

# WE246: Random Number Generation A Practitioner's Overview

Prof. Michael Mascagni

Department of Computer Science  
Department of Mathematics  
Department of Scientific Computing  
Florida State University, Tallahassee, FL 32306 **USA**

E-mail: [mascagni@fsu.edu](mailto:mascagni@fsu.edu) or [mascagni@math.ethz.ch](mailto:mascagni@math.ethz.ch)

URL: <http://www.cs.fsu.edu/~mascagni>

Research supported by ARO, DOE/ASCI, NATO, and NSF



# Outline of the Talk

- 1 Types of random numbers and Monte Carlo Methods
- 2 Pseudorandom number generation
  - Types of pseudorandom numbers
  - Properties of these pseudorandom numbers
  - Parallelization of pseudorandom number generators
- 3 Quasirandom number generation
  - The Koksma-Hlawka inequality
  - Discrepancy
  - The van der Corput sequence
  - Methods of quasirandom number generation
  - Randomization and Derandomization
- 4 Conclusions

# Outline of the Talk

- 1 Types of random numbers and Monte Carlo Methods
- 2 Pseudorandom number generation
  - Types of pseudorandom numbers
  - Properties of these pseudorandom numbers
  - Parallelization of pseudorandom number generators
- 3 Quasirandom number generation
  - The Koksma-Hlawka inequality
  - Discrepancy
  - The van der Corput sequence
  - Methods of quasirandom number generation
  - Randomization and Derandomization
- 4 Conclusions



# Outline of the Talk

- 1 Types of random numbers and Monte Carlo Methods
- 2 Pseudorandom number generation
  - Types of pseudorandom numbers
  - Properties of these pseudorandom numbers
  - Parallelization of pseudorandom number generators
- 3 Quasirandom number generation
  - The Koksma-Hlawka inequality
  - Discrepancy
  - The van der Corput sequence
  - Methods of quasirandom number generation
  - Randomization and Derandomization
- 4 Conclusions

# Outline of the Talk

- 1 Types of random numbers and Monte Carlo Methods
- 2 Pseudorandom number generation
  - Types of pseudorandom numbers
  - Properties of these pseudorandom numbers
  - Parallelization of pseudorandom number generators
- 3 Quasirandom number generation
  - The Koksma-Hlawka inequality
  - Discrepancy
  - The van der Corput sequence
  - Methods of quasirandom number generation
  - Randomization and Derandomization
- 4 Conclusions

# Monte Carlo Methods: Numerical Experimental that Use Random Numbers

- A Monte Carlo method is any process that consumes random numbers
- ① Each calculation is a numerical experiment
  - Subject to known and unknown sources of error
  - Should be reproducible by peers
  - Should be easy to run anew with results that can be combined to reduce the variance
- ② Sources of errors must be controllable/isolatable
  - Programming/science errors under your control
  - Make possible RNG errors approachable
- ③ Reproducibility
  - Must be able to rerun a calculation with the same numbers
  - Across different machines (modulo arithmetic issues)
  - Parallel and distributed computers?

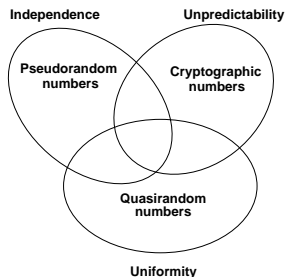


# What are Random Numbers Used For?

- 1 Random numbers are used extensively in simulation, statistics, and in *Monte Carlo* computations
  - Simulation: use random numbers to “randomly pick” event outcomes based on statistical or experiential data
  - Statistics: use random numbers to generate data with a particular distribution to calculate statistical properties (when analytic techniques fail)
- 2 There are many Monte Carlo applications of great interest
  - Numerical quadrature “all Monte Carlo is integration”
  - Quantum mechanics: Solving Schrödinger’s equation with Green’s function Monte Carlo via random walks
  - Mathematics: Using the Feynman-Kac/path integral methods to solve partial differential equations with random walks
  - Defense: neutronics, nuclear weapons design
  - Finance: options, mortgage-backed securities

## What are Random Numbers Used For?

- 3 There are many types of random numbers
- “Real” random numbers: uses a ‘physical source’ of randomness
  - Pseudorandom numbers: deterministic sequence that passes tests of randomness
  - Quasirandom numbers: well distributed (low discrepancy) points





# Why Monte Carlo?

- 1 Rules of thumb for Monte Carlo methods
  - Good for computing linear functionals of solution (linear algebra, PDEs, integral equations)
  - No discretization error but sampling error is  $O(N^{-1/2})$
  - High dimensionality is favorable, breaks the “curse of dimensionality”
  - Appropriate where high accuracy is not necessary
  - Often algorithms are “naturally” parallel
- 2 Exceptions
  - Complicated geometries often easy to deal with
  - Randomized geometries tractable
  - Some applications are insensitive to singularities in solution
  - Sometimes is the fastest high-accuracy algorithm (rare)

# The Classic Monte Carlo Application: Numerical Integration

- 1 Consider computing  $I = \int_0^1 f(x) dx$
- 2 Conventional quadrature methods:

$$I \approx \sum_{i=1}^N w_i f(x_i)$$

- *Rectangle*:  $w_i = \frac{1}{N}$ ,  $x_i = \frac{i}{N}$
- *Trapezoidal*:  $w_i = \frac{2}{N}$ ,  $w_1 = w_N = \frac{1}{N}$ ,  $x_i = \frac{i}{N}$

- 3 Monte Carlo quadrature

$$I \approx \frac{1}{N} \sum_{i=1}^N f(x_i), \quad x_i \sim U[0, 1], \text{ i.i.d.}$$

- 4 Big advantage seen in multidimensional integration, consider (s-dimensions):

$$I = \int_{[0,1]^s} f(x_1, \dots, x_s) dx_1 \dots dx_s$$



# The Classic Monte Carlo Application: Numerical Integration

- 1 Errors are significantly different, with  $N$  function evaluations we see the curse of dimensionality
  - *Product trapezoidal rule: Error =  $O(N^{-2/s})$*
  - *Monte Carlo: Error =  $O(N^{-1/2})$  (indep. of  $s$ !!)*
- 2 Note: the errors are deterministic for the trapezoidal rule whereas the MCM error is a variance bound
- 3 For  $s = 1$ ,  $E[f(x_i)] = I$  when  $x_i \sim U[0, 1]$ , so  
 $E[\frac{1}{N} \sum_{i=1}^N f(x_i)] = I$ , and  $Var[\frac{1}{N} \sum_{i=1}^N f(x_i)] = Var[f(x_i)]/N$ .  
 $Var[f(x_i)] = \int_0^1 (f(x) - I)^2 dx$



# Pseudorandom Numbers

- Pseudorandom numbers mimic the properties of 'real' random numbers
- A.** Pass statistical tests
- B.** Reduce error is  $O(N^{-\frac{1}{2}})$  in Monte Carlo
  - Some common pseudorandom number generators (RNG):
    - 1 Linear congruential:  $x_n = ax_{n-1} + c \pmod{m}$
    - 2 Implicit inversive congruential:  $x_n = a\overline{x_{n-1}} + c \pmod{p}$
    - 3 Explicit inversive congruential:  $x_n = a\overline{n} + c \pmod{p}$
    - 4 Shift register:  $y_n = y_{n-s} + y_{n-r} \pmod{2}$ ,  $r > s$
    - 5 Additive lagged-Fibonacci:  $z_n = z_{n-s} + z_{n-r} \pmod{2^k}$ ,  $r > s$
    - 6 Combined:  $w_n = y_n + z_n \pmod{p}$
    - 7 Multiplicative lagged-Fibonacci:  $x_n = x_{n-s} \times x_{n-r} \pmod{2^k}$ ,  $r > s$

# Pseudorandom Numbers

- Some properties of pseudorandom number generators, integers:  $\{x_n\}$  from modulo  $m$  recursion, and  $U[0, 1], z_n = \frac{x_n}{m}$ 
  - A. Should be a purely periodic sequence (e.g.: DES and IDEA are not provably periodic)
  - B. Period length:  $\text{Per}(x_n)$  should be large
  - C. Cost per bit should be moderate (not cryptography)
  - D. Should be based on theoretically solid and empirically tested recursions
  - E. Should be a totally reproducible sequence



# Pseudorandom Numbers

- Some common facts (rules of thumb) about pseudorandom number generators:
  - 1 Recursions modulo a power-of-two are cheap, but have simple structure
  - 2 Recursions modulo a prime are more costly, but have higher quality: use Mersenne primes:  $2^p - 1$ , where  $p$  is prime, too
  - 3 Shift-registers (Mersenne Twisters) are efficient and have good quality
  - 4 Lagged-Fibonacci generators are efficient, but have some structural flaws
  - 5 Combining generators is ‘provably good’
  - 6 Modular inversion is very costly
  - 7 All linear recursions ‘fall in the planes’
  - 8 Inversive (nonlinear) recursions ‘fall on hyperbolas’



## Periods of Pseudorandom Number Generators

- 1 Linear congruential:  $x_n = ax_{n-1} + c \pmod{m}$ ,  
 $\text{Per}(x_n) = m - 1$ ,  $m$  prime, with  $m$  a power-of-two,  
 $\text{Per}(x_n) = 2^k$ , or  $\text{Per}(x_n) = 2^{k-2}$  if  $c = 0$
- 2 Implicit inversive congruential:  $x_n = a\overline{x_{n-1}} + c \pmod{p}$ ,  
 $\text{Per}(x_n) = p$
- 3 Explicit inversive congruential:  $x_n = a\overline{n} + c \pmod{p}$ ,  
 $\text{Per}(x_n) = p$
- 4 Shift register:  $y_n = y_{n-s} + y_{n-r} \pmod{2}$ ,  $r > s$ ,  
 $\text{Per}(y_n) = 2^r - 1$
- 5 Additive lagged-Fibonacci:  $z_n = z_{n-s} + z_{n-r}$   
 $\pmod{2^k}$ ,  $r > s$ ,  $\text{Per}(z_n) = (2^r - 1)2^{k-1}$
- 6 Combined:  $w_n = y_n + z_n \pmod{p}$ ,  
 $\text{Per}(w_n) = \text{lcm}(\text{Per}(y_n), \text{Per}(z_n))$
- 7 Multiplicative lagged-Fibonacci:  $x_n = x_{n-s} \times x_{n-r}$   
 $\pmod{2^k}$ ,  $r > s$ ,  $\text{Per}(x_n) = (2^r - 1)2^{k-3}$



## Combining RNGs

- There are many methods to combine two streams of random numbers,  $\{x_n\}$  and  $\{y_n\}$ , where the  $x_n$  are integers modulo  $m_x$ , and  $y_n$ 's modulo  $m_y$ :
  - 1 Addition modulo one:  $z_n = \frac{x_n}{m_x} + \frac{y_n}{m_y} \pmod{1}$
  - 2 Addition modulo either  $m_x$  or  $m_y$
  - 3 Multiplication and reduction modulo either  $m_x$  or  $m_y$
  - 4 Exclusive "or-ing"
- Rigorously provable that linear combinations produce combined streams that are "no worse" than the worst
- Tony Warnock: all the above methods seem to do about the same



# Splitting RNGs for Use In Parallel

- We consider splitting a single PRNG:
  - Assume  $\{x_n\}$  has  $\text{Per}(x_n)$
  - Has the fast-leap ahead property: leaping  $L$  ahead costs no more than generating  $O(\log_2(L))$  numbers
- Then we associate a single block of length  $L$  to each parallel subsequence:

## 1 Blocking:

- First block:  $\{x_0, x_1, \dots, x_{L-1}\}$
- Second :  $\{x_L, x_{L+1}, \dots, x_{2L-1}\}$
- $i$ th block:  $\{x_{(i-1)L}, x_{(i-1)L+1}, \dots, x_{iL-1}\}$

## 2 The Leap Frog Technique: define the leap ahead of

$$\ell = \left\lfloor \frac{\text{Per}(x_i)}{L} \right\rfloor:$$

- First block:  $\{x_0, x_\ell, x_{2\ell}, \dots, x_{(L-1)\ell}\}$
- Second block:  $\{x_1, x_{1+\ell}, x_{1+2\ell}, \dots, x_{1+(L-1)\ell}\}$
- $i$ th block:  $\{x_i, x_{i+\ell}, x_{i+2\ell}, \dots, x_{i+(L-1)\ell}\}$



## Splitting RNGs for Use In Parallel

- 3 The Lehmer Tree, designed for splitting LCGs:
  - Define a right and left generator:  $R(x)$  and  $L(x)$
  - The right generator is used within a process
  - The left generator is used to spawn a new PRNG stream
  - Note:  $L(x) = R^W(x)$  for some  $W$  for **all**  $x$  for an LCG
  - Thus, spawning is just jumping a fixed,  $W$ , amount in the sequence
- 4 Recursive Halving Leap-Ahead, use fixed points or fixed leap aheads:
  - First split leap ahead:  $\left\lfloor \frac{\text{Per}(x_i)}{2} \right\rfloor$
  - $i$ th split leap ahead:  $\left\lfloor \frac{\text{Per}(x_i)}{2^{i+1}} \right\rfloor$
  - This permits effective user of all remaining numbers in  $\{x_n\}$  without the need for *a priori* bounds on the stream length  $L$



# Generic Problems Parallelizing via Splitting

- 1 Splitting for parallelization is not scalable:
  - It usually costs  $O(\log_2(\text{Per}(x_i)))$  bit operations to generate a random number
  - For parallel use, a given computation that requires  $L$  random numbers per process with  $P$  processes must have  $\text{Per}(x_i) = O((LP)^e)$
  - Rule of thumb: never use more than  $\sqrt{\text{Per}(x_i)}$  of a sequence  $\rightarrow e = 2$
  - Thus cost per random number is not constant with number of processors!!



## Generic Problems Parallelizing via Splitting

- 2 Correlations within sequences are generic!!
  - Certain offsets within any modular recursion will lead to extremely high correlations
  - Splitting in any way converts auto-correlations to cross-correlations between sequences
  - Therefore, splitting generically leads to interprocessor correlations in PRNGs



# New Results in Parallel RNGs: Using Distinct Parameterized Streams in Parallel

- 1 Default generator: additive lagged-Fibonacci,  
$$x_n = x_{n-s} + x_{n-r} \pmod{2^k}, r > s$$
  - Very efficient: 1 add & pointer update/number
  - Good empirical quality
  - Very easy to produce distinct parallel streams
- 2 Alternative generator #1: prime modulus LCG,  
$$x_n = ax_{n-1} + c \pmod{m}$$
  - Choice: Prime modulus (quality considerations)
  - Parameterize the multiplier
  - Less efficient than lagged-Fibonacci
  - Provably good quality
  - Multiprecise arithmetic in initialization



## New Results in Parallel RNGs: Using Distinct Parameterized Streams in Parallel

- 3 Alternative generator #2: power-of-two modulus LCG,  
 $x_n = ax_{n-1} + c \pmod{2^k}$
- Choice: Power-of-two modulus (efficiency considerations)
  - Parameterize the prime additive constant
  - Less efficient than lagged-Fibonacci
  - Provably good quality
  - Must compute as many primes as streams



## Parameterization Based on Seeding

- Consider the Lagged-Fibonacci generator:

$$x_n = x_{n-5} + x_{n-17} \pmod{2^{32}} \text{ or in general:}$$

$$x_n = x_{n-s} + x_{n-r} \pmod{2^k}, r > s$$

- The seed is 17 32-bit integers; 544 bits, longest possible period for this linear generator is  $2^{17 \times 32} - 1 = 2^{544} - 1$
- Maximal period is  $\text{Per}(x_n) = (2^{17} - 1) \times 2^{31}$
- Period is maximal  $\iff$  at least one of the 17 32-bit integers is odd
- This seeding failure results in only even “random numbers”
- Are  $(2^{17} - 1) \times 2^{31 \times 17}$  seeds with full period
- Thus there are the following number of full-period equivalence classes (ECs):

$$E = \frac{(2^{17} - 1) \times 2^{31 \times 17}}{(2^{17} - 1) \times 2^{31}} = 2^{31 \times 16} = 2^{496}$$



# The Equivalence Class Structure

With the “standard” l.s.b.,  $b_0$ :

m.s.b.				l.s.b.	
$b_{k-1}$	$b_{k-2}$	...	$b_1$	$b_0$	
□	□	...	0	0	$x_{r-1}$
0	□	...	□	0	$x_{r-2}$
⋮	⋮	⋮	⋮	⋮	
□	0	...	□	0	$x_1$
□	□	...	□	1	$x_0$

or a special  $b_0$  (adjoining 1's):

m.s.b.				l.s.b.	
$b_{k-1}$	$b_{k-2}$	...	$b_1$	$b_0$	
□	□	...	□	$b_{0n-1}$	$x_{r-1}$
□	□	...	□	$b_{0n-2}$	$x_{r-2}$
⋮	⋮	⋮	⋮	⋮	
□	□	...	□	$b_{01}$	$x_1$
0	0	...	0	$b_{00}$	$x_0$





## Parameterization of Prime Modulus LCGs

- Consider only  $x_n = ax_{n-1} \pmod{m}$ , with  $m$  prime has maximal period when  $a$  is a primitive root modulo  $m$
- If  $\alpha$  and  $a$  are primitive roots modulo  $m$  then  $\exists l$  s.t.  $\gcd(l, m-1) = 1$  and  $\alpha \equiv a^l \pmod{m}$
- If  $m = 2^{2^n} + 1$  (Fermat prime) then all odd powers of  $\alpha$  are primitive elements also
- If  $m = 2q + 1$  with  $q$  also prime (Sophie-Germain prime) then all odd powers (save the  $q$ th) of  $\alpha$  are primitive elements



## Parameterization of Prime Modulus LCGs

- Consider  $x_n = ax_{n-1} \pmod{m}$  and  $y_n = a'y_{n-1} \pmod{m}$  and define the full-period exponential-sum cross-correlation between them as:

$$C(j, l) = \sum_{n=0}^{m-1} e^{\frac{2\pi i}{m}(x_n - y_{n-j})}$$

then the Riemann hypothesis over finite-fields implies

$$|C(j, l)| \leq (l-1)\sqrt{m}$$



# Parameterization of Prime Modulus LCGs

- Mersenne modulus: relatively easy to do modular multiplication
- With Mersenne prime modulus,  $m = 2^p - 1$  must compute  $\phi_{m-1}^{-1}(k)$ , the  $k$ th number relatively prime to  $m - 1$
- Can compute  $\phi_{m-1}(x)$  with a variant of the Meissel-Lehmer algorithm fairly quickly:
  - Use partial sieve functions to trade off memory for more than  $2^j$  operations,  $j = \#$  of factors of  $m - 1$
  - Have fast implementation for  $p = 31, 61, 127, 521, 607$



## Parameterization of Power-of-Two Modulus LCGs

- $x_n = ax_{n-1} + c_i \pmod{2^k}$ , here the  $c_i$ 's are distinct primes
- Can prove (Percus and Kalos) that streams have good spectral test properties among themselves
- Best to choose  $c_i \approx \sqrt{2^k} = 2^{k/2}$
- Must enumerate the primes, uniquely, not necessarily exhaustively to get a unique parameterization
- Note: in  $0 \leq i < m$  there are  $\approx \frac{m}{\log_2 m}$  primes via the prime number theorem, thus if  $m \approx 2^k$  streams are required, then must exhaust all the primes modulo  $\approx 2^{k+\log_2 k} = 2^k k = m \log_2 m$
- Must compute distinct primes on the fly either with table or something like Meissel-Lehmer algorithm



## Parameterization of MLFGs

- 1 Recall the MLFG recurrence:  
$$x_n = x_{n-s} \times x_{n-r} \pmod{2^k}, r > s$$
- 2 One of the  $r$  seed elements is even  $\rightarrow$  eventually all become even
- 3 Restrict to only odd numbers in the MLFG seeds
- 4 Allows the following parameterization for odd integers modulo a power-of-two  $x_n = (-1)^{y_n} 3^{z_n} \pmod{2^k}$ , where  $y_n \in \{0, 1\}$  and where
  - $y_n = y_{n-s} + y_{n-r} \pmod{2}$
  - $z_n = z_{n-s} + z_{n-r} \pmod{2^{k-2}}$
- 5 Last recurrence means we can use ALFG parameterization,  $z_n$ , and map to MLFGs via modular exponentiation



# Quality Issues in Serial and Parallel PRNGs

- Empirical tests (more later)
- Provable measures of quality:
  - 1 Full- and partial-period discrepancy (Niederreiter) test  
equidistribution of overlapping  $k$ -tuples
  - 2 Also full- ( $k = \text{Per}(x_n)$ ) and partial-period exponential sums:

$$C(j, k) = \sum_{n=0}^{k-1} e^{\frac{2\pi i}{m}(x_n - x_{n-j})}$$



## Quality Issues in Serial and Parallel PRNGs

- For LCGs and SRGs full-period and partial-period results are similar

$$\triangleright |C(\cdot, \text{Per}(x_n))| < O(\sqrt{\text{Per}(x_n)})$$

$$\triangleright |C(\cdot, j)| < O(\sqrt{\text{Per}(x_n)})$$

- Additive lagged-Fibonacci generators have poor provable results, yet empirical evidence suggests

$$|C(\cdot, \text{Per}(x_n))| < O(\sqrt{\text{Per}(x_n)})$$



# Parallel Neutronics: A Difficult Example

- 1 The structure of parallel neutronics
  - Use a parallel queue to hold unfinished work
  - Each processor follows a distinct neutron
  - Fission event places a new neutron(s) in queue with initial conditions
- 2 Problems and solutions
  - Reproducibility: each neutron is queued with a new generator (and with the next generator)
  - Using the binary tree mapping prevents generator reuse, even with extensive branching
  - A global seed reorders the generators to obtain a statistically significant new but reproducible result





# Many Parameterized Streams Facilitate Implementation/Use

- 1 Advantages of using parameterized generators
  - Each unique parameter value gives an “independent” stream
  - Each stream is uniquely numbered
  - Numbering allows for absolute reproducibility, even with MIMD queuing
  - Effective serial implementation + enumeration yield a portable scalable implementation
  - Provides theoretical testing basis



# Many Parameterized Streams Facilitate Implementation/Use

- 2 Implementation details
  - Generators mapped canonically to a binary tree
  - Extended seed data structure contains current seed and next generator
  - Spawning uses new next generator as starting point: assures no reuse of generators
- 3 All these ideas in the **Scalable Parallel Random Number Generators (SPRNG) library**: <http://sprng.org>



# Many Different Generators and A Unified Interface

- 1 Advantages of having more than one generator
  - An application exists that stumbles on a given generator
  - Generators based on different recursions allow comparison to rule out spurious results
  - Makes the generators real experimental tools
- 2 Two interfaces to the `SPRNG` library: simple and default
  - Initialization returns a pointer to the generator state:  
`init_SPRNG()`
  - Single call for new random number: `SPRNG()`
  - Generator type chosen with parameters in `init_SPRNG()`
  - Makes changing generator very easy
  - Can use more than one generator *type* in code
  - Parallel structure is extensible to new generators through dummy routines



# Quasirandom Numbers

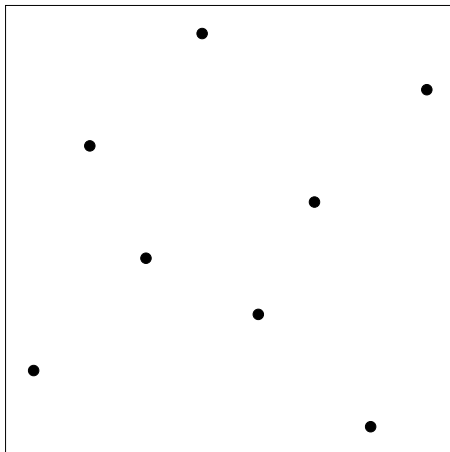
- Many problems require uniformity, not randomness: “quasirandom” numbers are highly uniform deterministic sequences with small *star discrepancy*
- **Definition:** The *star discrepancy*  $D_N^*$  of  $x_1, \dots, x_N$ :

$$\begin{aligned} D_N^* &= D_N^*(x_1, \dots, x_N) \\ &= \sup_{0 \leq u \leq 1} \left| \frac{1}{N} \sum_{n=1}^N \chi_{[0,u)}(x_n) - u \right|, \end{aligned}$$

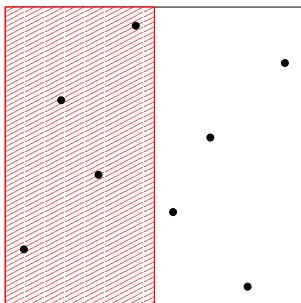
where  $\chi$  is the characteristic function



# Star Discrepancy in 2D



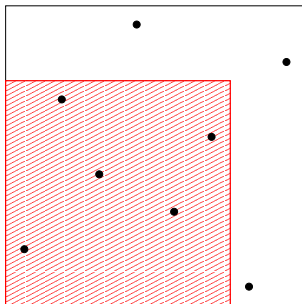
## Star Discrepancy in 2D



•  $\left| \frac{1}{2} - \frac{4}{8} \right| = 0$

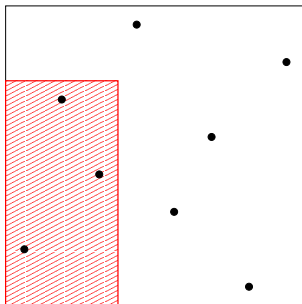
- 
- 
-

## Star Discrepancy in 2D



- $\left| \frac{1}{2} - \frac{4}{8} \right| = 0$
- $\left| \frac{9}{16} - \frac{5}{8} \right| = \frac{1}{16} = 0.0625$
- 
-

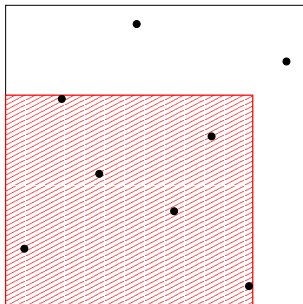
## Star Discrepancy in 2D



- $\left| \frac{1}{2} - \frac{4}{8} \right| = 0$
- $\left| \frac{9}{16} - \frac{5}{8} \right| = \frac{1}{16} = 0.0625$
- $\left| \frac{9}{32} - \frac{3}{8} \right| = \frac{3}{32} = 0.09375$
-



## Star Discrepancy in 2D



- $\left| \frac{1}{2} - \frac{4}{8} \right| = 0$
- $\left| \frac{9}{16} - \frac{5}{8} \right| = \frac{1}{16} = 0.0625$
- $\left| \frac{9}{32} - \frac{3}{8} \right| = \frac{3}{32} = 0.09375$
- $\left| \frac{143}{256} - \frac{6}{8} \right| = \frac{49}{256} \approx 0.19140625$

# Quasirandom Numbers

- **Theorem** (Koksma, 1942): if  $f(x)$  has bounded variation  $V(f)$  on  $[0, 1]$  and  $x_1, \dots, x_N \in [0, 1]$  with star discrepancy  $D_N^*$ , then:

$$\left| \frac{1}{N} \sum_{n=1}^N f(x_n) - \int_0^1 f(x) dx \right| \leq V(f) D_N^*,$$

this is the Koksma-Hlawka inequality

- Note: Many different types of discrepancies are definable



## Discrepancy Facts

- Real random numbers have (the law of the iterated logarithm):

$$D_N^* = O(N^{-1/2}(\log \log N)^{-1/2})$$

- Klaus F. Roth (Fields medalist in 1958) proved the following lower bound in 1954 for the star discrepancy of  $N$  points in  $s$  dimensions:

$$D_N^* \geq O(N^{-1}(\log N)^{\frac{s-1}{2}})$$

- Sequences (indefinite length) and point sets have different "best discrepancies" at present
  - Sequence:  $D_N^* \leq O(N^{-1}(\log N)^{s-1})$
  - Point set:  $D_N^* \leq O(N^{-1}(\log N)^{s-2})$



## Some Types of Quasirandom Numbers

- Must choose point sets (finite #) or sequences (infinite #) with small  $D_N^*$
- Often used is the *van der Corput sequence* in base  $b$ :  
 $x_n = \Phi_b(n - 1)$ ,  $n = 1, 2, \dots$ , where for  $b \in \mathbb{Z}$ ,  $b \geq 2$ :

$$\Phi_b \left( \sum_{j=0}^{\infty} a_j b^j \right) = \sum_{j=0}^{\infty} a_j b^{-j-1} \quad \text{with}$$
$$a_j \in \{0, 1, \dots, b - 1\}$$



## Some Types of Quasirandom Numbers

- For the van der Corput sequence

$$ND_N^* \leq \frac{\log N}{3 \log 2} + O(1)$$

- With  $b = 2$ , we get  $\{\frac{1}{2}, \frac{1}{4}, \frac{3}{4}, \frac{1}{8}, \frac{5}{8}, \frac{3}{8}, \frac{7}{8} \dots\}$
- With  $b = 3$ , we get  $\{\frac{1}{3}, \frac{2}{3}, \frac{1}{9}, \frac{4}{9}, \frac{7}{9}, \frac{2}{9}, \frac{5}{9}, \frac{8}{9} \dots\}$

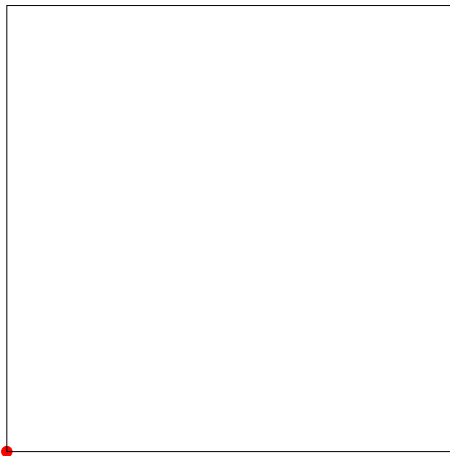


## Some Types of Quasirandom Numbers

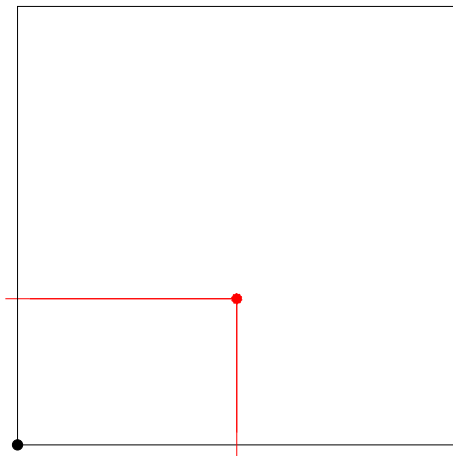
- Other small  $D_N^*$  points sets and sequences:
  - 1 Halton sequence:  $\mathbf{x}_n = (\Phi_{b_1}(n-1), \dots, \Phi_{b_s}(n-1))$ ,  
 $n = 1, 2, \dots$ ,  $D_N^* = O(N^{-1}(\log N)^s)$  if  $b_1, \dots, b_s$  pairwise relatively prime
  - 2 Hammersley point set:  
 $\mathbf{x}_n = (\frac{n-1}{N}, \Phi_{b_1}(n-1), \dots, \Phi_{b_{s-1}}(n-1))$ ,  $n = 1, 2, \dots, N$ ,  
 $D_N^* = O(N^{-1}(\log N)^{s-1})$  if  $b_1, \dots, b_{s-1}$  are pairwise relatively prime



# Halton sequence: example

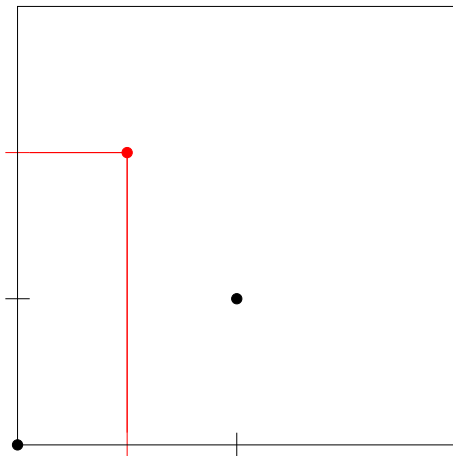


# Halton sequence: example

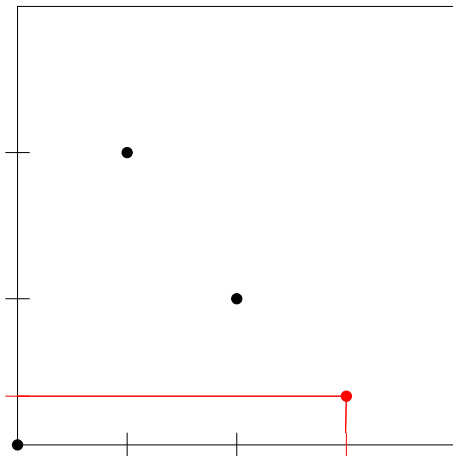




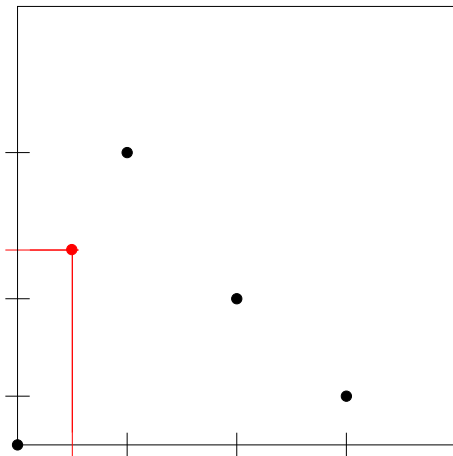
# Halton sequence: example



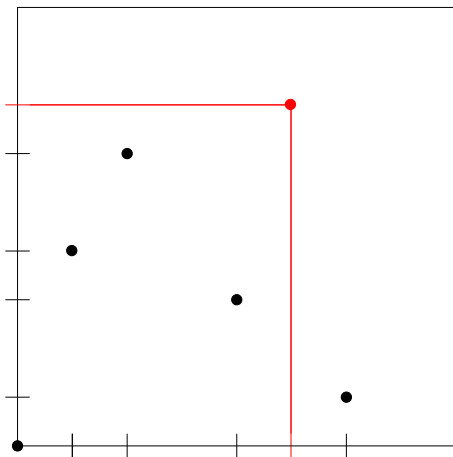
# Halton sequence: example



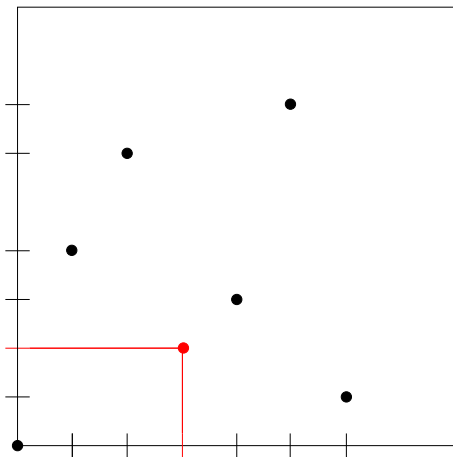
# Halton sequence: example



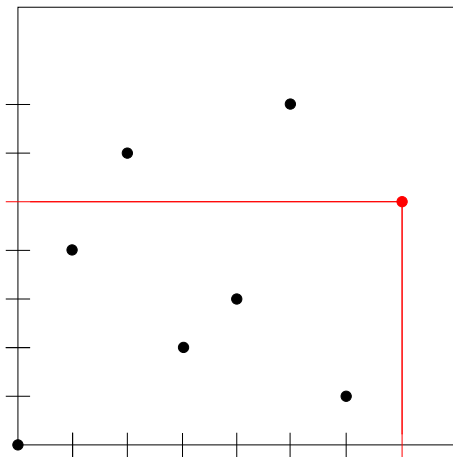
# Halton sequence: example



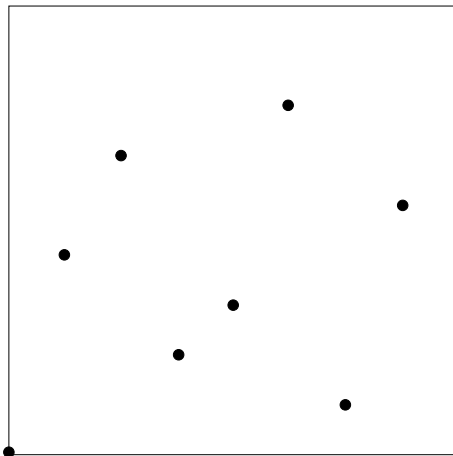
# Halton sequence: example



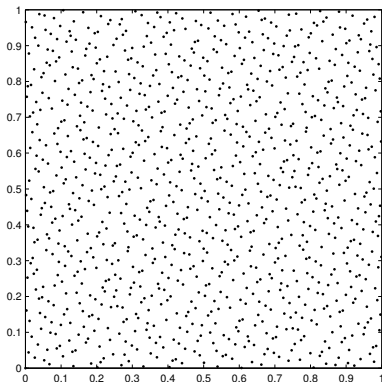
# Halton sequence: example



# Halton sequence: example

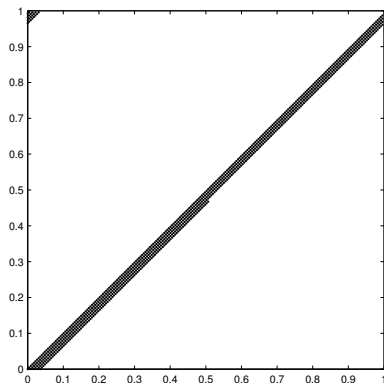
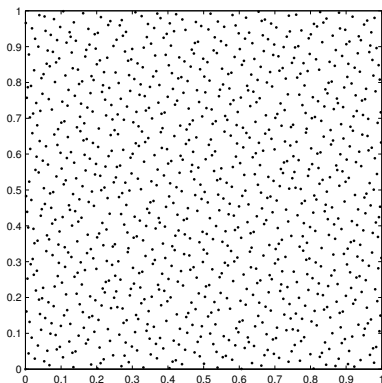


# Good Halton points vs poor Halton points





# Good Halton points vs poor Halton points



## Some Types of Quasirandom Numbers

- ③ Ergodic dynamics:  $\mathbf{x}_n = \{n\alpha\}$ , where  $\alpha = (\alpha_1, \dots, \alpha_s)$  is irrational and  $\alpha_1, \dots, \alpha_s$  are linearly independent over the rationals then for almost all  $\alpha \in \mathbb{R}^s$ ,  
 $D_N^* = O(N^{-1}(\log N)^{s+1+\epsilon})$  for all  $\epsilon > 0$
- ④ Other methods of generation
  - Method of good lattice points (Sloan and Joe)
  - Sobol' sequences
  - Faure sequences (more later)
  - Niederreiter sequences



## Continued-Fractions and Irrationals

Infinite continued-fraction expansion for choosing good irrationals:

$$r = a_0 + \frac{1}{a_1 + \frac{1}{a_2 + \dots}}$$

$a_i \leq K \rightarrow$  sequence is a low-discrepancy sequence  
Choose all  $a_i = 1$ . Then

$$r = 1 + \frac{1}{1 + \frac{1}{1 + \dots}}$$

is the golden ratio.

0.618, 0.236, 0.854, 0.472, 0.090, ...

Irrational sequence in more dimensions is not a low-discrepancy sequence.

# Lattice

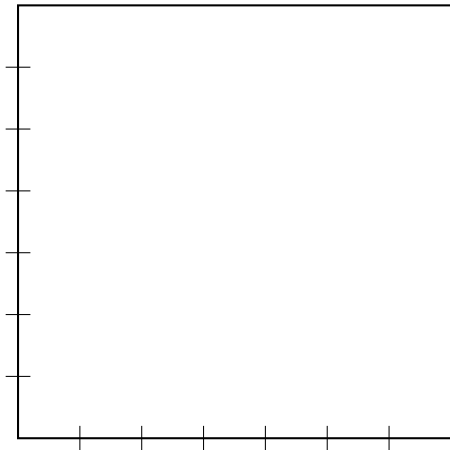
- Fixed  $N$
- Generator vector  $\vec{g} = (g_1, \dots, g_d) \in \mathbb{Z}^d$ .

We define a rank-1 lattice as

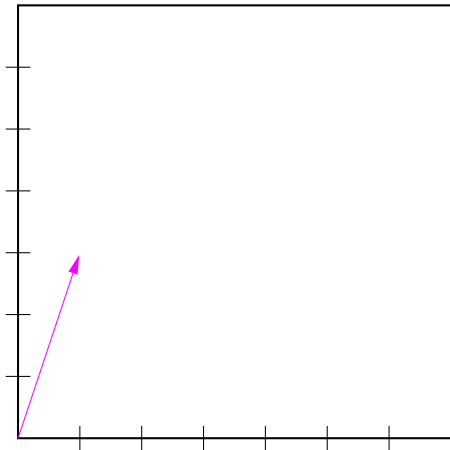
$$P_{\text{lattice}} := \left\{ \vec{x}_i = \frac{i\vec{g}}{N} \bmod 1 \right\}.$$



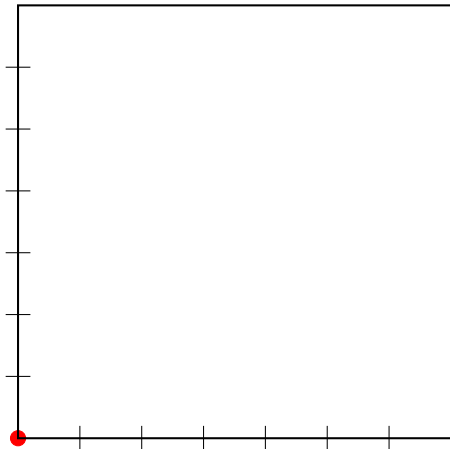
## An example lattice



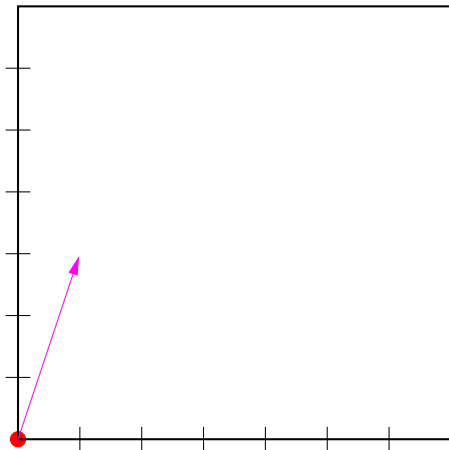
## An example lattice



# An example lattice

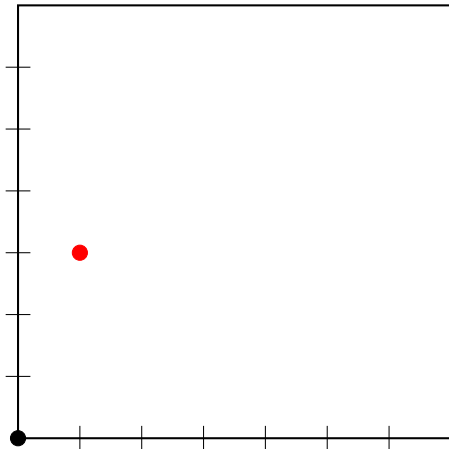


# An example lattice

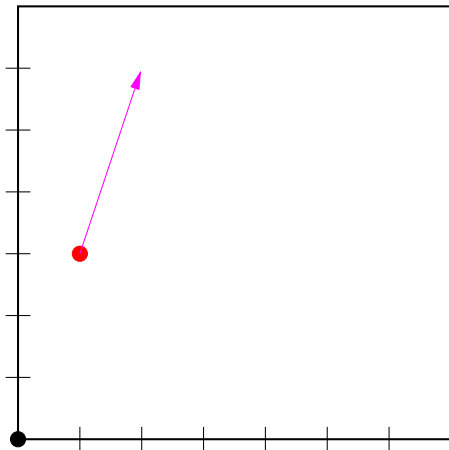




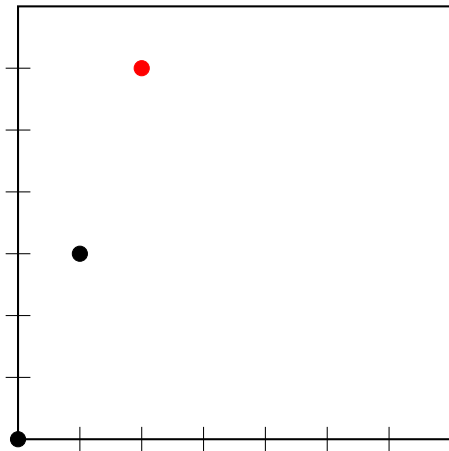
## An example lattice



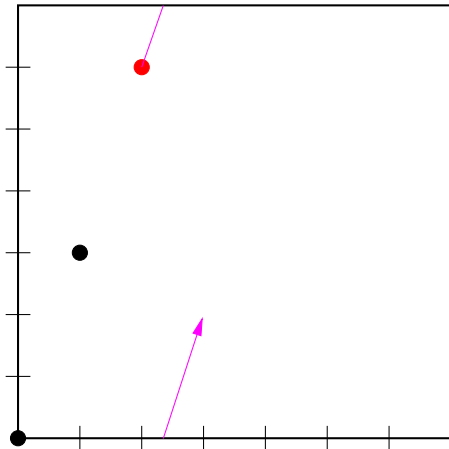
## An example lattice



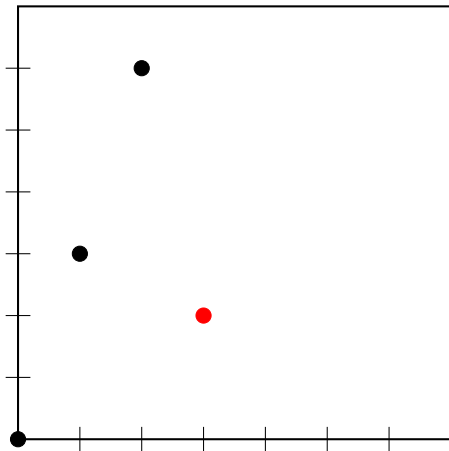
## An example lattice



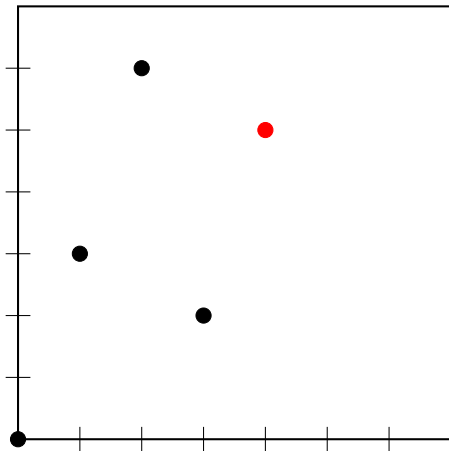
## An example lattice



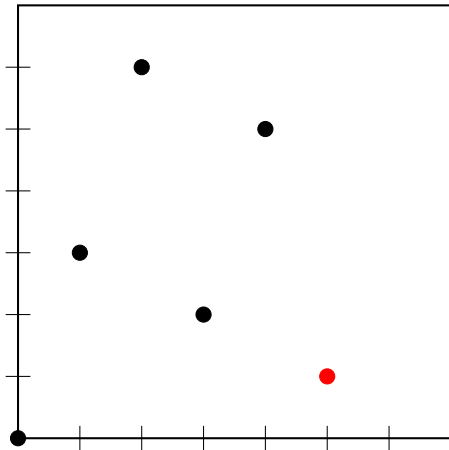
## An example lattice



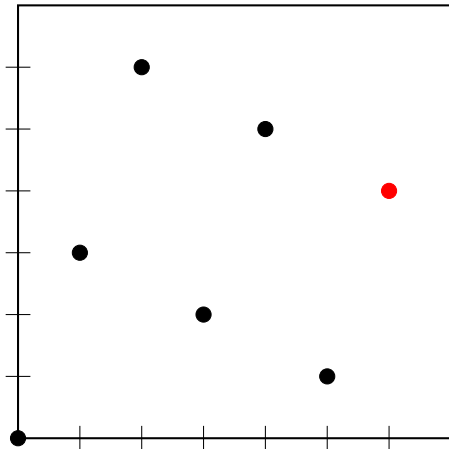
## An example lattice



## An example lattice

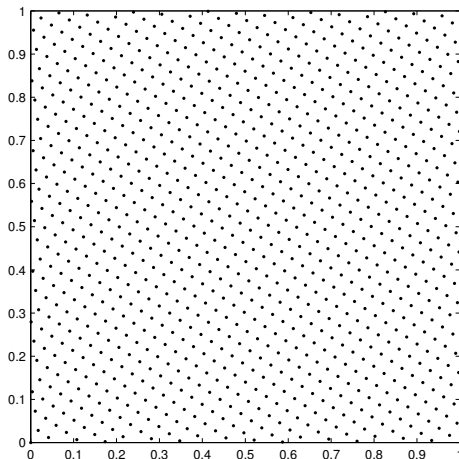


## An example lattice





# Lattice with 1031 points

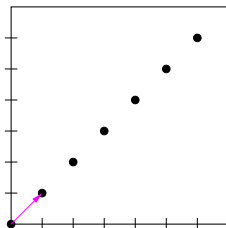


# Lattice

- After  $N$  points the sequence repeats itself,
- Projection on each axe gives the set  $\{\frac{0}{N}, \frac{1}{N}, \dots, \frac{N-1}{N}\}$ .

Not every generator gives a good point set.

E.g.  $g_1 = g_2 = \dots = g_d = 1$ , gives  $\{(\frac{i}{N}, \dots, \frac{i}{N})\}$ .



## Some Types of Quasirandom Numbers

### 1 Another interpretation of the v.d. Corput sequence:

- Define the  $i$ th  $\ell$ -bit “direction number” as:  $v_i = 2^i$  (think of this as a bit vector)
- Represent  $n - 1$  via its base-2 representation  
 $n - 1 = b_{\ell-1}b_{\ell-2} \dots b_1b_0$

- Thus we have
- $$\Phi_2(n - 1) = 2^{-\ell} \bigoplus_{i=0, b_i=1}^{i=\ell-1} v_i$$

### 2 The Sobol' sequence works the same!!

- Use recursions with a primitive binary polynomial define the (dense)  $v_i$
- The Sobol' sequence is defined as:

$$s_n = 2^{-\ell} \bigoplus_{i=0, b_i=1}^{i=\ell-1} v_i$$

- Use Gray-code ordering for speed

## Some Types of Quasirandom Numbers

- $(t, m, s)$ -nets and  $(t, s)$ -sequences and generalized Niederreiter sequences
- ① Let  $b \geq 2$ ,  $s > 1$  and  $0 \leq t \leq m \in \mathbb{Z}$  then a  $b$ -ary box,  $J \subset [0, 1)^s$ , is given by

$$J = \prod_{i=1}^s \left[ \frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right)$$

where  $d_i \geq 0$  and the  $a_i$  are  $b$ -ary digits, note that  
 $|J| = b^{-\sum_{i=1}^s d_i}$

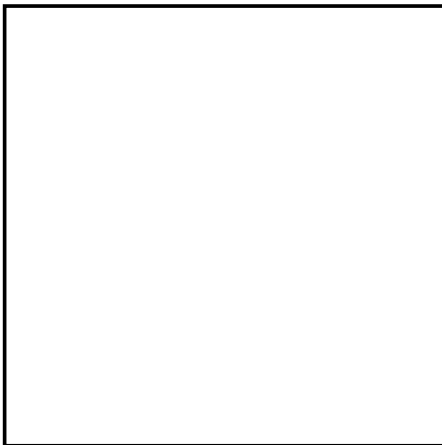


## Some Types of Quasirandom Numbers

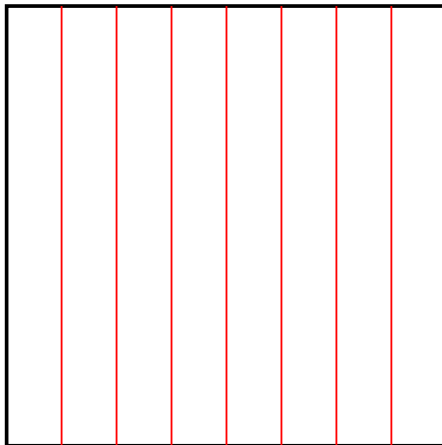
- 2 A set of  $b^m$  points is a  $(t, m, s)$ -net if each  $b$ -ary box of volume  $b^{t-m}$  has exactly  $b^t$  points in it
- 3 Such  $(t, m, s)$ -nets can be obtained via Generalized Niederreiter sequences, in dimension  $j$  of  $s$ :  
 $y_i^{(j)}(n) = C^{(j)} a_i(n)$ , where  $n$  has the  $b$ -ary representation  
 $n = \sum_{k=0}^{\infty} a_k(n) b^k$  and  $x_i^{(j)}(n) = \sum_{k=1}^m y_k^{(j)}(n) q^{-k}$



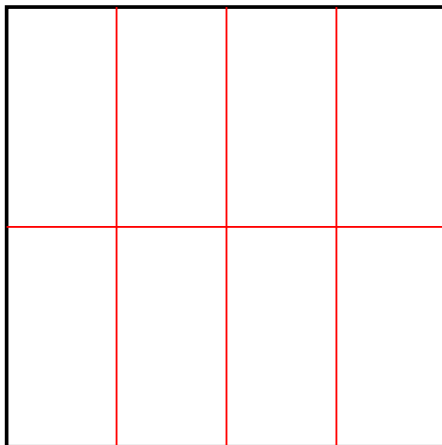
# Nets: Example



# Nets: Example

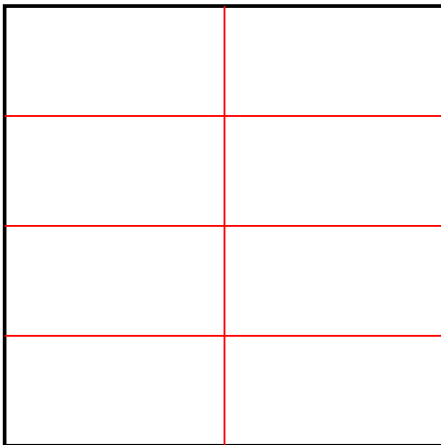


# Nets: Example

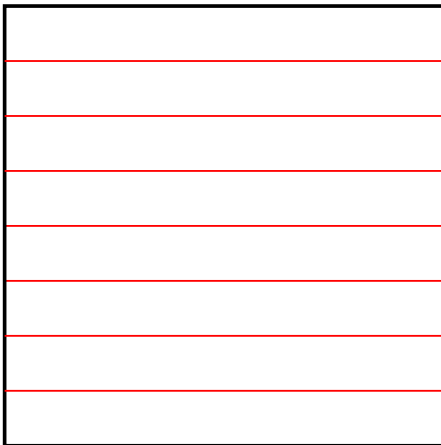




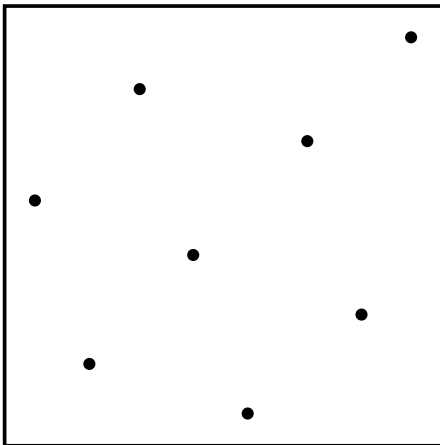
# Nets: Example



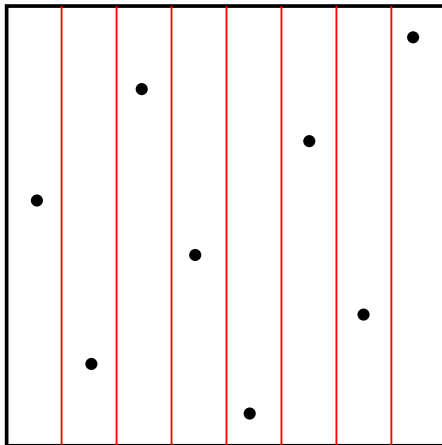
# Nets: Example



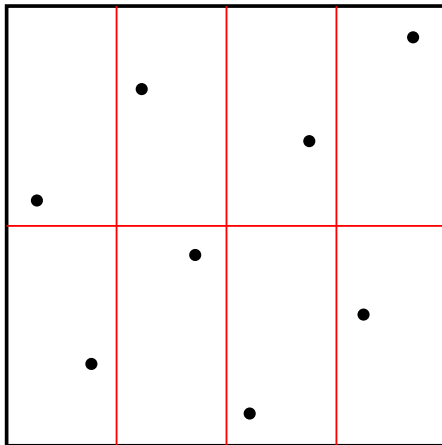
# Nets: Example



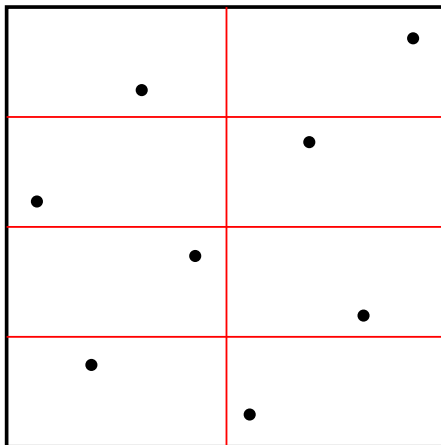
# Nets: Example



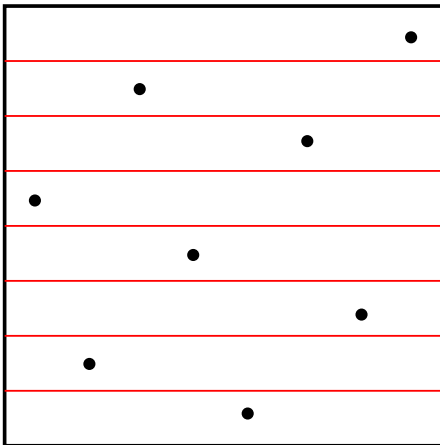
# Nets: Example



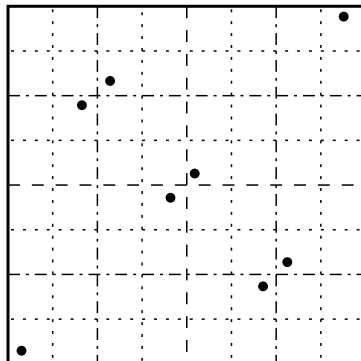
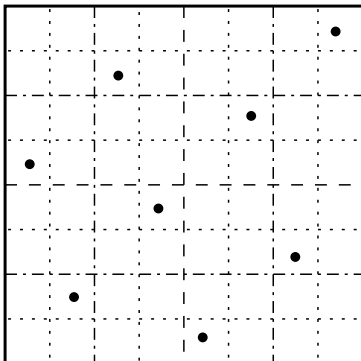
# Nets: Example



# Nets: Example



# Good vs poor net





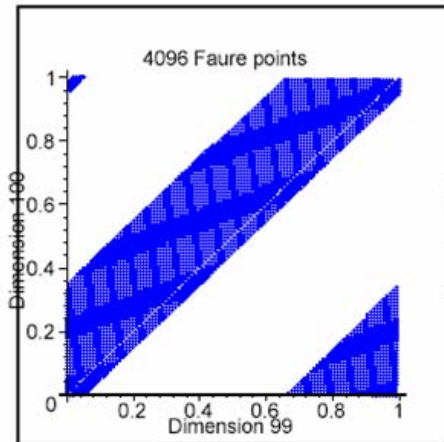
# Randomization of the Faure Sequence

- 1 A problem with all QRNs is that the Koksma-Hlawka inequality provides no practical error estimate
- 2 A solution is to randomize the QRNs and then consider each randomized sequence as providing an independent sample for constructing confidence intervals
- 3 Consider the  $s$ -dimensional Faure series is:  
 $(\phi_p(C^{(0)}(n)), \phi_p(C^{(1)}(n)), \dots, \phi_p(P^{s-1}(n)))$ 
  - $p > s$  is prime
  - $C^{(j-1)}$  is the generator matrix for dimension  $1 \leq j \leq s$
  - For Faure  $C^{(j)} = P^{j-1}$  is the Pascal matrix:  
$$P_{r,k}^{j-1} = \binom{r-1}{k-1} (j-1)^{(r-k)} \pmod{p}$$



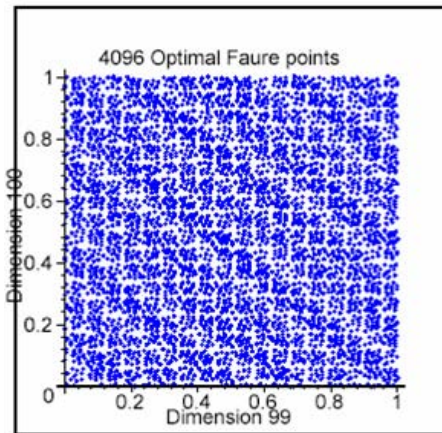
## Another Reason for Randomization

QRNs have inherently bad low-dimensional projections



## Another Reason for Randomization

Randomization (scrambling) helps



# General Randomization Techniques

- 1 Random shifting:  $z_n = x_n + r \pmod{1}$ 
  - $x_n \in [0, 1]^s$  is the original QRN
  - $r \in [0, 1]^s$  is a random point
  - $z_n \in [0, 1]^s$  scrambled point
- 2 Digit permutation
  - Nested scrambling (Owen)
  - Single digit scrambling like linear scrambling
- 3 Randomization of the generator matrices, i.e. Tezuka's  $\text{GFaure}$ ,  $C^{(j)} = A^{(j)} P^{j-1}$  where  $A^j$  is a random nonsingular lower-triangular matrix modulo  $p$

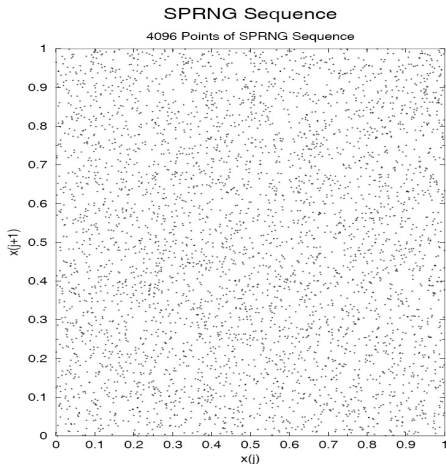


# Derandomization and Applications

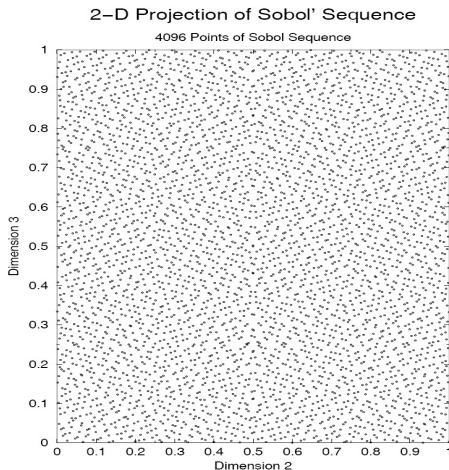
- 1 Given that a randomization leads to a family of QRNs, is there a best?
  - Must make the family small enough to exhaust over, so one uses a small family of permutations like the linear scramblings
  - There must be a quality criterion that is indicative and cheap to evaluate
- 2 Applications of randomization: tractable error bounds, parallel QRNs
- 3 Applications of derandomization: finding more rapidly converging families of QRNs



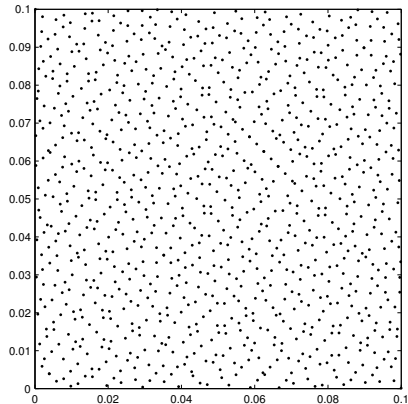
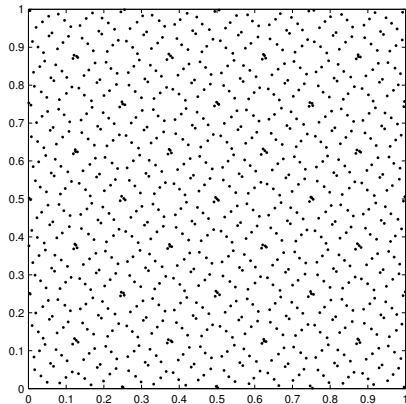
# A Picture is Worth a 1000 Words: 4K Pseudorandom Pairs



# A Picture is Worth a 1000 Words: 4K Quasirandom Pairs



# Sobol' sequence





# Future Work on Random Numbers (not yet completed)

- 1 SPRNG and pseudorandom number generation work
  - New generators: Well, Mersenne Twister
  - Spawn-intensive/small-memory footprint generators: MLFGs
  - C++ implementation
  - Grid-based tools
  - More comprehensive testing suite; improved theoretical tests
  - New version incorporating the completed work

# Future Work on Random Numbers (not yet completed)

## 2 Quasirandom number work




- Scrambling (parameterization) for parallelization
- Optimal scramblings
- Grid-based tools
- Application-based comparison/testing suite
- Comparison to sparse grids
- "QPRNG"

## 3 Commercialization of SPRNG



- FSU-supported startup company
- Commercial licenses and SPRNG consulting
- Funds will support continued development and support
- SPRNG will continue to be free to academic and government researchers



## For Further Reading I

-  [Y. Li and M. Mascagni (2005)]  
Grid-based Quasi-Monte Carlo Applications,  
*Monte Carlo Methods and Applications*, **11**: 39–55.
-  [H. Chi, M. Mascagni and T. Warnock (2005)]  
On the Optimal Halton Sequence,  
*Mathematics and Computers in Simulation*, **70(1)**: 9–21.
-  [M. Mascagni and H. Chi (2004)]  
Parallel Linear Congruential Generators with  
Sophie-Germain Moduli,  
*Parallel Computing*, **30**: 1217–1231.

## For Further Reading II

-  [M. Mascagni and A. Srinivasan (2004)]  
Parameterizing Parallel Multiplicative Lagged-Fibonacci  
Generators,  
*Parallel Computing*, **30**: 899–916.
-  [M. Mascagni and A. Srinivasan (2000)]  
Algorithm 806: SPRNG: A Scalable Library for  
Pseudorandom Number Generation,  
*ACM Transactions on Mathematical Software*, **26**: 436–461.

© Michael Mascagni, 2005-2010