Super-polynomial accuracy of median of means

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Annotated I

These are slides that I presented at MCQMC 2022 in Linz after Zexin Pan was unable to attend. That's a pity. He would have interacted well with much that took place.

The project began with the question about what would happen if base 2 generator matrices were chosen completely at random. The matrices could be bad (e.g., all zeros) but they could also be good (e.g., Niederreiter-Xing) and as it turns out good choices are much more common than bad ones. Better than random generator matrices is to use a random Matousek scramble. Those also are mostly good but every once in a while bad. If we take the median of a modest number of replicates the result can be much more accurate than taking the mean.

Annotated II

We choose some example functions. For instance $x\exp(x)$ is analytic as our theory requires. It is not highly oscillatory which would make it less likely that we see the asymptotic behavior in a modest sample size. It is a ‘positive control’. However, it is not symmetric or anti-symmetric or a polynomial or trigonometric polynomial or specially sensitive to dyadic numbers. Those are things that might make it artificially easy.

We also use $\max(0,(x-1/3))$. This is a harder function than our theory assumes because it is not smooth. Also the value $1/3$ has a slowly converging base 2 expansion which we think is a disadvantage for Sobol’ points.

Zexin Pan

- Sobol' Gains are powers of 2
- Where are the logs?

  There are functions in BVHK with error $> c\log(n)^{(d-1)/2-\epsilon}/n$ infinitely often

  E. Novak $\longrightarrow$ Traub, Wasilkowski, Wozniakowski (1988) $\longrightarrow$ unpublished Trojan
- What if Sobol' had used completely random generator matrices?

Idea in brief

Usual randomized QMC:

- Randomize via Matousek (1998)
- Replicate R times

$$\hat{\mu}_r = \frac{1}{n}\sum_{i=0}^{n-1} f(\boldsymbol{x}_i^{(r)}), \quad r = 1, \dots, R$$

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

Our proposal

$$\hat{\mu} = \textbf{median}\big(\hat{\mu}_1, \dots, \hat{\mu}_R\big)$$

Because

Most of the $\hat{\mu}_r$ are very good

A few are very bad outliers

Median of means

Classic method in theoretical computer science

Jerrum, Valiant, Vazirani (1986), Lecué & Lerasle (2020)

Uses in information based complexity

Kunsch, Novak, Rudolf (2019)

Recent uses in (R)QMC

Goda, L'Ecuyer (2022) [Random lattices]

Hofstadler, Rudolf (2022) [Laws of large numbers]

Gobet, Lerasle, Métivier (2022) [Robust RQMC]

Superpolynomial accuracy

For $d = 1$ and $(0, m, 1)$-net in base $b = 2$

Analytic f

error like $O(n^{-c\log_2(n)})$

$c < 3\log(2)/\pi^2 \approx 0.21$

$f^{(\alpha)}$ is Hölder-λ

error like $O(n^{-\alpha-\lambda+\epsilon})$

P & O (2021) arXiv:2111.12676

Conjecture

Analytic f

Error like $O(n^{-c\log_2(n)/d})$ for $d \geqslant 1$

Work in progress.

Algorithm for $d = 1$

$$\mathbb{N}_0 \longrightarrow \{0,1\}^m \longrightarrow [0,1)$$

$$i = \sum_{k=1}^m i_k 2^{k-1} \qquad \vec{i} = (i_1, i_2, \dots, i_m)^\mathsf{T} \in \{0,1\}^m$$
$$a = \sum_{k=1}^\infty a_k 2^{-k} \qquad \vec{a} = (a_1, a_2, \dots, a_m)^\mathsf{T} \in \{0,1\}^m$$

Unscrambled net

$a_0, a_1, \dots, a_{2^m-1}$ with

$$\vec{a}_i = C\vec{i} \ \text{ mod } 2$$
$$C \in \{0,1\}^{m\times m}$$

C has full rank over $\mathbb{Z}_2$

$C = I_m$ for van Der Corput

Linearly scrambled net

$$\vec{x}_i = M\vec{a}_i = MC\vec{i} \mod 2$$

$$M = \begin{pmatrix} 1 & & & & & \\ u & 1 & & & & \\ u & u & 1 & & & \\ u & u & u & 1 & & \\ \vdots & \vdots & \vdots & \vdots & \ddots & \\ u & u & u & u & \cdots & 1 \\ u & u & u & u & \cdots & u \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ u & u & u & u & \cdots & u \end{pmatrix} \in \{0,1\}^{E\times m} \qquad E \geqslant m$$

$u \sim$ IID $\mathbf{U}\{0,1\}$

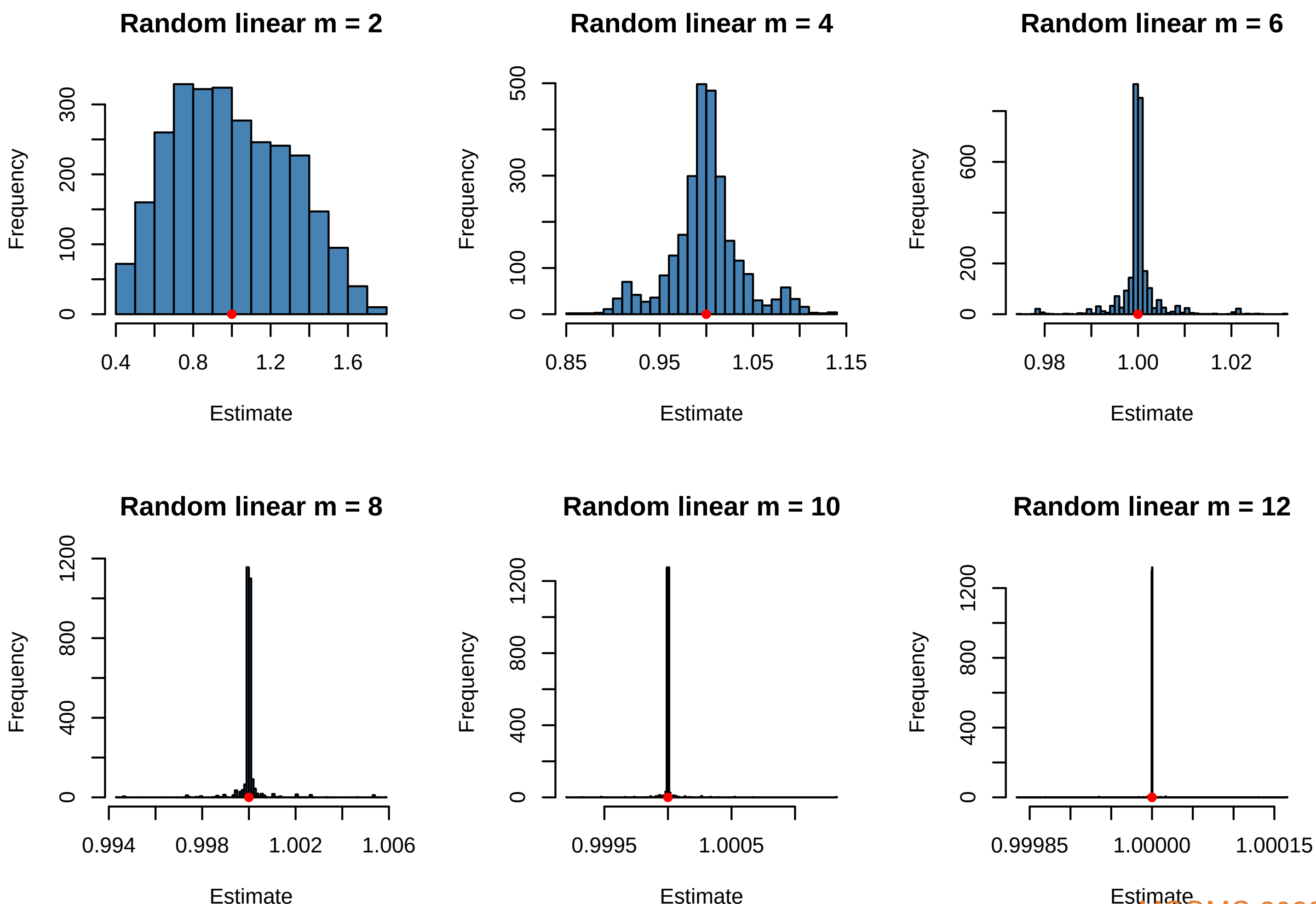
Apply digital shift

$$\vec{x}_i = MC\vec{i} + \vec{D} \mod 2 \qquad D_k \overset{\text{iid}}{\sim} \mathbf{U}\{0,1\}$$

$\Longrightarrow$ each $x_i \sim \mathbf{U}[0,1]$ for $E = \infty$

$$\int_0^1 xe^x \, \mathrm{d}x = 1$$

$n = 2^m$ random linear Same shift D for all n points



QMCPy, Hickernell, Sorokin

Precision

$M \in \{0,1\}^{E\times m}$ produces x_i to E bits

Infinite precision $E=\infty$ and $M \in \{0,1\}^{\infty\times m}$

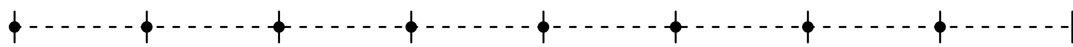
Produces $\hat\mu_\infty$

based on $n = 2^m$ points

Stratification

Without randomization we get

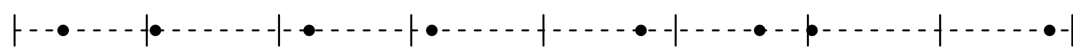
i/n for $0 \leqslant i < n$



in some order

With randomization we get one point in

$[i/n, (i+1)/n)$



each $0 \leqslant i < n$

Bottleneck

Maybe

$$M(m+1,:) = (0,0,\dots,0) = \mathbf{0} \in \{0,1\}^m$$

Then

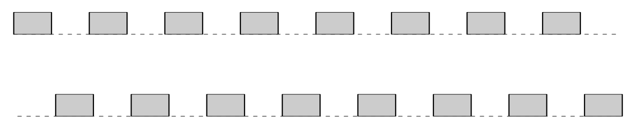
$$x_{0,m+1} = x_{1,m+1} = \cdots = x_{n-1,m+1} = D_{m+1}$$

This has probability $2^{-m} = 1/n$

Consequence

$D_{m+1} = 0 \implies$ all points in $\bigl[\frac{i}{n}, \frac{i+1/2}{n}\bigr)$'s

$D_{m+1} = 1 \implies$ all points in $\bigl[\frac{i+1/2}{n}, \frac{i+1}{n}\bigr)$'s



$\implies$ Half of $[0,1)$ is empty

$\mathbb{E}\bigl(|\hat\mu - \mu| \mid M(m+1,:) = \mathbf{0}\bigr) = O(1/n)$ (Taylor)

Summary

This rare event contributes $O(1/n^3)$ to $\mathrm{Var}(\hat\mu_\infty)$

Cannot reduce by more smoothness

More trouble

Problematic whenever

$$\sum_{\ell\in L} M(\ell,:) = \mathbf{0} \quad \text{for some } L \subseteq \mathbb{N}$$

Can't happen if $L \subseteq \{1,2,\dots,m\}$ because M has full rank

Probability 2^{-m} otherwise: "last row" of $M(L,:)$ does it

That is

$$\Pr\Bigl(\sum_{\ell\in L} M(\ell,:) = \mathbf{0}\Bigr) = \begin{cases} 0, & L \subseteq \{1,2,\dots,m\} \\ 2^{-m}, & L \not\subseteq \{1,2,\dots,m\} \end{cases}$$

Magnitudes

$$|L| = \text{card}(L) \qquad \|L\|_1 = \sum_{\ell\in L} \ell$$

Decomposition

$$\mathcal{L} := \{L \subset \mathbb{N} \mid 0 < |L| < \infty\}$$

Let f be analytic on $[0,1]$ with

$$\Bigl|f^{(k)}\bigl(\tfrac{1}{2}\bigr)\Bigr| \leqslant A\alpha^k k!, \quad A < \infty, \quad \alpha < 2, \quad \text{all } k \in \mathbb{N}$$

$C \in \{0,1\}^{m\times m}$ full rank

Theorem 3.1

$$\hat{\mu}_\infty - \mu = \sum_{L\in\mathcal{L}} \mathbf{1}\Biggl\{\sum_{\ell\in L} M(\ell,:) = \mathbf{0}\Biggr\} S_L(D) 2^{-\|L\|_1} B_L$$

$$S_L(D) = \prod_{\ell\in L} (-1)^{D_\ell}$$

$$|B_L| \leqslant 6A(|L|-1)!\Bigl(\frac{\alpha/2}{1-\alpha/2}\Bigr)^{|L|}$$

The B_L involve Walsh coefficients of f

Significant use of Dick & Pillichshammer (2010)

Norm of L

The bound includes $2^{-\|L\|_1}$

Things are bad for small $\|L\|_1$

worst is $L = \{m+1\}$ (bottleneck example)

Fortunately

Not too many $L \in \mathcal{L}$ with $\|L\|_1 = N$ small

$p(N) = \#$ ways to partition $N \in \mathbb{N}$ into a sum of natural numbers.

Analytic combinatorics

Hardy & Ramanujan (1918) show that

$$p(N) \sim \frac{1}{N4\sqrt{3}} \exp\Bigl(\pi\Bigl(\frac{2N}{3}\Bigr)^{1/2}\Bigr) = o(2^N)$$

Bidar (2012) reduces this for ***distinct*** natural numbers

$$\frac{\pi}{2\sqrt{3N}} \exp\Bigl(\pi\Bigl(\frac{N}{3}\Bigr)^{1/2}\Bigr)$$

Trouble spots

Let $m = 3$

$\|L\|_1$	L
4	$\{4\}$
5	$\{5\}, \{1,4\}$
6	$\{6\}, \{1,5\}, \{2,4\}$
7	$\{7\}, \{1,6\}, \{2,5\}, \{1,2,4\}$
8	$\{8\}, \{1,7\}, \{2,6\}, \{3,5\}, \{1,2,5\}, \{1,3,4\}$
$\vdots$	$\vdots$ $\qquad\qquad\qquad\qquad\qquad\qquad \ddots$

Weighted by $2^{-\|L\|_1}$

The rows grow in cardinality but they do not double in size.

Controlling bad $L \in \mathcal{L}$

For $\lambda = 3(\log(2)/\pi)^2 \approx 0.146$

$$\bigl|\{L \in \mathcal{L} \mid \|L\|_1 \leqslant \lambda m^2\}\bigr| \sim \frac{3^{1/4}}{2\pi\lambda^{1/4}} \frac{2^m}{\sqrt{m}}$$

$$\Pr\left(\sum_{\ell \in L} M(\ell, :)\right) = \mathbf{0}) = 2^{-m}$$

Expect $O\left(\frac{1}{\sqrt{m}}\right)$ problematic sets L

Quality of estimate

Bound $\Pr\bigl(|\hat{\mu}_\infty - \mu| \gg 2^{-\lambda m^2}\bigr)$

Then median over infinite replicates has

$$\bigl|\text{median}(\hat{\mu}_\infty) - \mu)\bigr| = o(2^{-(\lambda-\epsilon)m^2})$$

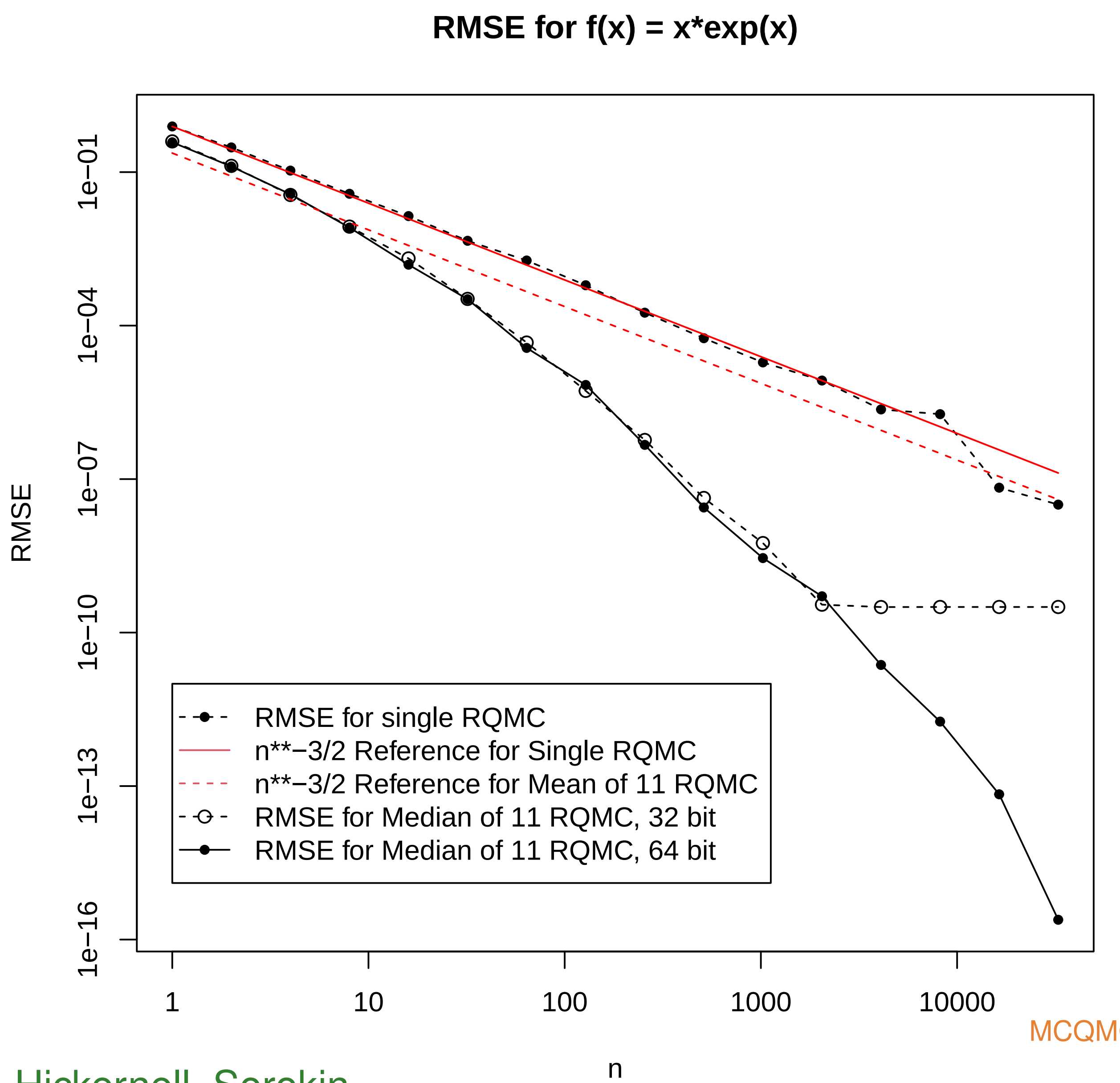
Sample median

$$\Bigl|\text{median}\bigl(\hat{\mu}_{\infty,1}, \hat{\mu}_{\infty,2}, \dots, \hat{\mu}_{\infty,2k-1}\bigr) - \text{median}\bigl(\hat{\mu}_\infty\bigr)\Bigr|$$

letting $k = \Omega(m) = \Omega(\log_2(n))$.

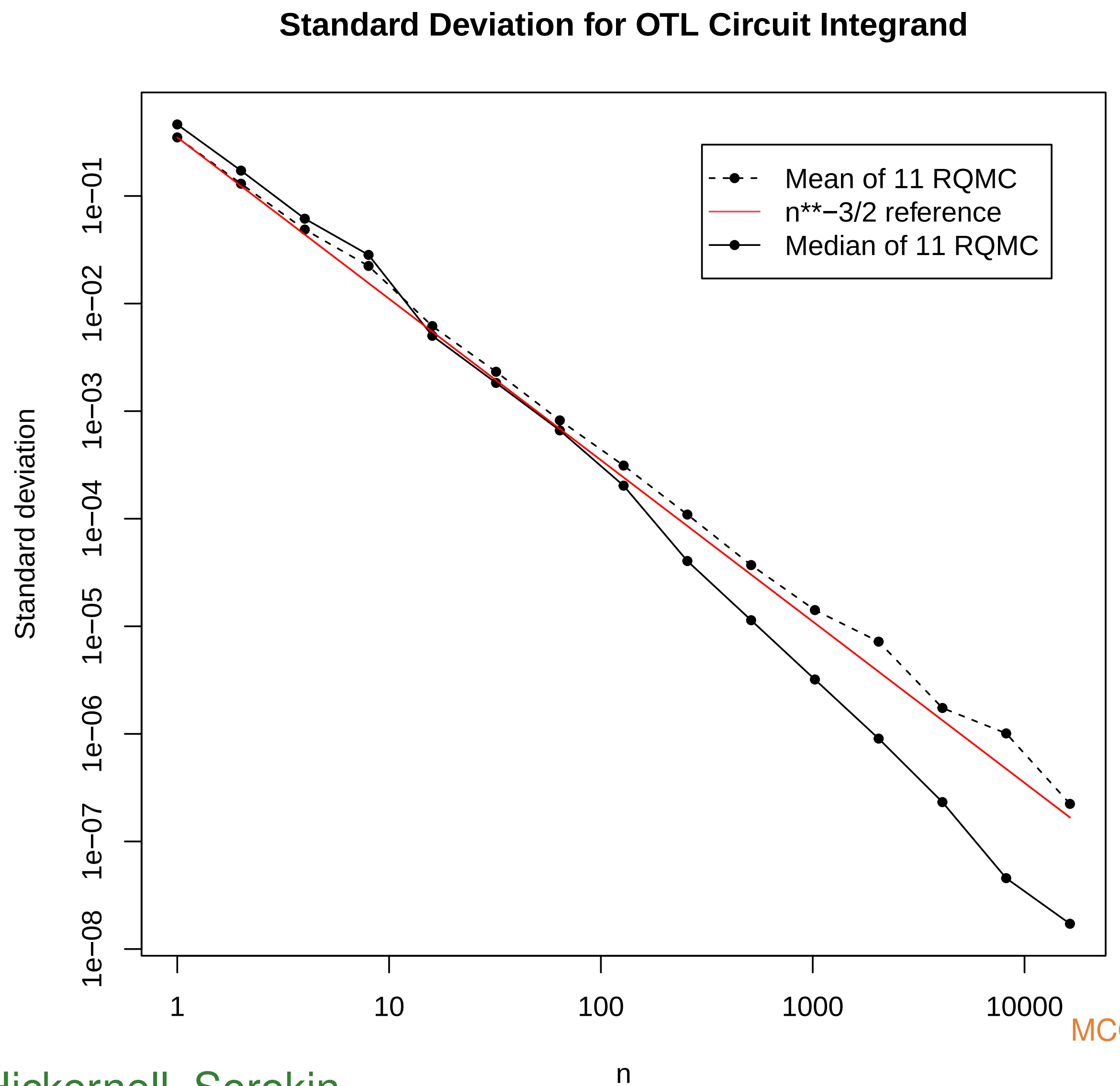
Cost is now $O(n\log(n))$

Example $d = 1$


RMSE for f(x) = x*exp(x)
RMSE
n
1e−01
1e−04
1e−07
1e−10
1e−13
1e−16
1
10
100
1000
10000
RMSE for single RQMC
n**−3/2 Reference for Single RQMC
n**−3/2 Reference for Mean of 11 RQMC
RMSE for Median of 11 RQMC, 32 bit
RMSE for Median of 11 RQMC, 64 bit

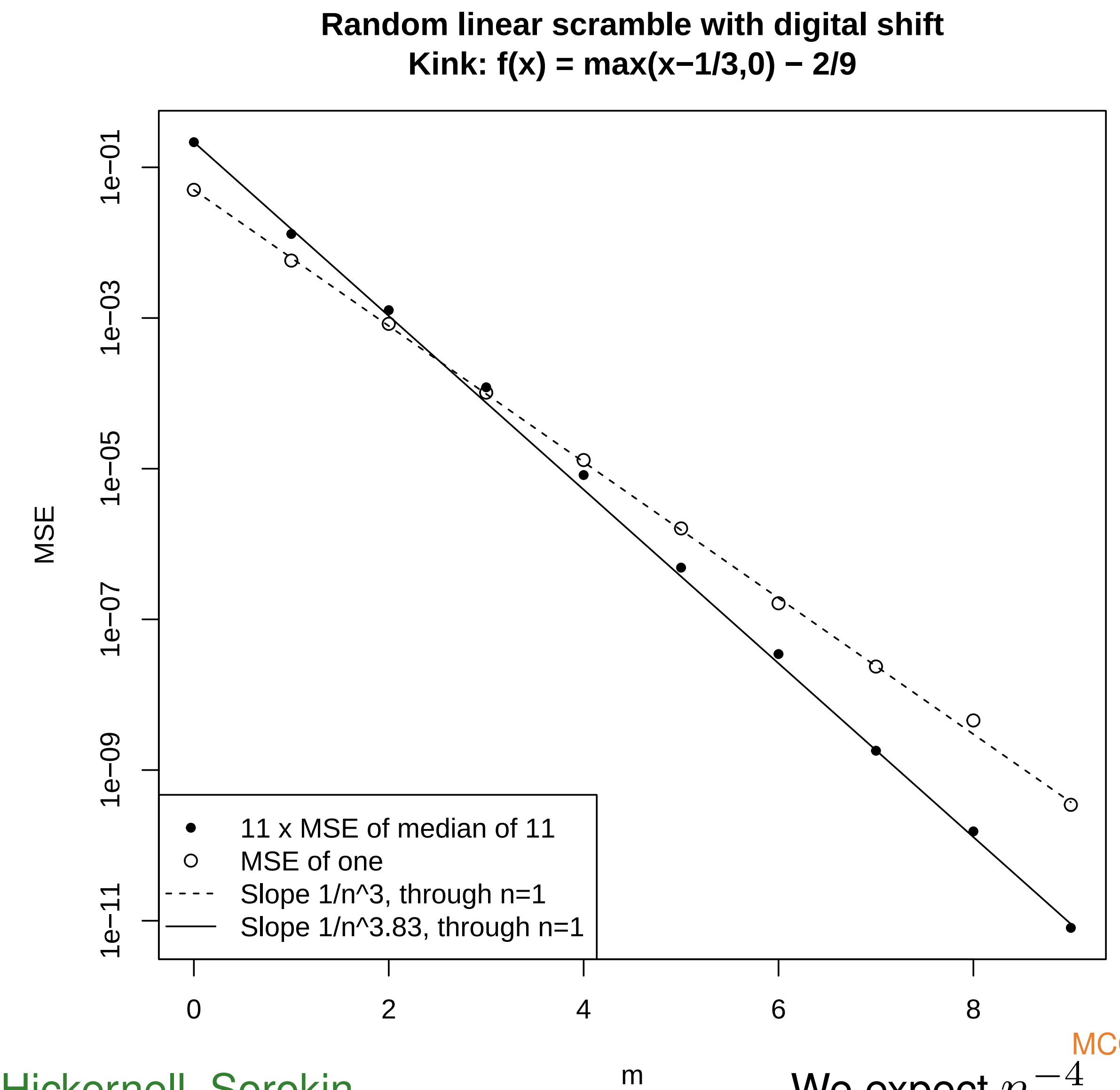
Example $d = 6$

Surjanovic & Bingham



QMCPy, Hickernell, Sorokin

$$\int_0^1 (x-1/3)_+ \, \mathrm{d}x = 2/9$$



We expect n^{-4}

Challenge

It is ***hard*** to estimate

$$\mathrm{Var}\bigl(\text{median}(\hat{\mu}_1,\dots,\hat{\mu}_{2k-1})\bigr)$$

It is ***easy*** to get a confidence interval for

$$\text{median}\bigl(\text{Distribution of } \hat{\mu}_r\bigr)$$

But we ***want*** to know about

$$\int f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \text{mean}\bigl(\text{Distribution of } \hat{\mu}_r\bigr)$$

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