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Chapter 9 Notes
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
- 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
- Retort to 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 do exist deterministic methods which converge at rate $N^{-1/2}$ for any dimension d.
  - Therefore, under MC propaganda logic, $0 = 1$.

- Questions
  - What is rate of convergence when using pseudorandom numbers?
  - Why do pseudorandom methods converge at rate $N^{-1/2}$ in practice even though they are deterministic?
- Answer: MC propagandists pull a bait-and-switch
  - They use worst-case analysis when they say "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* - since there always is some sequence where MC does not converge
  - Some pseudorandom methods converge at $N^{-1/2}$ *in worst case*; proofs are number-theoretic.
  - If f is C^k there are deterministic rules which converge 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 logical 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* $\{x^j\}_{j=1}^{\infty} \subset D \subset R^d$ *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 θ irrational

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

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

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

    is equidistributed

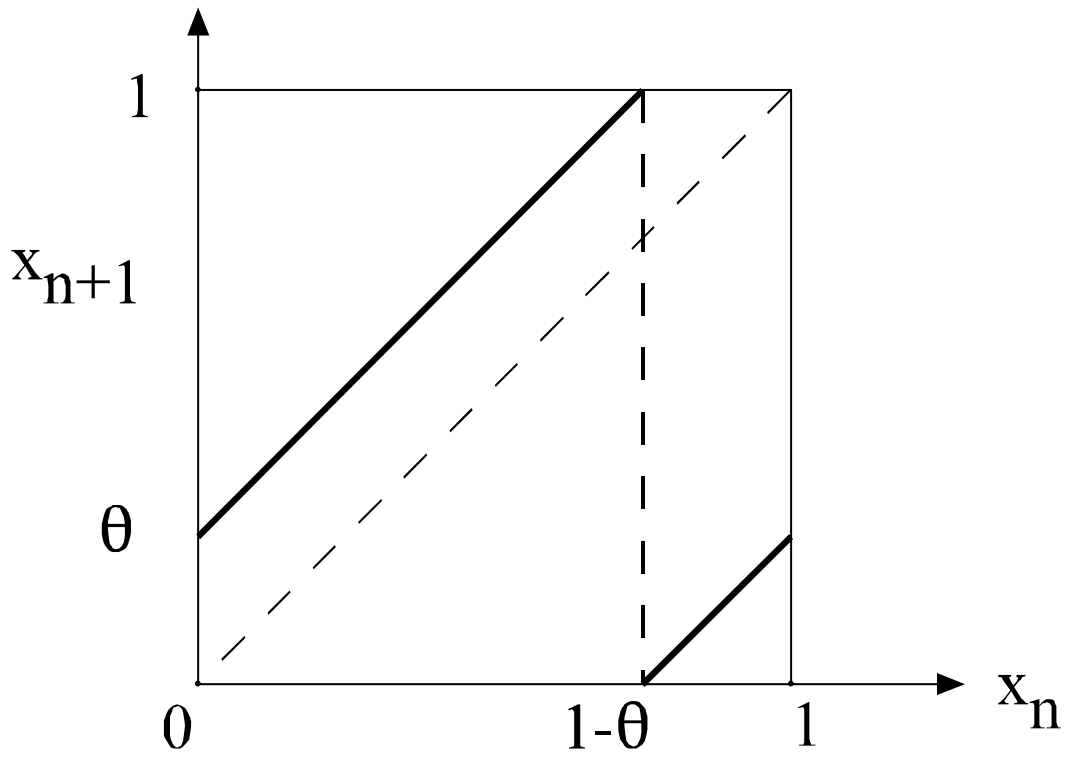
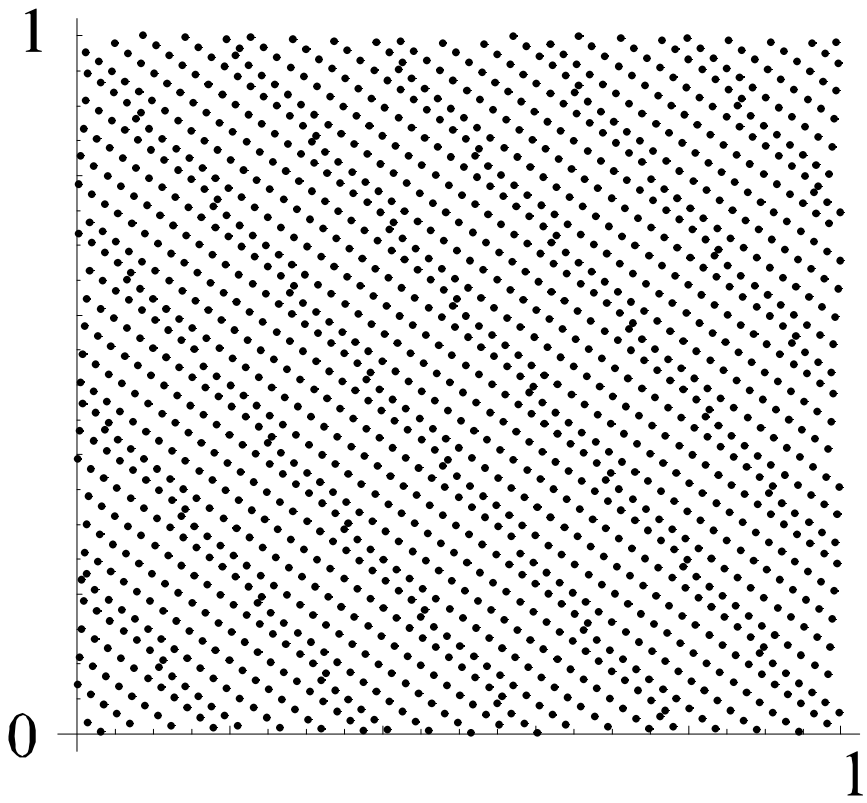


Figure 1: Weyl function



First 1500 Weyl points

Table 9.1: Equidistributed Sequences in 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	$(\{n\,e^{r_1}\},\cdots,\{n\,e^{r_d}\})$, r_j rational and distinct

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

Discrepancy

We want measures of deviation from uniformity for sets of points

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

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

Definition 3 *The star discrepancy D_N^* of the set $X \equiv \{x_1, \cdots, x_N\} \subset [0,1]$ is*

$$D_N^*(X) = \sup_{0 \le t \le 1} |\frac{card([0,t) \cap X)}{N} - t|$$

Definition 4 *If X is a sequence $x_1, x_2, \cdots \subset [0,1]$, then $D_N(X)(D_N^*(X))$ is $D_N(X^N)(D_N^*(X^N))$ where $X^N = \{x_j \in X \mid j = 1, \cdots, N\}$.*

Definition 5 *The star discrepancy D_N^* of the set $X = \{x_1, \cdots, x_N\} \subset I^d$ is*

$$D_N^*(X) = \sup_{0 \le t_1, \cdots t_d \le 1} | \frac{card([0,\, t_1) \times \cdots \times [0, t_d) \cap X)}{N} - \Pi_{j=1}^d t_j|$$

and $D_N^*(X)$ for sequences in I^d is defined as in the case $d = 1$. $D_N(X)$ is generalized similarly from $d = 1$.

- **Small discrepancy sets**
  - On $[0,1]$, the set with minimal D_N and 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):

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

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

    $$\begin{aligned} D_N &< \frac{d}{N^2} + \frac{1}{N} \prod_{j=1}^{d} \left(\frac{p_j - 1}{2\log p_j} \log N + \frac{p_j + 1}{2} \right) \qquad (9.2.4) \\ &\sim \frac{(\log N)^d}{N} \le \mathcal{O}\left(N^{-1+\varepsilon}\right) \end{aligned}$$

  - Bound not good for moderate N and large d.

Theorem 6 *The total variation of f, $V(f)$, on $[0,1]$ is*

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

Theorem 7 *(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 8 *(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 $O\left(N^{-1/d}\right)$, not as good as some other sets with discrepancy $\mathcal{O}\left(N^{-1+\varepsilon}\right)$

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

N(1000s)	MC	Weyl	Haber	Niederreiter
d = 10:				
1	1(-3)	3(-4)	4(-4)	4(-4)
10	2(-4)	6(-5)	1(-3)	3(-5)
100	1(-3)	7(-6)	2(-4)	2(-6)
1000	4(-5)	6(-7)	2(-4)	2(-7)
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)

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

N(1000s)	MC	Weyl	Haber	Niederreiter
d = 10:				
1	1(-2)	6(-2)	8(-2)	9(-3)
10	3(-2)	8(-3)	5(-3)	5(-4)
100	9(-3)	2(-3)	1(-3)	6(-4)
1000	2(-3)	3(-5)	6(-3)	2(-4)
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

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

  - Error analysis: error is approximation, and

$$\begin{aligned}
&\tfrac{1}{N} \textstyle\sum_{n=1}^{N} \tfrac{1}{2}(e^{2\pi i n\alpha} + e^{-2\pi i n\alpha}) \\
&= \tfrac{1}{2N} \textstyle\sum_{n=1}^{N} \left(e^{2\pi i\alpha}\right)^n + \tfrac{1}{2N} \textstyle\sum_{n=1}^{N} \left(e^{-2\pi i\alpha}\right)^n \\
&\le \tfrac{1}{2N} \left(\left| \tfrac{e^{2\pi i N\alpha} - 1}{e^{2\pi i\alpha} - 1} \right| + \left| \tfrac{e^{-2\pi i N\alpha} - 1}{e^{-2\pi i\alpha} - 1} \right| \right) \qquad (9.3.1) \\
&\le \tfrac{1}{2N} \left(\tfrac{2}{|e^{2\pi i\alpha} - 1|} + \tfrac{2}{|e^{-2\pi i\alpha} - 1|} \right) \le \tfrac{C}{N}
\end{aligned}$$

    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 $e^{2\pi i k x}$ terms; can be generalized to arbitrary Fourier series.

- The following theorem summarizes results reported in book.

Theorem 9 *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 $f \in \mathcal{C}^k$ 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
    $$\hat{I} \equiv \frac{1}{m}\sum_{j=1}^{m} Q(f;\beta_j) \tag{9.5.2}$$
    is an unbiased estimator of $I(f)$ with standard error $\sigma_{\hat{I}}$ approximated by
    $$\hat{\sigma}^2_{\hat{I}} \equiv \frac{\sum_{j=1}^{m}(Q(f;\beta_j) - \hat{I})^2}{m-1} \tag{9.5.3}$$
- Example: Random shifts to Weyl rules, because if x_j is equidistributed on $[0,1]$, then so is $x_j + \beta$ for any random β.

Conclusion

- *All* sampling methods use deterministic sequences
- Probability theory does not apply to *any* practical sampling scheme
- Pseudorandom schemes seem to have $O\left(N^{-1/2}\right)$ convergence; this is proven for LCM
- There are $O\left(N^{-1}\right)$ 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