f}(1)$.



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For smooth f, can reduce the variance to $O(n^{-4+\epsilon})$ (Hickernell 2002). The resulting \tilde{f} is symmetric with respect to u = 1/2.

In practice, we transform the points \mathbf{U}_i instead of f.

Random shift followed by baker's transformation. Along each coordinate, stretch everything by a factor of 2 and fold. Same as replacing U_j by min $[2U_j, 2(1 - U_j)]$.



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Gives locally antithetic points in intervals of size 2/n.

This implies that linear pieces over these intervals are integrated exactly.

Intuition: when f is smooth, it is well-approximated by a piecewise linear function, which is integrated exactly, so the error is small.

Example: A stochastic activity network

Gives precedence relations between activities. Activity k has random duration Y_k (also length of arc k) with known cumulative distribution function (cdf) $F_k(y) := \mathbb{P}[Y_k \leq y]$.

Project duration T = (random) length of longest path from source to sink.

May want to estimate $\mathbb{E}[T]$, $\mathbb{P}[T > x]$, a quantile, density of T, etc.



Simulation

Algorithm: to generate T:

for k = 0, ..., 12 do Generate $U_k \sim U(0, 1)$ and let $Y_k = F_k^{-1}(U_k)$ Compute $X = T = h(Y_0, ..., Y_{12}) = f(U_0, ..., U_{12})$

Monte Carlo: Repeat *n* times independently to obtain *n* realizations X_1, \ldots, X_n of *T*. Estimate $\mathbb{E}[\mathcal{T}] = \int_{(0,1)^s} f(\mathbf{u}) d\mathbf{u}$ by $\overline{X}_n = \frac{1}{n} \sum_{i=0}^{n-1} X_i$.

To estimate $\mathbb{P}(T > x)$, take $X = \mathbb{I}[T > x]$ instead.

RQMC: Replace the n independent points by an RQMC point set of size n.

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Numerical illustration from Elmaghraby (1977): $Y_k \sim N(\mu_k, \sigma_k^2)$ for k = 0, 1, 3, 10, 11, and $V_k \sim \text{Expon}(1/\mu_k)$ otherwise. μ_0, \ldots, μ_{12} : 13.0, 5.5, 7.0, 5.2, 16.5, 14.7, 10.3, 6.0, 4.0, 20.0, 3.2, 3.2, 16.5. Naive idea: replace each Y_k by its expectation. Gives T = 48.2.

Results of an experiment with n = 100000.

Histogram of values of T is a density estimator that gives more information than a confidence interval on $\mathbb{E}[T]$ or $\mathbb{P}[T > x]$. Values range from 14.4 to 268.6; 11.57% exceed x = 90.



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Histogram of values of T is a density estimator that gives more information than a confidence interval on $\mathbb{E}[T]$ or $\mathbb{P}[T > x]$. Values range from 14.4 to 268.6; 11.57% exceed x = 90. RQMC can also reduce the error (e.g., the MISE) of a density estimator!



Alternative estimator of $\mathbb{P}[T > x] = \mathbb{E}[\mathbb{I}(T > x)]$ for SAN.

Naive estimator: Generate T and compute $X = \mathbb{I}[T > x]$. Repeat *n* times and average. Alternative estimator of $\mathbb{P}[T > x] = \mathbb{E}[\mathbb{I}(T > x)]$ for SAN.

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Conditional Monte Carlo estimator of $\mathbb{P}[T > x]$. Generate the Y_j 's only for the 8 arcs that do not belong to the cut $\mathcal{L} = \{4, 5, 6, 8, 9\}$, and replace $\mathbb{I}[T > x]$ by its conditional expectation given those Y_j 's,

$$X_{\mathrm{e}} = \mathbb{P}[T > x \mid \{Y_j, j \notin \mathcal{L}\}].$$

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To compute X_e : for each $l \in \mathcal{L}$, say from a_l to b_l , compute the length α_l of the longest path from 1 to a_l , and the length β_l of the longest path from b_l to the destination.

The longest path that passes through link *I* does not exceed x iff $\alpha_I + Y_I + \beta_I \leq x$, which occurs with probability $\mathbb{P}[Y_I \leq x - \alpha_I - \beta_I] = F_I[x - \alpha_I - \beta_I]$.

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Since the Y_l are independent, we obtain

$$X_{\mathbf{e}} = 1 - \prod_{l \in \mathcal{L}} F_l[\mathbf{x} - \alpha_l - \beta_l].$$

Can be faster to compute than X, and always has less variance.

ANOVA Variances for estimator of $\mathbb{P}[T > x]$ in Stochastic Activity Network



Stochastic Activity Network

Variance for estimator of $\mathbb{P}[T > x]$ for SAN



Variance for estimator of $\mathbb{P}[T > x]$ with CMC



Histograms, with n = 8191 and m = 10,000



Histograms, with n = 8191 and m = 10,000



Effective dimension

(Caflisch, Morokoff, and Owen 1997).

A function f has effective dimension d in proportion ρ in the superposition sense if

$$\sum_{|\mathfrak{u}| \leq \boldsymbol{d}} \sigma_{\mathfrak{u}}^2 \geq \rho \sigma^2.$$

It has effective dimension d in the truncation sense if

$$\sum_{\mathfrak{u}\subseteq\{1,\ldots,d\}}\sigma_{\mathfrak{u}}^2\geq\rho\sigma^2.$$

High-dimensional functions with low effective dimension are frequent. One may change f to make this happen.

Let $\mu = E[f(\mathbf{U})] = E[g(\mathbf{Y})]$ where $\mathbf{Y} = (Y_1, \dots, Y_s) \sim N(\mathbf{0}, \mathbf{\Sigma})$.

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To generate **Y**: Decompose $\Sigma = AA^t$, generate $\mathbf{Z} = (Z_1, \ldots, Z_s) \sim N(\mathbf{0}, \mathbf{I})$ where the (independent) Z_j 's are generated by inversion: $Z_j = \Phi^{-1}(U_j)$, and return $\mathbf{Y} = A\mathbf{Z}$.

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Choice of A?

Cholesky factorization: **A** is lower triangular.

 $\mathbf{A} = \mathbf{P}\mathbf{D}^{1/2}$ where $\mathbf{D} = \text{diag}(\lambda_s, \dots, \lambda_1)$ (eigenvalues of $\mathbf{\Sigma}$ in decreasing order) and the columns of \mathbf{P} are the corresponding unit-length eigenvectors.

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Function of a Brownian motion (or other Lévy process):

Payoff depends on *c*-dimensional Brownian motion $\{\mathbf{X}(t), t \ge 0\}$ observed at times $0 = t_0 < t_1 < \cdots < t_d = T$.

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The first few N(0,1) r.v.'s already sketch the path trajectory.

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Each of these methods corresponds to some matrix \mathbf{A} . Choice has a large impact on the ANOVA decomposition of f.

Example: Pricing an Asian basket option

We have *c* assets, *d* observation times. Want to estimate $\mathbb{E}[f(\mathbf{U})]$, where

$$f(\mathbf{U}) = e^{-rT} \max\left[0, \ rac{1}{cd} \sum_{i=1}^{c} \sum_{j=1}^{d} S_i(t_j) - K
ight]$$

is the net discounted payoff and $S_i(t_j)$ is the price of asset *i* at time t_j .

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Suppose $(S_1(t), \ldots, S_c(t))$ obeys a geometric Brownian motion. Then, $f(\mathbf{U}) = g(\mathbf{Y})$ where $\mathbf{Y} = (Y_1, \ldots, Y_s) \sim N(\mathbf{0}, \mathbf{\Sigma})$ and s = cd.

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Even with Cholesky decompositions of Σ , the two-dimensional projections often account for more than 99% of the variance: low effective dimension in the superposition sense.

With PCA or bridge sampling, we get low effective dimension in the truncation sense. In realistic examples, the first two coordinates Z_1 and Z_2 often account for more than 99.99% of the variance!

Numerical experiment with c = 10 and d = 25

This gives a 250-dimensional integration problem.

Let $\rho_{i,j} = 0.4$ for all $i \neq j$, T = 1, $\sigma_i = 0.1 + 0.4(i-1)/9$ for all i, r = 0.04, S(0) = 100, and K = 100. (Imai and Tan 2002).

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Variance reduction factors for Cholesky (left) and PCA (right) (experiment from 2003):

n = 16381		n = 65521		n = 262139	
<i>a</i> = 5693		<i>a</i> = 944		<i>a</i> = 21876	
18	878	18	1504	9	2643
50	4553	46	3657	43	7553
Sobol' Nets					
$n = 2^{14}$		$n = 2^{16}$		$n = 2^{18}$	
10	1299	17	3184	32	6046
6	4232	4	9219	35	16557
	n = a = 18 50 Sc $n = 10$ 6	$n = 16381$ $a = 5693$ $18 878$ $50 4553$ $Sobol' Ne'$ $n = 2^{14}$ $10 1299$ $6 4232$	n = 16381 n =	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$n = 16381$ $n = 65521$ $n =$ $a = 5693$ $a = 944$ $a =$ 18 878 18 1504 9 50 4553 46 3657 43 Sobol' Nets $n = 2^{14}$ $n = 2^{16}$ n 10 1299 17 3184 32 6 4232 4 9219 35

Korobov Lattice Rules

Note: The payoff function is not smooth and also unbounded!

ANOVA Variances for ordinary Asian Option



Total Variance per Coordinate for the Asian Option



Variance with good lattices rules and Sobol points



Polynomial lattice rules

Integers and real numbers are replaced by polynomials and formal series, respectively.

Select prime base $b \ge 2$. Usually b = 2. Replace \mathbb{Z} by $\mathbb{F}_b[z]$, the ring of polynomials over finite field $\mathbb{F}_b \equiv \mathbb{Z}_b$; Replace \mathbb{R} by $\mathbb{L}_b = \mathbb{F}_b((z^{-1}))$, the field of formal Laurent series over \mathbb{F}_b , of the form $\sum_{\ell=\omega}^{\infty} x_{\ell} z^{-\ell}$, where $x_{\ell} \in \mathbb{F}_b$.

Polynomial lattice

$$\mathcal{L}_{s} = \left\{ \mathbf{v}(z) = \sum_{j=1}^{s} q_{j}(z) \mathbf{v}_{j}(z) \text{ such that each } q_{j}(z) \in \mathbb{F}_{b}[z]
ight\},$$

where $\mathbf{v}_1(z), \ldots, \mathbf{v}_s(z)$ are independent vectors in \mathbb{L}_b^s , of the form $\mathbf{v}_j(\mathbf{z}) = \mathbf{a}_j(z)/P(z)$, where $P(z) = z^k + \alpha_1 z^{k-1} + \cdots + \alpha_k \in \mathbb{Z}_b[z]$ and each $\mathbf{a}_j(z)$ is a vector of polynomials of degree less than k. Note that $(\mathbb{Z}_b[z])^s \subseteq \mathcal{L}_s$ (integration lattice) and $\mathcal{L}_s \mod \mathbb{F}_b[z]$ contains exactly b^k points in \mathbb{L}_b^s .

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$$\mathcal{L}_s = \left\{ \mathbf{v}(z) = \sum_{j=1}^s q_j(z) \mathbf{v}_j(z) \text{ such that each } q_j(z) \in \mathbb{F}_b[z]
ight\},$$

where $\mathbf{v}_1(z), \ldots, \mathbf{v}_s(z)$ are independent vectors in \mathbb{L}_b^s , of the form $\mathbf{v}_j(\mathbf{z}) = \mathbf{a}_j(z)/P(z)$, where $P(z) = z^k + \alpha_1 z^{k-1} + \cdots + \alpha_k \in \mathbb{Z}_b[z]$ and each $\mathbf{a}_j(z)$ is a vector of polynomials of degree less than k. Note that $(\mathbb{Z}_b[z])^s \subseteq \mathcal{L}_s$ (integration lattice) and $\mathcal{L}_s \mod \mathbb{F}_b[z]$ contains exactly b^k points in \mathbb{L}_b^s .

For a rule of rank 1, $\mathbf{v}_2(z), \ldots, \mathbf{v}_s(z)$ are the unit vectors.

Define $\varphi : \mathbb{L} \to \mathbb{R}$ by

$$\varphi\left(\sum_{\ell=\omega}^{\infty} x_{\ell} z^{-\ell}\right) = \sum_{\ell=\omega}^{\infty} x_{\ell} b^{-\ell}.$$

The polynomial lattice rule (PLR) uses the node set $P_n = \varphi(\mathcal{L}_s) \cap [0, 1)^s = \varphi(\mathcal{L}_s \mod \mathbb{F}_b[z])$.

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PLRs were first studied by Niederreiter, Larcher, Tezuka (circa 1990), with rank 1. They were generalized and further studied by Lemieux and L'Ecuyer (circa 2000), then by Dick, Pillischammer, Nuyens, Goda, and others. Most of the properties of ordinary lattice rules have counterparts for the polynomial rules.

The Fourier expansion is replaced by a Walsh expansion, the weighted $\mathcal{P}_{\gamma,\alpha}$ has a counterpart $\mathcal{P}_{\gamma,\alpha,\text{PRL}}$, CBC constructions can provide good parameters, fast CBC also works, etc.

Walsh expansion For $\mathbf{h} \equiv \mathbf{h}(z) = (h_1(z), \dots, h_s(z)) \in (\mathbb{F}_b[z])^s$ and $\mathbf{u} = (u_1, \dots, u_s) \in [0, 1)^s$, where

$$h_i(z)=\sum_{j=1}^{\ell_i}h_{i,j}z^{j-1}$$
 and $u_i=\sum_{j\geq 1}u_{i,j}b^{-j}\in [0,1),$ define $\langle \mathbf{h},\mathbf{u}
angle =\sum_{i=1}^s\sum_{j=1}^{\ell_i}h_{i,j}u_{i,j}$ in $\mathbb{F}_b.$

The Walsh expansion in \mathbb{F}_b of $f:[0,1)^s \to \mathbb{R}$ is

$$f(\mathbf{u}) = \sum_{\mathbf{h} \in (\mathbb{F}_b[z])^s} ilde{f}(\mathbf{h}) e^{2\pi \mathrm{i} \langle \mathbf{h}, \mathbf{u}
angle / b},$$

with Walsh coefficients

$$ilde{f}(\mathbf{h}) = \int_{[0,1)^s} f(\mathbf{u}) e^{-2\pi \mathrm{i} \langle \mathbf{h}, \mathbf{u}
angle / b} d\mathbf{u}.$$

Theorem: For a PLR with a random digital shift, $\operatorname{Var}[Q_n] = \sum_{\mathbf{0} \neq \mathbf{h} \in \mathcal{L}_s^*} |\tilde{f}(\mathbf{h})|^2$.

Again, we want to kick out of the dual lattice the **h**'s for which $|\tilde{f}(\mathbf{h})|^2$ is large. For smooth f, the small **h** are the most important.

Version of $\mathcal{P}_{\gamma,\alpha}$ for PLRs

A similar reasoning as for ordinary lattice rules leads to

$$\begin{aligned} \mathcal{P}_{\gamma,\alpha,\mathrm{PLR}} &= \sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \gamma_{\mathfrak{u}} \prod_{j \in \mathfrak{u}, \ h_{j} \neq 0} 2^{\alpha \lfloor \log_{2} h_{j} \rfloor} \\ &= \sum_{\mathfrak{u} \subseteq \{1,\dots,s\}} \gamma_{\mathfrak{u}} \frac{1}{n} \sum_{i} i = 0^{n-1} \prod_{j \in \mathfrak{u}} \left(\mu(\alpha) - 2^{(1 + \lfloor \log_{2}(x_{i,j}) \rfloor)(\alpha-1)} (\mu(\alpha) + 1) \right). \end{aligned}$$

where $\mu(\alpha) = (1 - 2^{1-\alpha})^{-1}$.

For $\alpha=$ 2, this simplifies to $\mu(2)=$ 2 and

$$\mathcal{P}_{\gamma,2,\mathrm{PLR}} = \sum_{\mathfrak{u} \subseteq \{1,\ldots,s\}} \gamma_{\mathfrak{u}} \frac{1}{n} \sum_{i=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(2 - 6 \cdot 2^{\lfloor \log_2(x_{i,j}) \rfloor} \right).$$

Example in s = 2 dimensions

Base
$$b = 2$$
, $k = 8$, $n = 2^8 = 256$,
 $P(z) = 1 + z + z^3 + z^5 + z^8 \equiv [110101001]$,
 $q_1(z) = 1$, $q_2(z) = 1 + z + z^2 + z^3 + z^5 + z^7 \equiv [11110101]$.



61
A PLR is also a special case of a digital net in base b, and this can be used to generate the points efficiently: compute the generating matrices and use the digital net implementation. This is particularly fast in base b = 2.

Random shift in space of formal series: equivalent to a random digital shift in base *b*, applied to all the points. It preserves equidistribution.

Random digital shift for digital net

Equidistribution in digital boxes is lost with random shift modulo 1, but can be kept with a random digital shift in base b.

In base 2: Generate $\mathbf{U} \sim U(0,1)^s$ and XOR it bitwise with each \mathbf{u}_i .

Example for s = 2:

$$\mathbf{u}_i = (0.01100100..., 0.10011000...)_2$$
$$\mathbf{U} = (0.01001010..., 0.11101001...)_2$$
$$\mathbf{u}_i \oplus \mathbf{U} = (0.00101110..., 0.01110001...)_2.$$

Each point has U(0,1) distribution.

Preservation of the equidistribution ($k_1 = 3, k_2 = 5$):

$$u_i = (0.***, 0.****)$$
$$U = (0.010, 0.11101)_2$$
$$u_i \oplus U = (0.***, 0.****)$$

Example with

 $U = (0.1270111220, 0.3185275653)_{10}$ = (0.0010 0000100000111100, 0.0101 0001100010110000)_2.

Changes the bits 3, 9, 15, 16, 17, 18 of $u_{i,1}$ and the bits 2, 4, 8, 9, 13, 15, 16 of $u_{i,2}$.



Red and green squares are permuted ($k_1 = k_2 = 4$, first 4 bits of **U**).

Array-RQMC for Markov Chains Setting: A Markov chain with state space $\mathcal{X} \subseteq \mathbb{R}^{\ell}$, evolves as

$$X_0 = x_0, \qquad X_j = \varphi_j(X_{j-1}, \mathbf{U}_j), \ j \ge 1,$$

where the U_j are i.i.d. uniform r.v.'s over $(0,1)^d$. Want to estimate

$$\mu = \mathbb{E}[Y]$$
 where $Y = \sum_{j=1}^{ au} extsf{g}_j(X_j).$

Ordinary MC: *n* i.i.d. realizations of *Y*. Requires $s = \tau d$ uniforms.

Array-RQMC: L., Lécot, Tuffin, et al. [2004, 2006, 2008, etc.] Simulate an "array" (or population) of *n* chains in "parallel." **Goal**: Want small discrepancy between empirical distribution of states $S_{n,j} = \{X_{0,j}, \ldots, X_{n-1,j}\}$ and theoretical distribution of X_j , at each step *j*. At each step, use RQMC point set to advance all the chains by one step. **Some RQMC insight:** To simplify, suppose $X_j \sim U(0,1)^{\ell}$. We estimate

$$\mu_j = \mathbb{E}[g_j(X_j)] = \mathbb{E}[g_j(arphi_j(X_{j-1}, \mathbf{U}))] = \int_{[0,1)^{\ell+d}} g_j(arphi_j(\mathbf{x}, \mathbf{u})) d\mathbf{x} d\mathbf{u}$$

by

$$\hat{\mu}_{\mathrm{arqmc},j,n} = rac{1}{n} \sum_{i=0}^{n-1} g_j(X_{i,j}) = rac{1}{n} \sum_{i=0}^{n-1} g_j(\varphi_j(X_{i,j-1}, \mathbf{U}_{i,j}))$$

This is (roughly) RQMC with the point set $Q_n = \{(X_{i,j-1}, \mathbf{U}_{i,j}), 0 \le i < n\}$. We want Q_n to have low discrepancy (LD) over $[0, 1)^{\ell+d}$. **Some RQMC insight:** To simplify, suppose $X_j \sim U(0,1)^{\ell}$. We estimate

$$\mu_j = \mathbb{E}[g_j(X_j)] = \mathbb{E}[g_j(arphi_j(X_{j-1}, \mathbf{U}))] = \int_{[0,1)^{\ell+d}} g_j(arphi_j(\mathbf{x}, \mathbf{u})) d\mathbf{x} d\mathbf{u}$$

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This is (roughly) RQMC with the point set $Q_n = \{(X_{i,j-1}, \mathbf{U}_{i,j}), 0 \le i < n\}$. We want Q_n to have low discrepancy (LD) over $[0, 1)^{\ell+d}$.

We do not choose the $X_{i,j-1}$'s in Q_n : they come from the simulation. We select a LD point set

$$\ddot{\boldsymbol{Q}}_n = \{(\mathbf{w}_0, \mathbf{U}_{0,j}), \ldots, (\mathbf{w}_{n-1}, \mathbf{U}_{n-1,j})\},\$$

where the $\mathbf{w}_i \in [0, 1)^\ell$ are fixed and each $\mathbf{U}_{i,j} \sim U(0, 1)^d$. Permute the states $X_{i,j-1}$ so that $X_{\pi_j(i),j-1}$ is "close" to \mathbf{w}_i for each *i* (LD between the two sets), and compute $X_{i,j} = \varphi_j(X_{\pi_j(i),j-1}, \mathbf{U}_{i,j})$ for each *i*.

Example: If $\ell = 1$, can take $\mathbf{w}_i = (i + 0.5)/n$ and just sort the states. For $\ell > 1$, there are various ways to define the matching (multivariate sort).

Array-RQMC algorithm

$$\begin{split} & X_{i,0} \leftarrow x_0 \text{ (or } X_{i,0} \leftarrow x_{i,0}) \text{ for } i = 0, \dots, n-1; \\ & \text{for } j = 1, 2, \dots, \tau \text{ do} \\ & \text{Compute the permutation } \pi_j \text{ of the states (for matching)}; \\ & \text{Randomize afresh } \{\mathbf{U}_{0,j}, \dots, \mathbf{U}_{n-1,j}\} \text{ in } \tilde{Q}_n; \\ & X_{i,j} = \varphi_j(X_{\pi_j(i),j-1}, \mathbf{U}_{i,j}), \text{ for } i = 0, \dots, n-1; \\ & \hat{\mu}_{\operatorname{arqmc},j,n} = \bar{Y}_{n,j} = \frac{1}{n} \sum_{i=0}^{n-1} g(X_{i,j}); \\ & \text{Estimate } \mu \text{ by the average } \bar{Y}_n = \hat{\mu}_{\operatorname{arqmc},n} = \sum_{j=1}^{\tau} \hat{\mu}_{\operatorname{arqmc},j,n}. \end{split}$$

Array-RQMC algorithm

$$\begin{array}{l} X_{i,0} \leftarrow x_0 \ (\text{or} \ X_{i,0} \leftarrow x_{i,0}) \ \text{for} \ i = 0, \ldots, n-1; \\ \text{for} \ j = 1, 2, \ldots, \tau \ \text{do} \\ \text{Compute the permutation} \ \pi_j \ \text{of the states} \ (\text{for matching}); \\ \text{Randomize afresh} \ \{\mathbf{U}_{0,j}, \ldots, \mathbf{U}_{n-1,j}\} \ \text{in} \ \tilde{Q}_n; \\ X_{i,j} = \varphi_j(X_{\pi_j(i),j-1}, \mathbf{U}_{i,j}), \ \text{for} \ i = 0, \ldots, n-1; \\ \hat{\mu}_{\operatorname{arqmc},j,n} = \ \bar{Y}_{n,j} = \frac{1}{n} \sum_{i=0}^{n-1} g(X_{i,j}); \\ \text{Estimate} \ \mu \ \text{by the average} \ \tilde{Y}_n = \hat{\mu}_{\operatorname{arqmc},n} = \sum_{j=1}^{\tau} \hat{\mu}_{\operatorname{arqmc},j,n}. \end{array}$$

Proposition: (i) The average \bar{Y}_n is an unbiased estimator of μ . (ii) The empirical variance of *m* independent realizations gives an unbiased estimator of $Var[\bar{Y}_n]$.

Some generalizations

L., Lécot, and Tuffin [2008]: τ can be a random stopping time w.r.t. the filtration $\mathcal{F}\{(j, X_j), j \ge 0\}$.

L., Demers, and Tuffin [2006, 2007]: Combination with splitting techniques (multilevel and without levels), combination with importance sampling and weight windows. Covers particle filters.

L. and Sanvido [2010]: Combination with coupling from the past for exact sampling.

Dion and L. [2010]: Combination with approximate dynamic programming and for optimal stopping problems.

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Gerber and Chopin [2015]: Sequential QMC.
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Convergence results and applications

L., Lécot, and Tuffin [2006, 2008]: Special cases: convergence at MC rate, one-dimensional, stratification, etc. $O(n^{-3/2})$ variance.

Lécot and Tuffin [2004]: Deterministic, one-dimension, discrete state.

El Haddad, Lécot, L. [2008, 2010]: Deterministic, multidimensional. $O(n^{-1/(\ell+1)})$ worst-case error under some conditions.

Fakhererredine, El Haddad, Lécot [2012, 2013, 2014]: LHS, stratification, Sudoku sampling, ...

L., Lécot, Munger, and Tuffin [2016]: Survey, comparing sorts, and further examples, some with $O(n^{-3})$ empirical variance.

Wächter and Keller [2008]: Applications in computer graphics.

Gerber and Chopin [2015]: Sequential QMC (particle filters), Owen nested scrambling and Hilbert sort. $o(n^{-1})$ variance.



Sobol' net in 2 dimensions after random digital shift



Sobol' net in 2 dimensions after random digital shift



Sobol' net in 2 dimensions after random digital shift



Sobol' net in 2 dimensions after random digital shift

Map the states to [0, 1], then sort.



Map the states to [0, 1], then sort.



Map the states to [0,1], then sort.



Map the states to [0,1], then sort.



Example: Asian Call Option $S(0) = 100, K = 100, r = 0.05, \sigma = 0.15, t_j = j/52, j = 0, ..., \tau = 13.$ RQMC: Sobol' points with linear scrambling + random digital shift. Similar results for randomly-shifted lattice + baker's transform.



Example: Asian Call Option

Sort	RQMC points	$\frac{\log_2 \operatorname{Var}[\bar{Y}_{n,j}]}{\log_2 n}$	VRF	CPU (sec)
Batch sort	SS	-1.38	$2.0 imes10^2$	744
$(n_1 = n_2)$	Sobol	-2.03	$4.2 imes10^{6}$	532
	Sobol+NUS	-2.03	$2.8 imes10^6$	1035
	${\sf Korobov+baker}$	-2.04	$4.4 imes10^6$	482
Hilbert sort	SS	-1.55	$2.4 imes10^3$	840
(logistic map)	Sobol	-2.03	$2.6 imes10^6$	534
	Sobol+NUS	-2.02	$2.8 imes10^6$	724
	${\sf Korobov+baker}$	-2.01	$3.3 imes10^6$	567

VRF for $n = 2^{20}$. CPU time for m = 100 replications.

Conclusion, discussion, etc.

- ▶ RQMC can improve the accuracy of estimators considerably in some applications.
- Cleverly modifying the function f can often bring huge statistical efficiency improvements in simulations with RQMC.
- There are often many possibilities for how to change f to make it smoother, periodic, and reduce its effective dimension.
- Point set constructions should be based on discrepancies that take that into account.
- ► Nonlinear functions of expectations: RQMC also reduces the bias.
- RQMC for density estimation.
- RQMC for optimization.
- Array-RQMC and other QMC methods for Markov chains. Sequential RQMC.
- Still a lot to learn and do ...

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