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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."
 - "pseudo" means "false, feigned, fake, counterfeit, spurious, illusory"
 - Neither LLN nor CLT apply
 - Visual similarities are not mathematically relevant; for example, "optical regression" is not a valid technique.

- 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^0 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.
 - $-~\mathrm{pMC}$ 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

Equidistributed Sequences

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

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

for all Riemann-integrable f(x). More generally, a sequence $\{x^j\}_{j=1}^{\infty} \subset D \subset \mathbb{R}^d$ 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 $f(x) : \mathbb{R}^d \to \mathbb{R}$, 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 θ irrational

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

Table 9.1: Equidistributed Sequences in
$$\mathbb{R}^d$$
Name:Formula for x^n :Weyl $\left(\left\{n p_1^{1/2}\right\}, \cdots, \left\{n p_d^{1/2}\right\}\right)$ Haber $\left(\left\{\frac{n(n+1)}{2} p_1^{1/2}\right\}, \cdots, \left\{\frac{n(n+1)}{2} p_d^{1/2}\right\}\right)$ Niederreiter $\left(\left\{n 2^{1/(d+1)}\right\}, \cdots, \left\{n 2^{d/(d+1)}\right\}\right)$ Baker $\left(\left\{n e^{r_1}\right\}, \cdots, \left\{n e^{r_d}\right\}\right), r_j$ rational and distinct

• MC vs qMC

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

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 $x_1, x_2, \dots \in [0, 1]$, then $D_N(X)$ is $D_N(X^N)$ where $X^N = \{x_j \in X \mid j = 1, \dots, N\}$.

• Small discrepancy sets

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

– Discrepancy of lattice point set

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

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

$$D_N < \frac{d}{N^2} + \frac{1}{N} \prod_{j=1}^d \left(\frac{p_j - 1}{2\log p_j} \log N + \frac{p_j + 1}{2} \right)$$

$$\sim \frac{(\log N)^d}{N} \le \mathcal{O}\left(N^{-1+\varepsilon} \right)$$
(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 $x_j \in I, j = 1, \dots, N$, 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

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

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

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

1(-3)	3(-4)	4(-4)	4(-4)
2(-4)	6(-5)	1(-3)	3(-5)
1(-3)	7(-6)	2(-4)	2(-6)
4(-5)	6(-7)	2(-4)	2(-7)
	1(-3) 2(-4) 1(-3) 4(-5)	$\begin{array}{ll}1(-3) & 3(-4)\\2(-4) & 6(-5)\\1(-3) & 7(-6)\\4(-5) & 6(-7)\end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$

$$d = 40:$$

1	3(-3)	4(-4)	3(-3)	2(-4)
10	3(-4)	6(-5)	1(-3)	2(-6)
100	4(-6)	5(-6)	3(-4)	9(-6)
1000	1(-4)	6(-7)	1(-5)	4(-7)

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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 = 40:

1	4(-1)	5(-1)	5(-2)	7(-1)
10	2(-1)	4(-1)	4(-1)	8(-2)
100	1(-2)	2(-1)	3(-3)	5(-2)
1000	3(-2)	2(-1)	3(-2)	4(-3)

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

$$\frac{1}{N} \sum_{n=1}^{N} \frac{1}{2} (e^{2\pi i n \alpha} + e^{-2\pi i n \alpha})$$

$$= \frac{1}{2N} \sum_{n=1}^{N} (e^{2\pi i \alpha})^n + \frac{1}{2N} \sum_{n=1}^{N} (e^{-2\pi i \alpha})^n$$

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

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

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

- 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.

• 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

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

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

2. All partial derivatives

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

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

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

- Key observation:
 - If f is C^k we can find rules with $O(N^{-k+\varepsilon})$ 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 β ,

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

- For $\beta \sim U[0,1]$ $I(f) \equiv \int_D f(x) \, dx = E\{Q(f;\beta)\} \tag{9.5.1}$ - Then

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

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

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

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