Numerical Methods in Economics MIT Press, 1998

# Notes for Chapter 9: quasi-Monte Carlo Methods

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# Quasi-Monte Carlo Methods

- Observation:
	- MC uses "random" sequences to satisfy i.i.d. premise of LLN
	- Integration only needs sequences which are good for integration
	- Integration does not care about i.i.d. property
- Idea of quasi-Monte Carlo methods
	- Explicitly construct a sequence designed to be good for integration.
	- Do not leave integration up to mindless random choices
- Pseudorandom sequence are not random.
	- von Neumann: "Anyone who considers arithmetical methods of producing random digits is, of course, in a state of sin."

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- "pseudo" means "false, feigned, fake, counterfeit, spurious, illusory"
- Neither LLN nor CLT apply
- Visual similarities are not mathematically relevant
- Monte Carlo Propaganda
	- Best deterministic methods converge at rate  $N^{-1/d}$
	- MC converges at rate  $N^{-1/2}$  for any dimension d
	- So, MC is far better than any deterministic scheme
- Observations about Monte Carlo Propaganda
	- Implementations of MC use pseudorandom (hence, deterministic) sequences instead of random numbers
	- Implementations of MC converge at rate  $N^{-1/2}$  for any dimension d
	- Therefore, there exist deterministic methods which converge at rate  $N^{-1/2}$  for any dimension d.
	- Therefore, under MC propaganda logic,  $1/2=1/d$  for all  $d > 1$
- Questions
	- What is rate of convergence when using pseudorandom numbers?
	- Why do deterministic pseudorandom methods converge at rate  $N^{-1/2}$  in practice?
- Answer: MC propagandists pull a bait-and-switch
	- $-$  They use worst-case analysis in "Best deterministic methods for integrating  $C<sup>0</sup>$  functions converge at rate  $N^{-1/d}$
	- They use probability-one criterion when they say "MC methods converge at rate  $N^{-1/2}$ "
- Mathematical Facts:
	- MC worst-case convergence rate is  $N^{-0}$  no convergence there is some sequence where MC does not converge
	- Some pseudorandom methods converge at  $N^{-1/2}$  for smooth functions in worst case; proofs are number-theoretic.
	- If f is  $C^k$  and periodic, then there are deterministic rules converging at rate  $N^{-k}$  independent of dimension
- Practical facts
	- qMC has been used for many high-dimension (e.g., 360) problems.
	- pMC asymptotics kick in early; qMC asymptotics take longer
	- $-$  Therefore, pMC methods have *finite sample advantages*, not asymptotic advantages.
	- "quasi-MC" is bad name since qMC methods have no connection to probability theory

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Equidistributed Sequences

**Definition 1** A sequence  $\{x_j\}_{j=1}^{\infty} \subset R$  is equidistributed over  $[a, b]$  if

$$
\lim_{n \to \infty} \frac{b-a}{n} \sum_{j=1}^{n} f(x_j) = \int_{a}^{b} f(x) dx
$$
\n(9.1.1)

for all Riemann-integrable  $f(x)$ . More generally, a sequence  $\{x^j\}_{j=1}^{\infty} \subset D \subset R^d$  is equidistributed over  $D$  iff

$$
\lim_{n \to \infty} \frac{\mu(D)}{n} \sum_{j=1}^{n} f(x^j) = \int_D f(x) \, dx \tag{9.1.2}
$$

for all Riemann-integrable  $f(x) : R^d \to R$ , where  $\mu(D)$  is the Lebesgue measure of D.

- Examples:
	- $-0, 1/2, 1, 1/4, 3/4, 1/8, 3/8, 5/8, 7/8,$  etc., is not equidistributed over [0, 1] since  $\frac{b-a}{n} \sum_{j=1}^{n} x_j$ , the approximation to  $\int_0^1 x \, dx$ , oscillates.
	- Weyl sequence: for  $\theta$  irrational

$$
x_n = \{n\theta\}, \ n = 1, 2, \cdots,
$$
\n(9.1.3)

where  $\{x\}$  is *fractional part of* x and defined by

$$
\{x\} \equiv x - \max\{k \in Z \mid k \le x\}
$$

is equidistributed



Figure 1: Weyl function



First 1500 Weyl points



1500 Points generated by LCM

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• MC vs qMC

- qMC are not serially uncorrelated
- Similar iterations for Weyl since  $x_{n+1} = (x_n + \theta) \text{mod } 1$ , but slope term is 1, not some big number.

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## **Discrepancy**

We want measures of deviation from uniformity for sets of points

**Definition 2** The discrepancy  $D_N$  of the set  $X \equiv \{x_1, \dots, x_N\} \subset [0, 1]$  is

$$
D_N(X) = \sup_{0 \le a < b \le 1} |\frac{card([a, b] \cap X)}{N} - (b - a)|.
$$

**Definition 3** If X is a sequence  $x_1, x_2, \dots \subset [0, 1]$ , then  $D_N(X)$  is  $D_N(X^N)$  where  $X^N = \{x_j \in X \mid$  $j = 1, \cdots, N$ .

#### • Small discrepancy sets

 $-$  On [0, 1], the set with minimal  $D_N$  is  $\left\{\frac{1}{N+1}, \frac{2}{N+1}, \dots, \frac{N}{N+1}\right\}$ 

— Discrepancy of lattice point set

$$
U_{d,m} = \left\{ \left( \frac{2m_1 - 1}{2m} , \cdots , \frac{2m_d - 1}{2m} \right) \mid 1 \leq m_j \leq m, j = 1, \cdots, d \right\}
$$

is  $\mathcal{O}(m^{-1}) = \mathcal{O}\left(N^{-1/d}\right)$ 

- Star discrepancy of N random points is  $\mathcal{O}(N^{-\frac{1}{2}}(\log \log N)^{1/2})$ , a.s.
- Roth (1954) and Kuipers and Niederreiter (1974):

$$
D_N^* > 2^{-4d} \left( (d-1) \log 2 \right)^{(1-d)/2} N^{-1} \left( \log N \right)^{(d-1)/2}.
$$
 (9.2.1)

which is much lower than the Chung-Kiefer result on randomly generated point sets. – The Halton sequence in  $I^d$  has discrepancy

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$$
D_N < \frac{d}{N^2} + \frac{1}{N} \prod_{j=1}^d \left( \frac{p_j - 1}{2 \log p_j} \log N + \frac{p_j + 1}{2} \right)
$$
\n
$$
\sim \frac{(\log N)^d}{N} \leq \mathcal{O}\left(N^{-1+\varepsilon}\right)
$$
\n(9.2.4)

 $-$  Bound not good for moderate N and large d.

### Variation and Integration

**Theorem 4** The total variation of f,  $V(f)$ , on [0, 1] is

$$
V(f) = \sup_{n} \sup_{0 \le x_0 < x_1 < \dots < x_n \le 1} \sum_{j=1}^{n} |f(x_j) - f(x_{j-1})|
$$

**Theorem 5** (Koksma) If f has bounded total variation, i.e.,  $V(f) < \infty$ , on I, and the sequence  $x_j \in I, j = 1, \cdots, N$ , has discrepancy  $D_N^*$ , then

$$
\left| N^{-1} \sum_{j=1}^{N} f(x_j) - \int_0^1 f(x) \, dx \right| \le D_N^* V(f) \tag{9.2.5}
$$

Can generalize variation to multivariate functions,  $V^{HK}(f)$ .

**Theorem 6** (Hlawka) If  $V^{HK}(f)$  is finite and  $\{x^j\}_{j=1}^N \subset I^d$  has discrepancy  $D_N^*$ , then

$$
\frac{1}{N} \sum_{j=1}^{N} f(x^j) - \int_{I^d} f(x) \, dx \le V^{HK}(f) D_N^*.
$$

Product rules use lattice sets, which have discrepancy  $O(N^{-1/d})$ , not as good as some other sets with discrepancy  $\mathcal{O}(N^{-1+\varepsilon})$ 

Monte Carlo versus Quasi-Monte Carlo

Table 9.2: Integration Errors for  $\int_{I^d} d^{-1} \sum_{j=1}^d |4x_j - 2| dx$ 

N(1000s) MC Weyl Haber Niederreiter



$$
d = 40:
$$



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Table 9.3: Integration Errors for  $\int_{I^d} \prod_{j=1}^d \left(\frac{\pi}{2} \sin \pi x_j\right) dx$ 

N(1000s) MC Weyl Haber Niederreiter

$$
d = 10:
$$
\n
$$
1 \t1(-2) \t6(-2) \t8(-2) \t9(-3)
$$
\n
$$
10 \t3(-2) \t8(-3) \t5(-3) \t5(-4)
$$
\n
$$
100 \t9(-3) \t2(-3) \t1(-3) \t6(-4)
$$
\n
$$
1000 \t2(-3) \t3(-5) \t6(-3) \t2(-4)
$$

 $d = 40$ :



Fourier Analytic Methods

- Consider  $\int_0^1 \cos 2\pi x \, dx = 0$  and its approximation  $N^{-1} \sum_{n=1}^N \cos 2\pi x_n$ 
	- Choose  $x_n = \{n\alpha\}$ , a Weyl sequence
	- Periodicity of  $\cos x$  implies  $\cos 2\pi \{n\alpha\} = \cos 2\pi n\alpha$
	- Periodicity of  $\cos 2\pi x$  implies Fourier series representation

$$
\cos 2\pi x = \frac{1}{2} (e^{2\pi ix} + e^{-2\pi ix})
$$

— Error analysis: error is approximation, and

$$
\frac{1}{N} \sum_{n=1}^{N} \frac{1}{2} (e^{2\pi i n \alpha} + e^{-2\pi i n \alpha})
$$
\n
$$
= \frac{1}{2N} \sum_{n=1}^{N} (e^{2\pi i \alpha})^{n} + \frac{1}{2N} \sum_{n=1}^{N} (e^{-2\pi i \alpha})^{n}
$$
\n
$$
\leq \frac{1}{2N} \left( \left| \frac{e^{2\pi i N \alpha} - 1}{e^{2\pi i \alpha} - 1} \right| + \left| \frac{e^{-2\pi i N \alpha} - 1}{e^{-2\pi i \alpha} - 1} \right| \right)
$$
\n
$$
\leq \frac{1}{2N} \left( \frac{2}{|e^{2\pi i \alpha} - 1|} + \frac{2}{|e^{-2\pi i \alpha} - 1|} \right) \leq \frac{C}{N}
$$
\n(9.3.1)

for a finite C as long as  $e^{2\pi i \alpha} \neq 1$ , which is true for any irrational  $\alpha$ .

 $-$  So, convergence rate is  $N^{-1}$ .

 $-$  (9.3.1) applies to a finite sum of  $e^{2\pi i kx}$  terms; can be generalized to arbitrary Fourier series.

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• The following theorem summarizes results reported in book.

**Theorem 7** Suppose, for some integer k, that  $f : [0, 1]^d \to R$  satisfies the following two conditions: 1. All partial derivatives

$$
\frac{\partial^{m_1+\dots+m_d}f}{\partial x_1^{m_1}\cdots \partial x_d^{m_d}}, 0 \le m_j \le k-1, 1 \le j \le d
$$

exist and are of bounded variation in the sense of Hardy and Krause, and

2. All partial derivatives

$$
\frac{\partial^{m_1+\dots+m_d}f}{\partial x_1^{m_1}\dotsm\partial x_d^{m_d}}, 0 \le m_j \le k-2, 1 \le j \le d
$$

are periodic on  $[0, 1]^d$ .

Then, the error in integrating  $f \in \mathcal{C}^k$  with Korobov or Keast good lattice point set with sample size N is  $O(N^{-k}(\ln N)^{kd}).$ 

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- Key observation:
	- If f is  $C^k$  we can find rules with  $O(N^{-k+\epsilon})$  convergence.
	- For smooth functions, there are deterministic rules which far outperform MC
	- $-$  qMC asymptotics may not kick in until  $N$  is impractically large.

### Estimating Quasi-Monte Carlo Errors

- MC rules have standard errors
- Quasi-MC rules do not have standard errors
- Add "randomization" to construct standard errors
- Suppose
	- $-$  For each  $\beta$ ,

$$
I(f) \doteq Q(f;\beta)
$$

– For  $\beta \sim U$  [0, 1]  $I(f) \equiv$ " D  $f(x) dx = E\{Q(f; \beta)\}\$  (9.5.1) — Then

$$
\hat{I} \equiv \frac{1}{m} \sum_{j=1}^{m} Q(f; \beta_j)
$$
\n(9.5.2)

is an unbiased estimator of  $I(f)$  with standard error  $\sigma_{\hat{I}}$  approximated by

$$
\hat{\sigma}_{\hat{I}}^2 \equiv \frac{\sum_{j=1}^m (Q(f; \beta_j) - \hat{I})^2}{m - 1} \tag{9.5.3}
$$

• Example: Random shifts to Weyl rules, because if  $x_j$  is equidistributed on [0, 1], then so is  $x_j + \beta$ for any random  $\beta$ .

# **Conclusion**

- All sampling methods use deterministic sequences
- Probability theory does not apply to *any* practical sampling scheme
- Pseudorandom schemes seem to have  $O(N^{-1/2})$  convergence; this is proven for LCM
- There are  $O(N^{-1})$  schemes for continuously differentiable functions use equidistributional sequences
- There are  $O(N^{-k})$  schemes for  $C^k$  functions use Fourier analytic schemes
- qMC methods have done well in some problems with hundreds of dimensions
- Pseudorandom sequences appear to have finite sample advantages for very high dimension problems