Serial and Parallel Random Number Generation

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Outline of the Talk

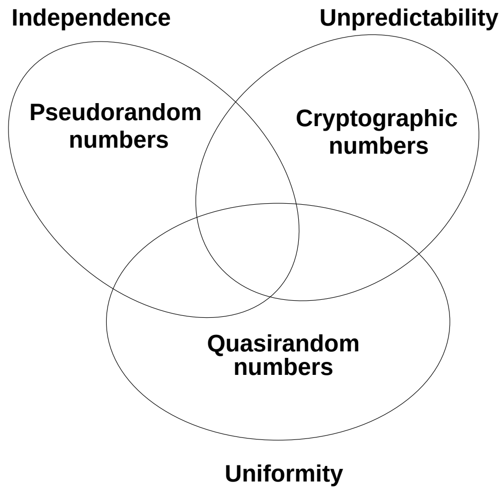
1. Types of random numbers and Monte Carlo Methods
2. Pseudorandom number generation
   - Types of pseudorandom numbers
   - Properties of these pseudorandom numbers
   - Parallelization of pseudorandom number generators
3. Quasirandom number generation
   - The Koksma-Hlawka inequality
   - Discrepancy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

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? (Cont.)

1. 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)

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:

1. Linear congruential: $x_n = ax_{n-1} + c \pmod{m}$
2. Shift register: $y_n = y_{n-s} + y_{n-r} \pmod{2}$, $r > s$
3. Additive lagged-Fibonacci: $z_n = z_{n-s} + z_{n-r} \pmod{2^k}$, $r > s$
4. Combined: $w_n = y_n + z_n \pmod{p}$
5. Multiplicative lagged-Fibonacci: $x_n = x_{n-s} \times x_{n-r} \pmod{2^k}$, $r > s$
6. Implicit inversive congruential: $x_n = a\overline{x_{n-1}} + c \pmod{p}$
7. Explicit inversive congruential: $x_n = a\overline{n} + c \pmod{p}$

Pseudorandom Numbers (Cont.)

- 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: $\mathrm{Per}(x_n)$ 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 (Cont.)

- 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 (RNGs)

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

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 $\mathrm{Per}(x_n)$
  - 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: $\{x_0, x_1, \ldots, x_{L-1}\}$
   - Second : $\{x_L, x_{L+1}, \ldots, x_{2L-1}\}$
   - ith block: $\{x_{(i-1)L}, x_{(i-1)L+1}, \ldots, x_{iL-1}\}$
2. The Leap Frog Technique: define the leap ahead of $\ell = \left\lfloor \frac{\mathrm{Per}(x_i)}{L} \right\rfloor$:
   - First block: $\{x_0, x_\ell, x_{2\ell}, \ldots, x_{(L-1)\ell}\}$
   - Second block: $\{x_1, x_{1+\ell}, x_{1+2\ell}, \ldots, x_{1+(L-1)\ell}\}$
   - ith block: $\{x_i, x_{i+\ell}, x_{i+2\ell}, \ldots, x_{i+(L-1)\ell}\}$

Splitting RNGs for Use In Parallel (Cont.)

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: $\left\lfloor \frac{\mathrm{Per}(x_i)}{2} \right\rfloor$
   - ith split leap ahead: $\left\lfloor \frac{\mathrm{Per}(x_i)}{2^{l+1}} \right\rfloor$
   - 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 with Splitting RNGs for Use In Parallel

1. Splitting for parallelization is not scalable:
   - It usually costs $O(\log_2(\mathrm{Per}(x_i)))$ 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 $\mathrm{Per}(x_i) = O((LP)^e)$
   - Rule of thumb: never use more than $\sqrt{\mathrm{Per}(x_i)}$ of a sequence $\rightarrow e = 2$
   - Thus cost per random number is not constant with number of processors!!
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,
   $x_n = a x_{n-1} + c \pmod{m}$
   - Choice: Prime modulus (quality considerations)
   - Parameterize the multiplier
   - Less efficient than lagged-Fibonacci
   - Provably good quality
   - Multiprecise arithmetic in initialization

New Results in PRNGs:

Using Distinct Parameterized Streams in Parallel (Cont.)

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 $\mathrm{Per}(x_n) = (2^{17} - 1) \times 2^{31}$
- 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}	$\ldots$	b_1	b_0	
$\Box$	$\Box$	$\ldots$	0	0	x_{r-1}
0	$\Box$	$\ldots$	$\Box$	0	x_{r-2}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$\Box$	0	$\ldots$	$\Box$	0	x_1
$\Box$	$\Box$	$\ldots$	$\Box$	1	x_0

or a special b_0 (adjoining 1's):

m.s.b.				l.s.b.	
b_{k-1}	b_{k-2}	$\ldots$	b_1	b_0	
$\Box$	$\Box$	$\ldots$	$\Box$	b_{0n-1}	x_{r-1}
$\Box$	$\Box$	$\ldots$	$\Box$	b_{0n-2}	x_{r-2}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
$\Box$	$\Box$	$\ldots$	$\Box$	b_{01}	x_1
0	0	$\ldots$	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 α 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 α are primitive elements also
- If $m = 2q + 1$ with q also prime (Sophie-Germain prime) then all odd powers (save the qth) of α are primitive elements
- Consider $x_n = ax_{n-1} \pmod{m}$ and $y_n = a^l y_{n-1} \pmod{m}$ and define the full-period exponential-sum cross-correlation between then 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 (Cont.)

- Mersenne modulus: relatively easy to do modular multiplication
- With Mersenne prime modulus, $m = 2^p - 1$ must compute $\phi_{m-1}^{-1}(k)$, the kth 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

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- ($k = \mathrm{Per}(x_n)$) and partial-period exponential sums:

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

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

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

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

- Additive lagged-Fibonacci generators have poor provable results, yet empirical evidence suggests $|C(\cdot, \mathrm{Per}(x_n))| < O(\sqrt{\mathrm{Per}(x_n)})$

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
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 **S**calable **P**arallel **R**andom **N**umber **G**enerators (`SPRNG`) library: `http://sprng.fsu.edu`

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 $x_1, \dots, x_N$:

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

  where χ is the characteristic function
- **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:

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

  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:
  $x_n = \Phi_b(n-1), n = 1, 2, \ldots,$ where for $b \in \mathbb{Z}, b \geq 2$:

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

$$a_j \in \{0, 1, \ldots, b-1\}$$

  For van der Corput sequence

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

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

Some Types of Quasirandom Numbers (Cont.)

- Other small D_N^* points sets and sequences:

1. Halton sequence: $\mathbf{x}_n = (\Phi_{b_1}(n-1), \ldots, \Phi_{b_s}(n-1))$, $n = 1, 2, \ldots,$ $D_N^* = O\left(N^{-1}(\log N)^s\right)$ if $b_1, \ldots, b_s$ pairwise relatively prime
2. Hammersley point set: $\mathbf{x}_n = \left(\frac{n-1}{N}, \Phi_{b_1}(n-1), \ldots, \Phi_{b_{s-1}}(n-1)\right)$, $n = 1, 2, \ldots, N$, $D_N^* = O\left(N^{-1}(\log N)^{s-1}\right)$ if $b_1, \ldots, b_{s-1}$ are pairwise relatively prime
3. Ergodic dynamics: $\mathbf{x}_n = \{n\alpha\}$, where $\alpha = (\alpha_1, \ldots, \alpha_s)$ is irrational and $\alpha_1, \ldots, \alpha_s$ 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)
   - Soboĺ sequences
   - Faure sequences
   - Niederreiter sequences

Some Types of Quasirandom Numbers (Cont.)

1. Another interpretation of the v.d. Corput sequence:
   - Define the ith ℓ-bit "direction number" as: $v_i = 2^i$ (think of this as a bit vector)
   - Represent $n-1$ via its base-2 representation $n-1 = b_{\ell-1}b_{\ell-2}\ldots b_1 b_0$
   - Thus we have

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

2. The Soboĺ sequence works the same!!
   - Use recursions with a primitive binary polynomial define the (dense) v_i
   - The Soboĺ sequence is defined as:

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

   - For speed of implementation, we use Gray-code ordering

Some Types of Quasirandom Numbers (Cont.)

- (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

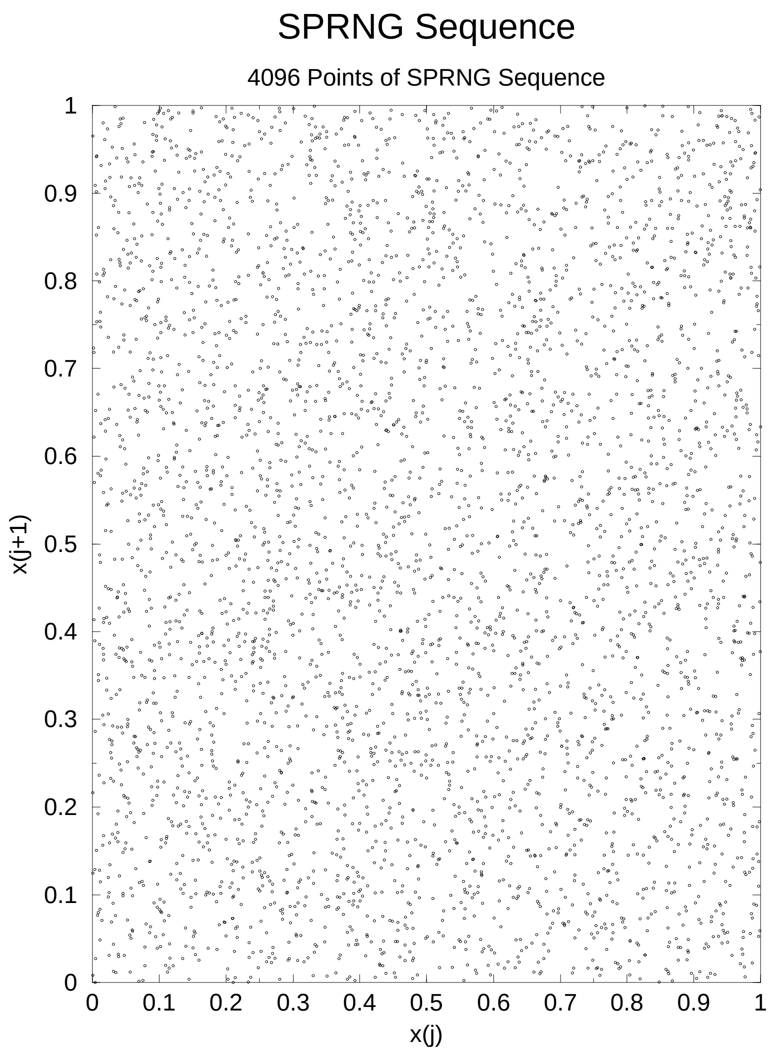
$$J = \prod_{i=1}^{s} [\frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}})$$

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

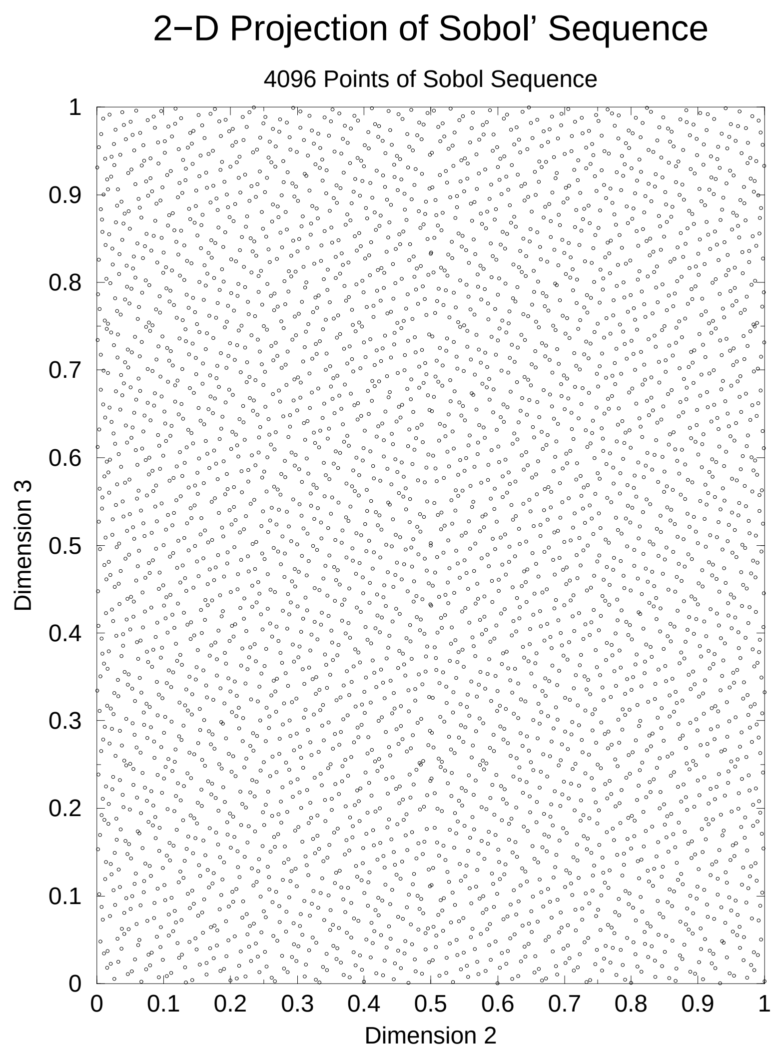
2. A set of b^m points is a (t, m, s)-net if each b-ary box of volume b^{t-m} has exactly b^t points in it

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 $x_i^{(j)}(n) = \sum_{k=1}^{m} y_k^{(j)}(n) q^{-k}$

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



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



Future Work on Random Numbers

1. `SPRNG` and pseudorandom number generation work
   - New generators: Well, Mersenne Twister, different LCGs, etc.
   - Spawn-intensive/small-memory footprint generators
   - More comprehensive testing suite
   - Improved theoretical tests
   - C++ implementation
   - Grid-based tools
2. Quasirandom number work
   - Scrambling (parameterization) for parallelization
   - Optimal scrambling
   - Comparison to sparse grids
   - “`QPRNG`”
   - Grid-based tools

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