

Randomized Quasi-Monte Carlo

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These slides are from a series of four lectures given at the Johann Radon Institute for Computational and Applied Mathematics (RICAM) held on March 24 and March 25 2021.

It was an honor to be asked to present on quasi-Monte Carlo (QMC) sampling in Austria, from where so much of QMC comes and has come. The talks were virtual; I would have otherwise made sure to get some Linzertorte. That will have to wait.

1. Quasi-Monte Carlo
2. Randomized Quasi-Monte Carlo
3. QMC Beyond the Cube
4. QMC and Variable Importance

A small number of corrections have been made since then.

Quasi-Monte Carlo

Estimate $\mu = \int_{[0,1]^d} f(\mathbf{x}) \, d\mathbf{x}$ by

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i)$$

getting

$$|\hat{\mu} - \mu| \leq D_n^*(\mathbf{x}_1, \dots, \mathbf{x}_n) \times V_{\text{HK}}(f)$$

with

$$D_n^*(\mathbf{x}_1, \dots, \mathbf{x}_n) = O\left(\frac{\log(n)^{d-1}}{n}\right) = o(n^{-1+\epsilon}), \quad \text{any } \epsilon > 0$$

Three problems

- 1) How to estimate $|\hat{\mu} - \mu|$ for given f and n ?
- 2) What about all those logs?
- 3) What if $V_{\text{HK}}(f) = \infty$?

$\frac{1}{2}$ of RQMC

I will leave out most of randomized lattice methods
focussing on scrambling of digital constructions

For lattices see works by

Hickernell, Joe, Kritzer, Kuo, L'Ecuyer, Lemieux, Nuyens, Sloan, Tuffin, Ulrich
and many others

Problem 1

Estimating $|\hat{\mu} - \mu|$

QMC is deterministic

Repeat $f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)$ get same $\hat{\mu}$

$|\hat{\mu}_n - \hat{\mu}_{n/2}|$ might describe accuracy of $\hat{\mu}_{n/2}$

Or it could be too small

Randomized QMC (RQMC)

Inject some randomness into \mathbf{x}_i

Keeping them at low discrepancy

$$\text{E.G. } \mathbb{P}\left(D_n^* < B \frac{(\log(n))^d}{n}\right) = 1$$

Then do independent repeats

RQMC

- 1) Make $\mathbf{x}_i \sim \mathbf{U}[0, 1]^d$ individually,
- 2) keeping $D_n^*(\mathbf{x}_1, \dots, \mathbf{x}_n) = O(n^{-1+\epsilon})$ collectively.

Then

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

$$\mathbb{E}(\hat{\mu}) = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(f(\mathbf{x}_i)) = \mu$$

$$|\hat{\mu} - \mu| \leq D_n^*(\mathbf{x}_1, \dots, \mathbf{x}_n) V_{\text{HK}}(f)$$

Ensure that

$$D_n^* \leq C n^{-1+\epsilon} \quad \text{with probability 1}$$

Therefore

$$\mathbb{E}((\hat{\mu} - \mu)^2) = O(n^{-2+2\epsilon})$$

R independent replicates

$$\hat{\mu} = \frac{1}{R} \sum_{r=1}^R \hat{\mu}_r$$

$$\widehat{\text{Var}}(\hat{\mu}) = \frac{1}{R(R-1)} \sum_{r=1}^R (\hat{\mu}_r - \hat{\mu})^2$$

If $V_{\text{HK}}(f) < \infty$ then

$$\mathbb{E}((\hat{\mu} - \mu)^2) = O\left(\frac{n^{-2+\epsilon}}{R}\right)$$

Random shift Cranley & Patterson (1976)

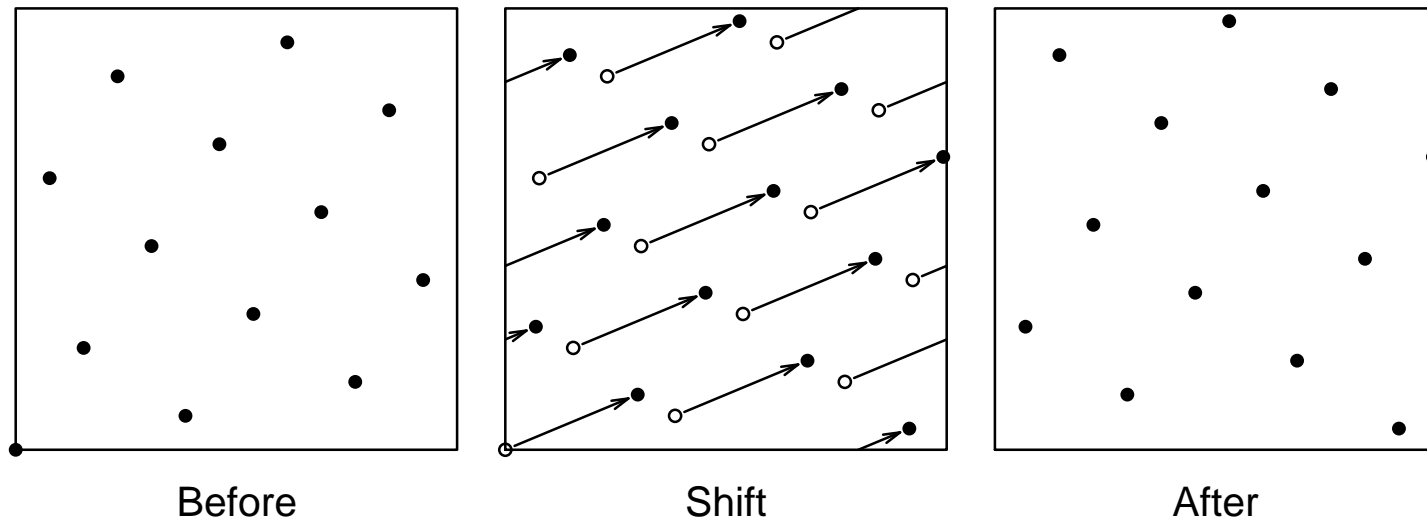
Scrambled nets O (1995,1997,1998)

Linear scramble Matousek (1998)

Survey in L'Ecuyer & Lemieux (2005)

Rotation modulo 1

Cranley–Patterson rotation



Shift the points by $\mathbf{u} \sim \mathbf{U}[0, 1)^s$ with wraparound:

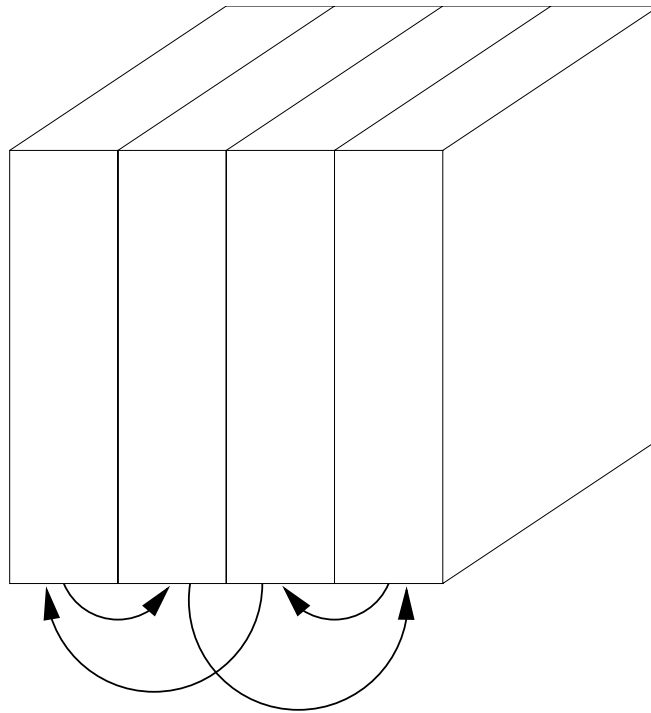
$$\mathbf{x}_i \rightarrow \mathbf{x}_i + \mathbf{u} \pmod{1}.$$

Shown for a lattice; can work with nets.

At least it removes $\mathbf{x}_1 = 0$:

$$\mathbb{P}(\mathbf{x}_i = 0) = 0.$$

Digit scrambling



- 1) Chop space into b slabs. Shuffle.
- 2) Repeat within each of b slabs.
- 3) Then within b^2 sub-slabs.
- 4) Ad infinitum b^3, b^4, \dots
- 5) And the same for all s coordinates.

Each $\mathbf{x}_i \sim \mathbf{U}[0, 1)^s$ and

$\mathbb{P}((\mathbf{x}_1, \dots, \mathbf{x}_n) \text{ are a net}) = 1 - O(n^{-1})$ (1995)

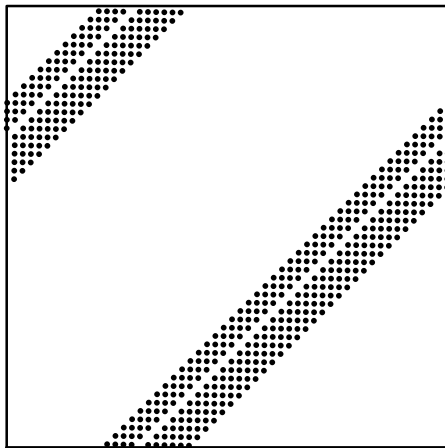
So Niederreiter (1987, 1992) still apply

Cheaper scrambles: digital shift and random linear.

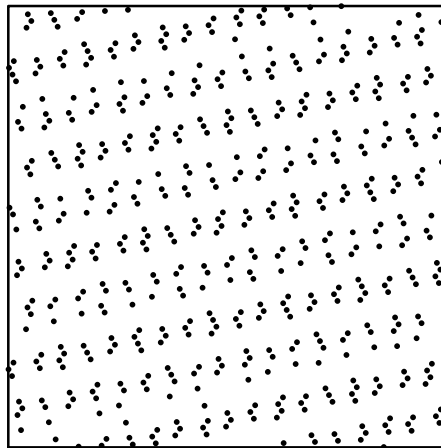
Example scrambles

Two components of the first 530 points of a Faure $(0, 53)$ -net in base 53.

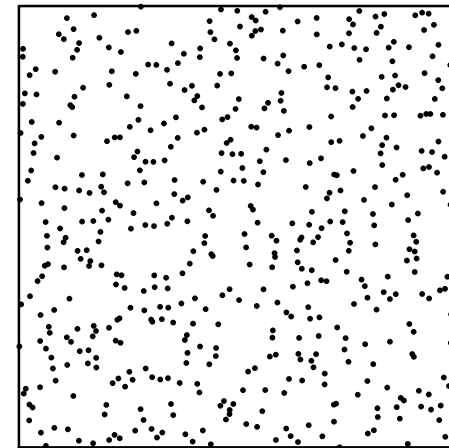
Randomized Faure points



Digital shift



Random linear



Nested uniform

The digital shift is much like a Cranley-Patterson rotation.

It uses just one random \mathbf{u} for all points: $\tilde{\mathbf{x}}_i = \mathbf{x}_i \oplus \mathbf{u}$. (bitwise)

Nested linear [Matousek \(1998\)](#) and nested uniform [O \(1995\)](#)

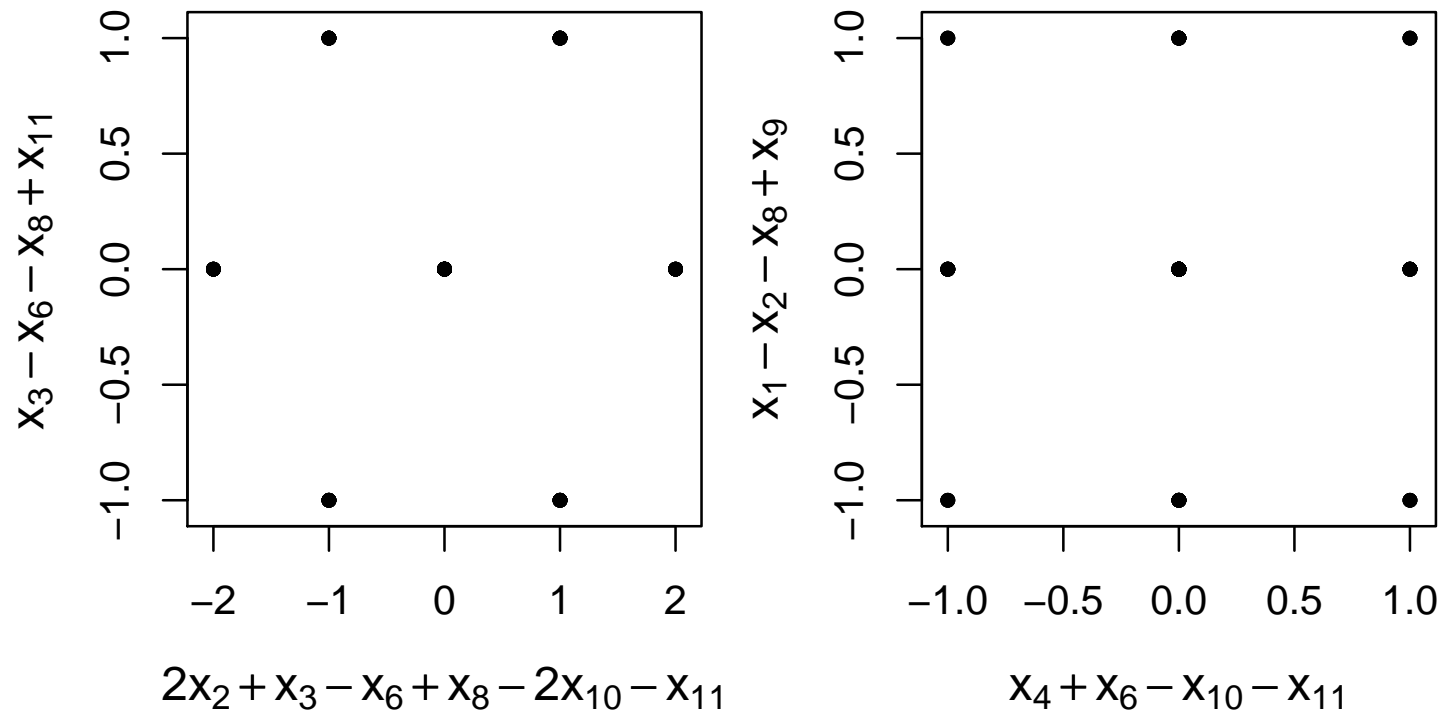
have the same $\text{Var}(\hat{\mu})$.

nested linear takes less memory

Unscrambled Faure

First $n = 11^2 = 121$ points of Faure $(0, 11)$ -net in $[0, 1]^{11}$.

Two projections of 121 Faure points



Unscrambled points are very structured.

Scrambling breaks it up.

Confidence intervals

Loh (2003):

central limit theorem for $\hat{\mu}$ when $t = 0$

$$\hat{\mu} \approx \mathcal{N}(\mu, \text{Var}(\hat{\mu}))$$

with nested uniform sampling

RMSE $O(n^{-1+\epsilon}R^{-1/2}) \implies$ small R popular

The bootstrap t of Efron (1982) gives good confidence intervals for small sample sizes O (1992)

Problem 2

Those logs

1) present the ANOVA

Hoefding (1948), Sobol' (1969), Efron & Stein (1981)

2) describe wavelet expansion

for QMC from O (1997)

3) control the variance

ANOVA Example

$$f(x_1, x_2) = 6x_1x_2^2$$

Write it as $\sum_{u \subseteq \{1,2\}} f_u(\mathbf{x})$

$$f_u(\mathbf{x}) = f_u(\mathbf{x}_u) \quad \mathbf{x}_u = (x_j)_{j \in u}$$

Recurse

$$f_{\emptyset}(x_1, x_2) = \int_0^1 \int_0^1 6x_1x_2^2 dx_1 dx_2 = 1$$

$$f_{\{1\}}(x_1, x_2) = \int_0^1 (6x_1x_2^2 - 1) dx_2 = 2x_1 - 1$$

$$f_{\{2\}}(x_1, x_2) = \int_0^1 (6x_1x_2^2 - 1) dx_1 = 3x_2^2 - 1$$

$$\begin{aligned} f_{\{1,2\}}(x_1, x_2) &= 6x_1x_2^2 - 1 - (2x_1 - 1) - (3x_2^2 - 1) \\ &= 6x_1x_2^2 - 2x_1 - 3x_2^2 + 1 \end{aligned}$$

For $f_{\{1,2\}}$ integrate over \mathbf{x}_{\emptyset} , i.e., no variables

ANOVA decomposition

$$f(\mathbf{x}) = \sum_{u \subseteq 1:d} f_u(\mathbf{x})$$

where f_u depends on \mathbf{x} only through $\mathbf{x}_u = (x_j)_{j \in u}$.

Don't attribute to \mathbf{x}_u what can be explained by \mathbf{x}_v for $v \subsetneq u$

Typographical conveniences

$$-u \equiv 1:d \setminus u \quad -j \equiv -\{j\} \quad d\mathbf{x}_u = \prod_{j \in u} dx_j$$

Recursive definition

$$f_{\emptyset}(\mathbf{x}) = \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} = \mu \quad (\text{constant})$$

$$f_{\{j\}}(\mathbf{x}) = \int_{[0,1]^{d-1}} (f(\mathbf{x}) - \mu) d\mathbf{x}_{-j} \quad (\text{function of } x_j)$$

$$f_u(\mathbf{x}) = \int_{[0,1]^{d-|u|}} \left(f(\mathbf{x}) - \sum_{v \subsetneq u} f_v(\mathbf{x}) \right) d\mathbf{x}_{-u} \quad (\text{function of } \mathbf{x}_u)$$

ANOVA properties

$$j \in u \implies \int_0^1 f_u(\mathbf{x}) dx_j = 0$$

$$u \neq v \implies \int_{[0,1]^d} f_u(\mathbf{x}) f_v(\mathbf{x}) d\mathbf{x} = 0$$

Variance components

$$\sigma_u^2 = \text{Var}(f_u(\mathbf{x})) = \begin{cases} 0, & u = \emptyset \\ \int f_u(\mathbf{x})^2 d\mathbf{x}, & \text{else.} \end{cases}$$

Decomposition

$$f(\mathbf{x}) = \sum_{u \subseteq 1:d} f_u(\mathbf{x})$$

$$\sigma^2 = \text{Var}(f(\mathbf{x})) = \sum_{u \subseteq 1:d} \sigma_u^2$$

Randomized QMC

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^n \sum_{u \subseteq 1:d} f_u(\mathbf{x}_i) = \sum_{u \subseteq 1:d} \hat{\mu}_u$$

$$\hat{\mu}_u \equiv \frac{1}{n} \sum_{i=1}^n f_u(\mathbf{x}_i)$$

For any RQMC method

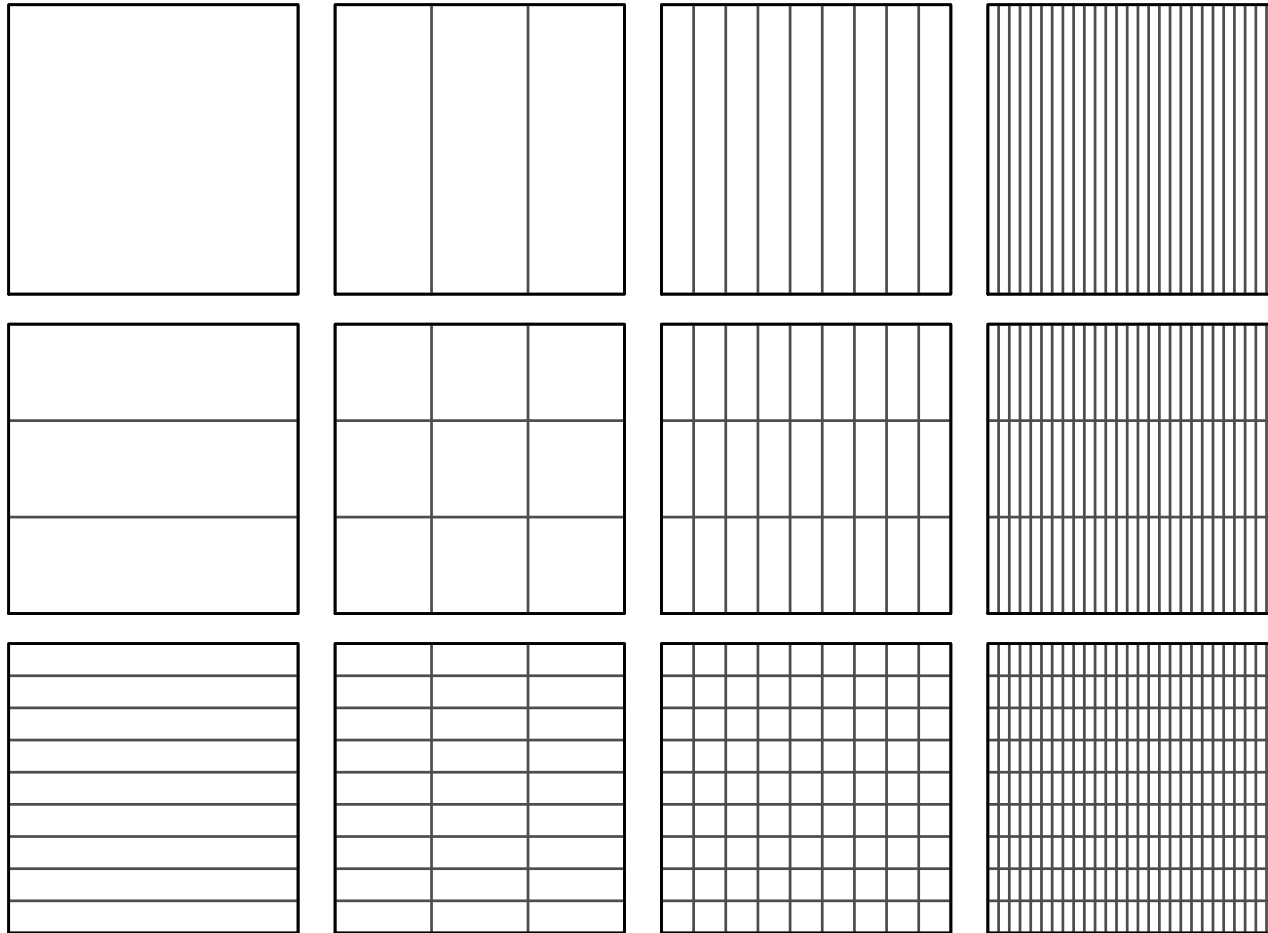
$$\text{Var}(\hat{\mu}) = \sum_{u \subseteq 1:d} \text{Var}(\hat{\mu}_u)$$

○ (2019) QMC notes online

Requires

x_{1j}, \dots, x_{nj} uniform and
independent of $x_{1j'}, \dots, x_{nj}'$

Elementary intervals



If f is constant with elementary intervals of volume b^{t-m}

then $\hat{\mu} = \mu$

Same if f is a sum of such functions

Wavelet expansion

From [O \(1997\) SINUM](#)

$\nu_{u,\mathbf{k}}(\mathbf{x})$ constant within cells of volume $\prod_{j \in u} b^{-k_j}$ $\mathbf{k} \in \mathbb{N}^{|u|}$

$$f_u(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}^{|u|}} \nu_{u,\mathbf{k}}(\mathbf{x}) \quad (\text{orthogonal})$$

Finding

$$\text{Var}(\hat{\mu}) = \sum_{u \subseteq 1:d} \sum_{\mathbf{k} \in \mathbb{N}^{|u|}} \text{Var}(\hat{\mu}_{u,\mathbf{k}})$$

$$\hat{\mu}_{u,\mathbf{k}} = \frac{1}{n} \sum_{i=1}^n \nu_{u,\mathbf{k}}(\mathbf{x}_i)$$

$$\sum_{j \in u} k_j \leq m - t \implies \text{Var}(\hat{\mu}_{u,\mathbf{k}}) = 0$$

One can use Walsh functions for digital nets

[Dick \(2008\)](#), [Dick & Pillichshammer \(2005\)](#), [Entacher \(1997,1998\)](#), [Larcher & Pillichshammer \(2001\)](#), and more

Gain coefficients

$$\text{Var}_{\text{RQMC}}(\hat{\mu}) = \frac{1}{n} \sum_u \sum_{\mathbf{k}} \Gamma_{u,\mathbf{k}} \sigma_{u,\mathbf{k}}^2$$

$$\text{Var}_{\text{MC}}(\hat{\mu}) = \frac{1}{n} \sum_u \sum_{\mathbf{k}} \sigma_{u,\mathbf{k}}^2$$

For $t = 0$

$$\Gamma_{u,\mathbf{k}} \leq \bar{\Gamma} = \left(\frac{b}{b-1}\right)^{d-1} \leq \exp(1) \approx 2.718$$

NB: When $t = 0$ we must have $b \geq d$

For $t > 0$

$$\Gamma_{u,\mathbf{k}} \leq \bar{\Gamma} = b^t \left(\frac{b+1}{b-1}\right)^s$$

O (1998)

Extends to first λb^m points of a (t, s) -sequence in base b $1 \leq \lambda < b$

Improved bounds in [Niederreiter & Pirsic \(2001\)](#)

Those logs

Let $f(\boldsymbol{x})$ have variance σ^2

$$\text{Var}(\hat{\mu}) \leq \frac{\bar{\Gamma}}{n} \sigma^2$$

For finite n

$$\text{RMSE} \leq \sigma \bar{\Gamma}^{1/2} n^{-1/2}$$

Without powers of $\log(n)$

Later

'smoothness' yields $\text{RMSE} = O(n^{-3/2} \log(n)^{(d-1)/2})$

Powers of $\log(n)$ can reappear only when they are negligible

Problem 3

What if $V_{\text{HK}}(f) = \infty$?

Converse

Riemann integrable f and $D_n^*(\mathbf{x}_1, \dots, \mathbf{x}_n) \rightarrow 0$

$$\implies \hat{\mu}_n \rightarrow \mu$$

Less well known

$|\hat{\mu}_n - \mu| \rightarrow 0$ whenever $D_n^* \rightarrow 0$

$$\implies f \text{ Riemann integrable} \quad \text{Niederreiter (1977)}$$

f not BVHK

1) integrable singularities

Sobol' (1973), O (2006), Hartinger & Kainhofer (2006), Basu & O (2018)

2) 'most' $f(\mathbf{x}) = \mathbf{1}\{\mathbf{x} \in A\}$ $A \subset [0, 1]^d$

He & Wang (2015)

3) f with 'kinks and jumps'

Sloan, Kuo, Griebel, Griewank

Gains $\Gamma_{u,\mathbf{k}} \rightarrow 0$

$$\text{Var}(\hat{\mu}) = \frac{1}{n} \sum_u \sum_{\mathbf{k}} \Gamma_{u,\mathbf{k}} \sigma_{u,\mathbf{k}}^2$$

$$\lim_{n=b^m \rightarrow 0} \Gamma_{u,\mathbf{k}} = 0$$

If $f \in L^2[0, 1]^d$

$$\text{RMSE}(\hat{\mu}) = \text{Var}(\hat{\mu}) = o\left(\frac{1}{n}\right)$$

This covers $f(\mathbf{x}) = \mathbf{1}_{\{\mathbf{x} \in A\}}$ for measurable A

Square integrable singularities / kinks / jumps

Laws of large numbers

From [O & Rudolf \(2020\)](#)

$$f \in L^{1+\delta}[0, 1]^d \quad \text{some } \delta > 0$$

Weak law

$$\lim_{n=b^m \rightarrow \infty} \mathbb{P}(|\hat{\mu}_n - \mu| > \epsilon) = 0$$

Strong law

$$\mathbb{P}\left(\limsup_{n \rightarrow \infty} |\hat{\mu}_n - \mu| > \epsilon\right) = 0, \quad \text{i.e.}$$

$$\mathbb{P}\left(\lim_{n \rightarrow \infty} \hat{\mu}_n = \mu\right) = 1$$

Needed by [Balandat et al. \(2020\)](#) for Bayesian optimization in NeurIPS

First prove for $f \in L^2$ adapting [Etemadi's \(1981\)](#) SLLN

then use Riesz-Thorin interpolation

Three problems

We can estimate the error \dots more work needed

For $f \in L^2$, RQMC cannot be powers of $\log n$ worse than MC

Don't need f to be BVHK

Smoothness

$$\partial^u f(\mathbf{x}) = \prod_{j \in u} \frac{\partial}{\partial x_j} f(\mathbf{x}) \quad \text{is continuous for all } u \subseteq 1:d$$

Consequence

$\text{Var}(\nu_{u,\mathbf{k}})$ decays quickly with $\sum_{j \in u} k_j$

$$\text{Var}(\hat{\mu}) = O(n^{-3} \log(n)^{d-1})$$

$$\text{Var}(\hat{\mu}) \leq \bar{\Gamma} \sigma^2 n^{-1} \quad \text{still holds}$$

O (1997, 2008)

Scrambled net properties

Using $\sigma^2 = \int (f(\mathbf{x}) - \mu)^2 d\mathbf{x}$

If	Then	N.B.
$f \in L^{1+\delta}$	$\mathbb{P}(\lim_{n \rightarrow \infty} \hat{\mu}_n = \mu) = 1$	O & Rudolf (2020)
$f \in L^2$	$\text{Var}(\hat{\mu}) = o(1/n)$	even if $V_{\text{HK}}(f) = \infty$
$f \in L^2$	$\text{Var}(\hat{\mu}) \leq \bar{\Gamma} \sigma^2 / n$	if $t = 0$, $\bar{\Gamma} \leq e \doteq 2.718$
all $\partial^u f \in L^2$	$\text{Var}(\hat{\mu}) = O(\log(n)^{d-1} / n^3)$	O (1997,2008)

Geometrically

Scrambling **Faure** breaks up the diagonal striping of the nets.

Scrambling **Sobol'** points moves the full / empty blocks around.

Scrambling vs shifting

Explanation from [Hickernell](#) Consider $n = 2^m$ points in $[0, 1)$.

QMC

van der Corput points



Shift

Shift all points by $U \sim \mathbf{U}(0, 1)$ with wraparound.



Scramble

Get a stratified sample, **independent** $x_i \sim \mathbf{U}[(i-1)/n, i/n)$



Random errors cancel yielding an $O(n^{-1/2})$ improvement.

New software

Three python language projects were mentioned at MCQMC 2020

- QMCPy Fred Hickernell++
- PyTorch Max Balandat++
- Scipy Pamphile Roy++

Especially scrambled Sobol'

Sobol'

First 8 Sobol' points in $[0, 1]^4$

```
0.000 0.000 0.000 0.000
0.500 0.500 0.500 0.500
0.250 0.750 0.750 0.750
0.750 0.250 0.250 0.250
0.125 0.625 0.375 0.125
0.625 0.125 0.875 0.625
0.375 0.375 0.625 0.875
0.875 0.875 0.125 0.375
```

Many implementations did not like the leading $\mathbf{0} = (0, 0, 0, 0, 0)$

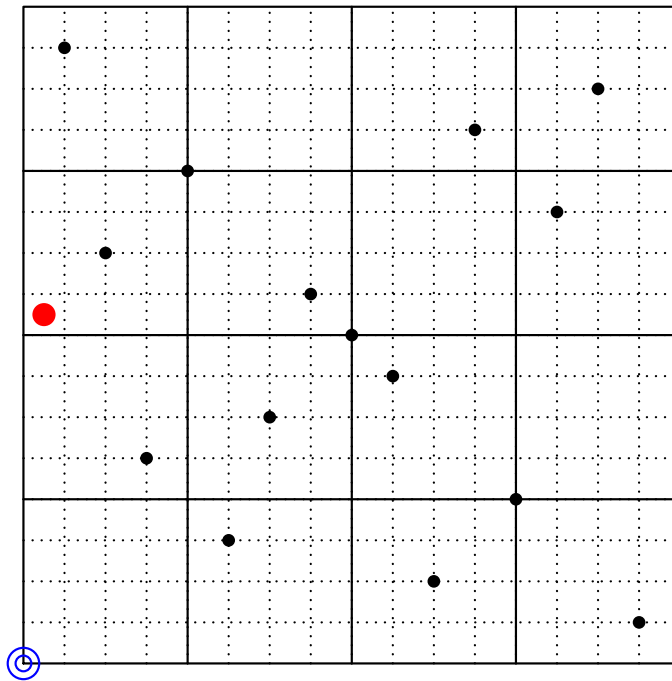
They dropped it and used $\mathbf{x}_2, \dots, \mathbf{x}_{2^m+1}$

starting at $(1/2, 1/2, 1/2, 1/2)$

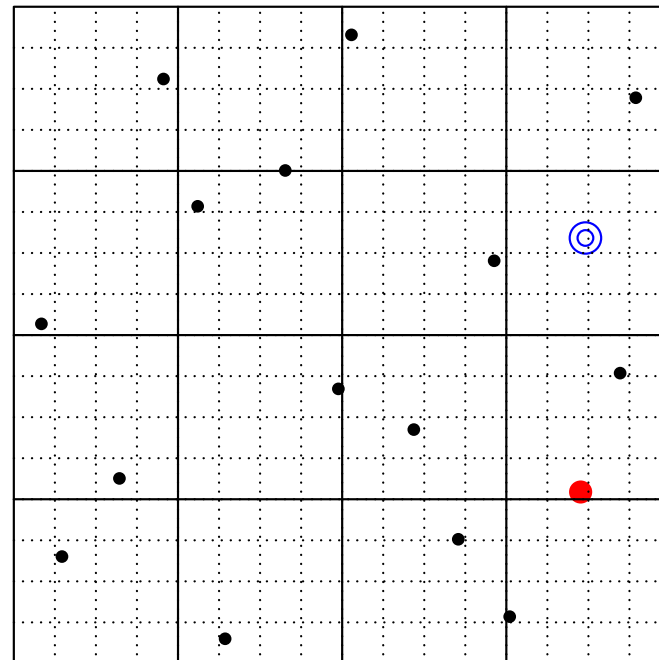
This is *not* a net

Dropping initial point

17 Sobol' points



17 scrambled Sobol' points

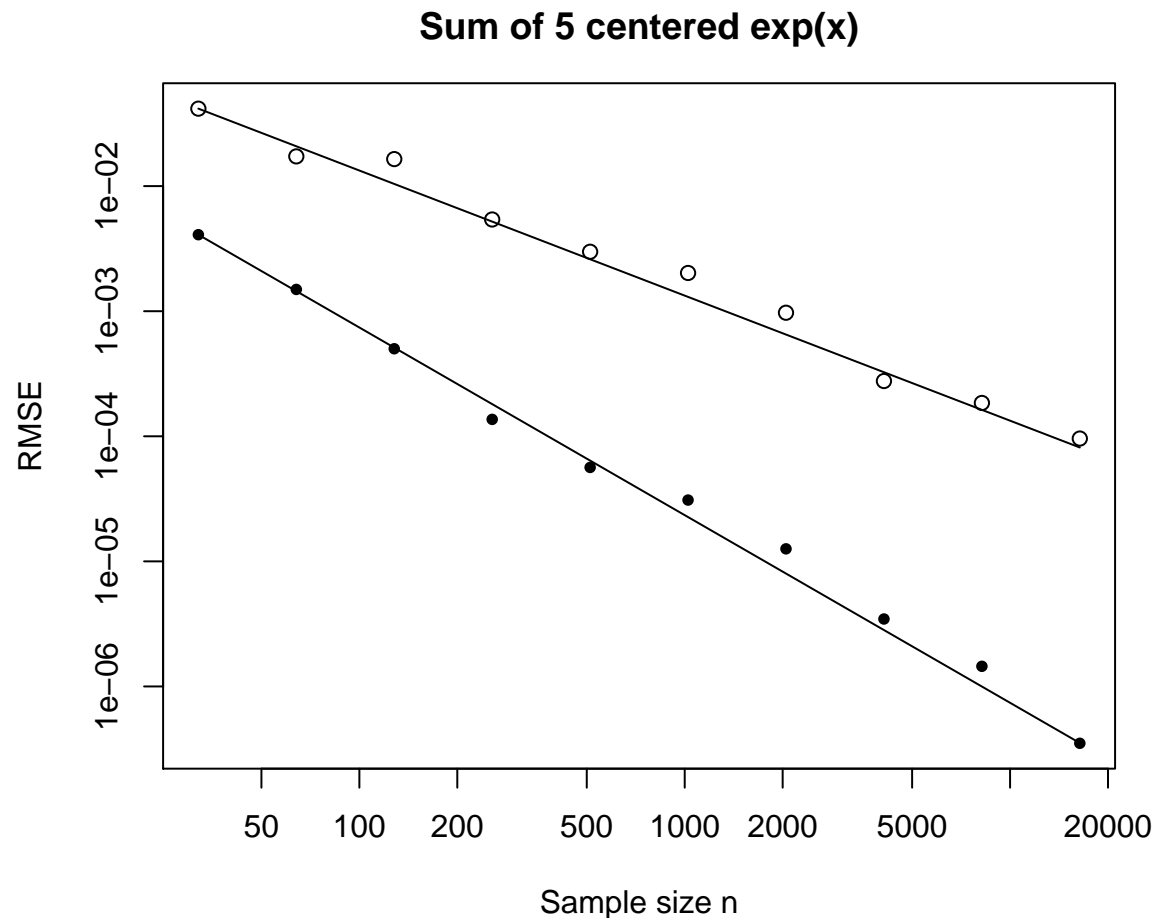


Can worsen the *rate* of convergence

Just one point

Can make a big difference:

- includes x_1
- skips x_1



Easy function: $f(\mathbf{x}) = \sum_{j=1}^5 (\exp(x_j) - e + 1)$

Reference lines $O(n^{-1})$ and $O(n^{-3/2})$

Reason

$$|\hat{\mu}_n - \mu| \approx n^{-3/2}$$

Changing one point is $O(1/n)$ change
larger than the error

Sobol' points out that

$$|\hat{\mu}_n - \mu| \leq \frac{C}{n} \quad \text{and} \quad |\hat{\mu}_{n+1} - \mu| \leq \frac{C}{n+1}$$

\implies

$$|f(\mathbf{x}_{n+1}) - \mu| = O\left(\frac{1}{n}\right)$$

Consequences

- 1) Don't use $n = 10^k$ for a net in base 2
- 2) Don't burn in / warm up RQMC
- 3) Don't take every k 'th RQMC

See [O \(2020\)](#) about "Dropping the first Sobol' point"

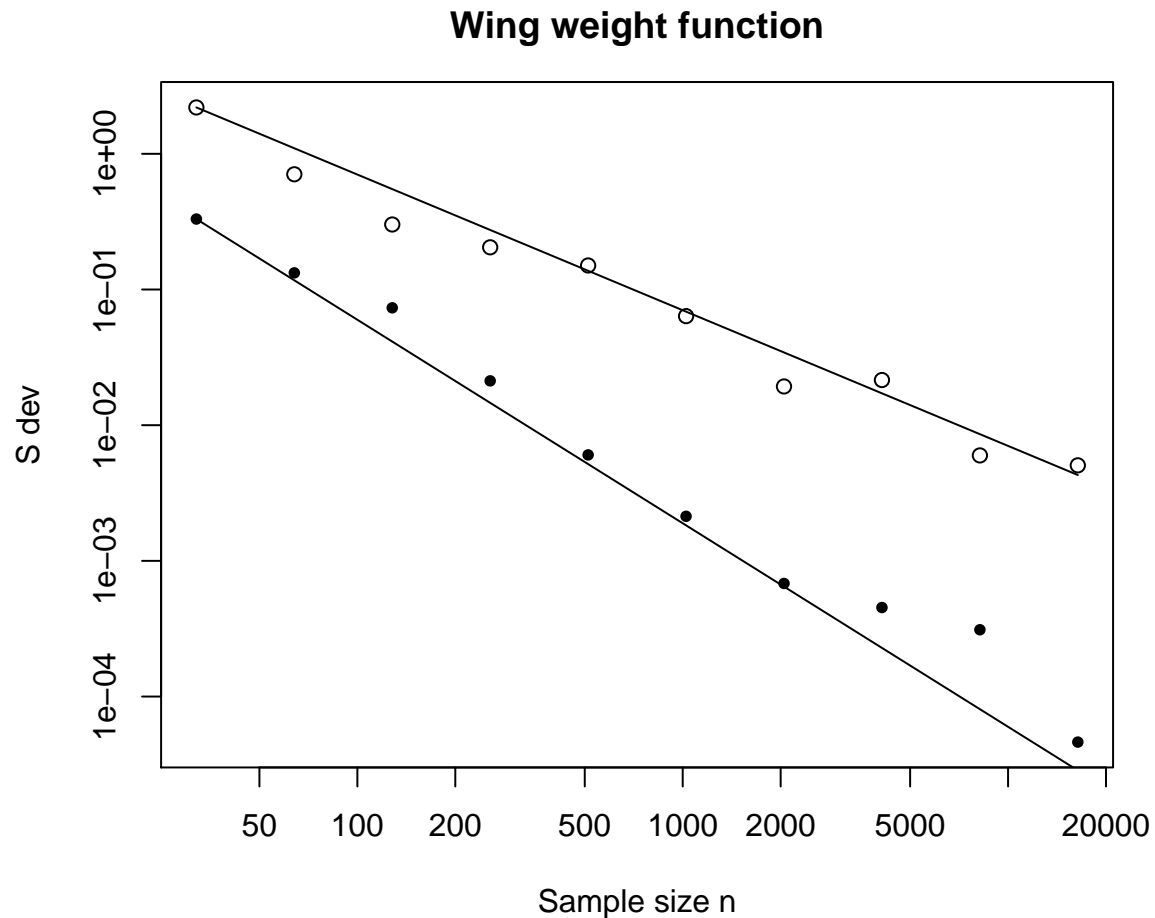
Wing weight function

Surjanovic & Bingham (2013)

$$0.036 S_w^{0.758} W_{fw}^{0.0035} \left(\frac{A}{\cos^2(\Lambda)} \right)^{0.6} q^{0.006} \lambda^{0.04} \left(\frac{100t_c}{\cos(\Lambda)} \right)^{-0.3} (N_x W_{dg})^{0.49} + S_w W_p$$

Variable	Range	Meaning
S_w	[150, 200]	wing area (ft ²)
W_{fw}	[220, 300]	weight of fuel in the wing (lb)
A	[6, 10]	aspect ratio
Λ	[-10, 10]	quarter-chord sweep (degrees)
q	[16, 45]	dynamic pressure at cruise (lb/ft ²)
λ	[0.5, 1]	taper ratio
t_c	[0.08, 0.18]	aerofoil thickness to chord ratio
N_z	[2.5, 6]	ultimate load factor
W_{dg}	[1700, 2500]	flight design gross weight (lb)
W_p	[0.025, 0.08]	paint weight (lb/ft ²)

Wing weight function



This function on $[a, b] \subset \mathbb{R}^{10}$ has low effective dimension.

We don't normally want the average weight of a randomly made wing.

This function has physical origin.

Accuracy from RQMC

Coordinate projection of a (t, m, d) -net

$$\mathbf{x}_{1,u}, \mathbf{x}_{2,u}, \dots, \mathbf{x}_{n,u} \in [0, 1]^{|u|} \quad u \subseteq 1:d$$

It is a $(t_u, m, |u|)$ -net with $t_u \leq t$

For Sobol' and $|u| = 1$ we get $t_u = 0$

Niederreiter & Pirsic (2001) 'Microstructure'

Schmid (2001) 'Projections'

Projection-based bound

$$\begin{aligned} \text{Var}(\hat{\mu}) &= \sum_{u \subseteq 1:d} \text{Var}(\hat{\mu}_u) \leq \frac{1}{n} \sum_{u \subseteq 1:d} \bar{\Gamma}_{|u|,m} \sigma_u^2 \\ &\leq \frac{1}{n} \sum_{u \subseteq 1:d} b^{t_u} \left(\frac{b+1}{b-1} \right)^{|u|} \sigma_u^2 \\ &\leq \frac{1}{n} \sum_{u \subseteq 1:d} 2^{t_u} 3^{|u|} \sigma_u^2 \quad \text{for } b = 2 \end{aligned}$$

Favorable cases dominated by σ_u^2 for small $|u|$

Rotated lattices

Cannot get $\text{Var}(\hat{\mu}) \leq \Gamma \sigma^2 / n$ for all $f \in L^2$

$\text{Var}(\hat{\mu}) = \sigma^2$ possible (for adversarial f)

Random shifts do not reduce error by $\approx n^{1/2}$

See however [Kritzer, Kuo, Nuyens, Ullrich \(2019\)](#) who use random n

No apparent central limit theorem

[L'Ecuyer](#)

No strong law of large numbers

(yet)

Challenges

1)

$$\mu = \int_{\Omega} f(\mathbf{x}) \, d\mathbf{x} \quad \Omega \neq [0, 1]^d$$

E.g. triangles, balls, spheres, simplices, Markov chains

2)

$$\sup_{\mathbf{x}} |f(\mathbf{x})| = \infty$$

Cannot easily get $O(n^{-3/2+\epsilon})$

Work in progress with [S. Liu](#)

Thanks

- Johannes Kepler Universität Linz
- RICAM: Johann·Radon·Institute for Computational and Applied Mathematics
- MCQMC series & Harald Niederreiter
- U.S. NSF: grants up to and including IIS-1837931
- Invitation: Peter Kritzer, Gerhard Larcher, Lucia Del Chicca
- Introductions: Peter Kritzer, Gerhard Larcher, Gunther Leobacher
- Organization: Melanie Traxler

Especially **Daniel Rudolf**