DON'T TRUST PARALLEL MONTE CARLO!

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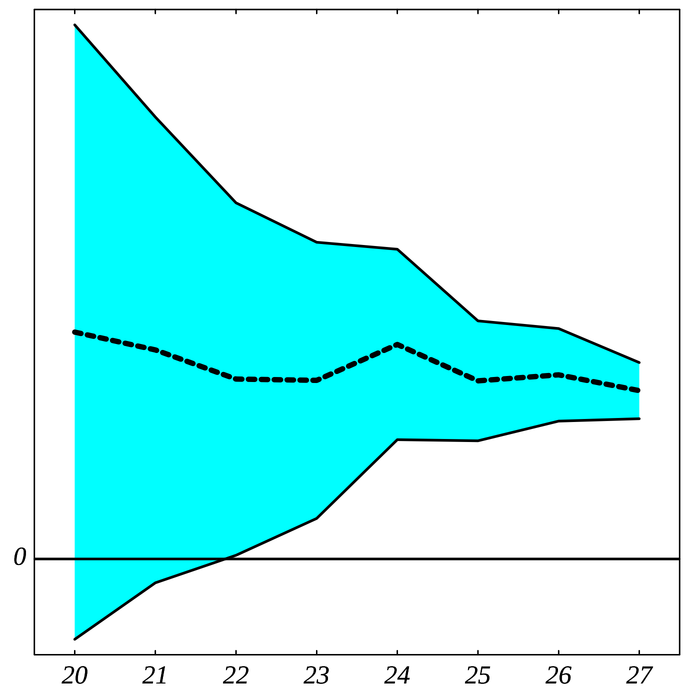
WHY NOT TRUST PARALLEL MONTE CARLO?

ANSWER

For the following reason



MC Integration Error
CRAY Generator
True Value: 0

DETAILS

Later in this talk

TABLE OF CONTENTS

RANDOM NUMBER GENERATORS (RNGs)

RNG

- *Deterministic* algorithm
- Produces numbers with certain *distribution properties*
  Standard case: Uniform distribution on $[0, 1[$
- A *fundamental tool* of applied mathematics

SOME FACTS

- RNGs produce *periodic* sequences
- Every RNG has its *unwanted side-effects*
- *No* RNG is appropriate for all tasks

RANDOM NUMBER GENERATORS: THE SETTING

SIMULATION PROBLEM
User Dependent

EMPIRICAL TESTS
Prototypical Simulations
Test 1
Test 2
Test 3
etc.

RNG

THEORETICAL TESTS
Figures of Merit
Discrepancy
Spectral Test
Weighted Spectral Test
?

DETAILS OF THE SETTING

SIMULATION PROBLEM
Unknown in advance

RNG

EMPIRICAL TESTS
Prototypical Simulations
Sample size N: varies widely
Dimension d: rather restricted

THEORETICAL TESTS
Figures of Merit
Sample size N: rather restricted
Dimension d: varies widely

RNG CHECKLIST

Theoretical Support		
Period Length	Conditions	
	Algorithms for parameters	
Structural Properties	Intrinsic structures	
	Points on hyperplanes	
	Equidistribution prop.	
Correlation Analysis	For particular parameters	
	For particular initializations	
	For parts of the period	
	For subsequences	
	For combinations of RNGs	

Empirical Evidence	
• Variable sample size • Two- or higher level tests	
Bit-oriented tests	
Geometric test quantities	
Complexity	
Transformation methods: sensitivity	

Practical Aspects	
Tables of parameters available	
Portable implementations available	
Parallelization techniques apply	
Large samples available	

CORRELATION ANALYSIS: THE APPROACH

THE APPROACH

- GIVEN
  Random numbers
  $$x_0, x_1, \ldots \in [0,1[$$
- CONSTRUCT
  $$\mathbf{x}_n := (x_n, x_{n+1}, \ldots, x_{n+d-1})$$
  … *overlapping d-tuples*
  $$\mathbf{x}_n := (x_{nd}, x_{nd+1}, \ldots, x_{nd+d-1})$$
  … *non-overlapping d-tuples*
- ASSESS
  The empirical distribution of
  $$\omega := (\mathbf{x}_n)_{n=0}^{N-1} \quad \text{in } [0,1[^d$$

THE QUESTION

When will ω have a *"good"* distribution?

CORRELATIONS: THE BACKGROUND

FACT

> *"Monte Carlo results are misleading when correlations hidden in the random numbers and in the simulated system interfere constructively."*

... A. Compagner, Phys. Rev. E **52**(1995)

QUESTION

How to assess such correlations?

APPROACH

- Theoretical Analysis: *a priori*, with *Figures of Merit*
  - Estimation of their order of magnitude (e.g. discrepancy)
  - Numerical evaluation of point distributions: full period (e.g. Spectral Test)
- Empirical Analysis: *for Samples*
  - "Statistical testing" of samples
  - Numerical calculation of figures of merit
  - Application-specific tests

THEORY VS. PRACTICE

EMPIRICAL FACT

The behavior of the *full cycle* point sets in dimension $d = 2, 3, \ldots$ with respect to theoretical figures of merit allows *very reliable predictions* of the performance of the random numbers themselves.

Practical evidence shows that many target distributions will be simulated very well.

EMPIRICAL EVIDENCE

(G: good, B: bad performance)

Forecasting Empirical Performance				
Theoretical Test	G	G	B	B
Empirical Test	G	B	B	G
Type of Event	Usual	Rare	Usual	Sometimes

REMARK

We always have to take into account the period length of the RNG vs. the sample size.

DISCREPANCY: THE DEFINITION

GIVEN

Finite point set $\omega = (\mathbf{x}_n)_{n=0}^{N-1}$ in $[0,1[^d$
Distribution function F of uniform distribution on $[0,1[^d$

COMPUTE

Empirical distribution function (e.d.f.) of ω,

$$F_N(\mathbf{x}), \quad \mathbf{x} \in [0,1[^d$$

COMPARE

Measure the deviation of F_N from the target distribution F:

$$\|F_N - F\|_p, \quad p \geq 1$$

$p = \infty$: star discrepancy
i.e. two-sided Kolmogoroff-Smirnov test statistics
$p = 2$: L^2-discrepancy
i.e. Cramer - von Mises test statistics

DISCREPANCY: THE DEFINITION

APPROACH

F_N ... Empirical Distribution Function of $\omega = (\mathbf{x}_n)_{n=0}^{N-1}$ in $[0,1[^d$
F ... Uniform Distribution on $[0,1[^d$

COMPARE

$$||F_N - F||_\infty$$

DEFINITION

$\omega = (\mathbf{x}_n)_{n\geq 0}$ in $[0,1[^d$

$$D_N^*(\omega) := \sup_{J\in\mathcal{J}^*} \left| \frac{1}{N} \cdot \sharp\{n, 0 \leq n < N : \mathbf{x}_n \in J\} - \lambda_d(J) \right| ,$$

... *(Star) Discrepancy* $D_N^*(\omega)$

where

- $\mathcal{J}^*$: class of all subintervals J of $[0,1[^d$:

$$J = \prod_{i=1}^{d} [0, v_i[, \quad 0 < v_i \leq 1, \quad 1 \leq i \leq d,$$

- $\lambda_d(J)$: volume of J

THE SPECTRAL TEST

TEST DESIGN

Coveyou and MacPherson (1967)
Knuth (1967)

$$\mathcal{F} = \mathcal{T}$$

TEST QUANTITY

$\omega = (\mathbf{x}_n)_{n=0}^{N-1}$ N-point node set of a d-dimensional lattice rule

$$\sigma(\omega) := \frac{1}{min\{\sqrt{k_1^2 + \ldots + k_d^2} : \mathbf{k} \neq \mathbf{0},\ S_N(e_{\mathbf{k}}, \omega) \neq 0\}}$$

REMARKS

- Highly successful for linear generators (LCG, ...)
- Practical limitation: only for point sets *with lattice structure*
- Strong relation to the geometry of numbers
- No relation to statistics known
- No general approach:

> *"The difficulty here is to find a convincing quantitative formulation of this idea."*

... Niederreiter(1992)

WHAT IS QUASI-MONTE CARLO?

FACTS

- MC convergence rate (in any dimension d):

$$\mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

- Koksma-Hlawka Inequality ($\omega = (\mathbf{x}_n)_{n=0}^{N-1}$ in $[0,1[^d$)

$$\left| \int_{[0,1]^d} f(\mathbf{x})\, d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n) \right| \leq v(f)\, \delta_N(\omega)$$

SETUP

Search for node sets ω with small figure of merit $\delta_N(\omega)$

PRACTICE

- Good Lattice Points modulo N (Korobov 1959):

$$\omega = \left(\left\{ \frac{n}{N}\, \mathbf{g} \right\} \right)_{n=0}^{N-1}, \quad \mathbf{g} \in \mathbb{Z}^d$$

- (t, m, s)-Nets (Sobol' 1967, Niederreiter 1987)

$\omega =$ much more complicated to define

- Rate of convergence

$$\mathcal{O}\left(\frac{(\log N)^{d-1}}{N}\right)$$

QMC: AN ILLUSTRATION

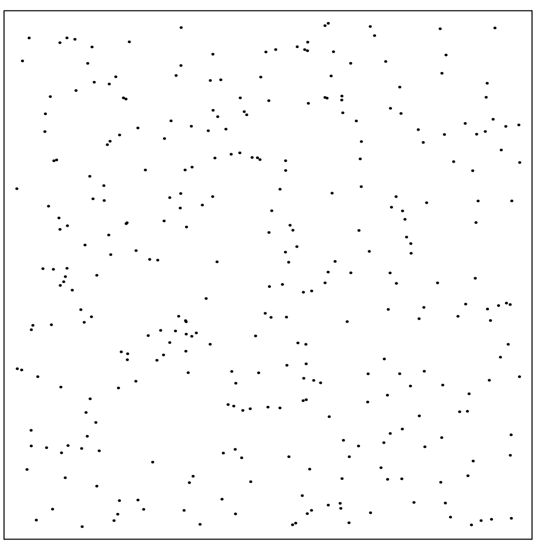
THE PROBLEM

Integration error as small as possible

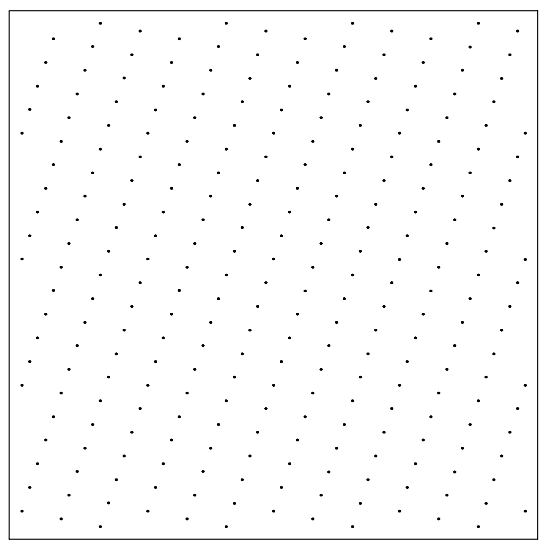
$$\int_{[0,1]^d} f(\mathbf{x})\, d\mathbf{x} - \frac{1}{N}\sum_{n=0}^{N-1} f(\mathbf{x}_n)$$

$\ldots \omega = (\mathbf{x}_n)_{n=0}^{N-1}$ node set

EXAMPLE



MC Node Set



QMC Node Set

QMC: TWO EXAMPLES of GLPs

KOROBOV GLPs

Good lattice point $\mathbf{g} = (1, a, a^2, \dots, a^{d-1})$ modulo N, $a \in \mathbb{Z}$, N prime

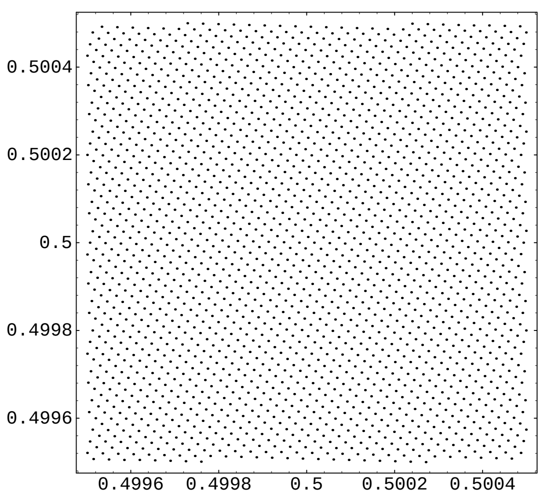
ASSOCIATED LDP

Node set ω in $[0,1[^d$

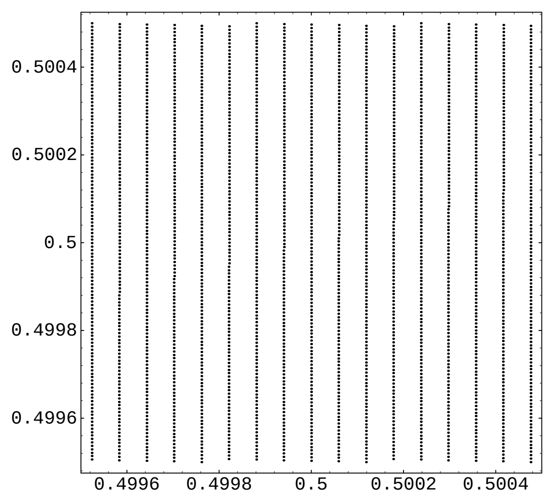
$$\omega = \omega(a) = \left(\left\{ \frac{n}{N} \mathbf{g} \right\} \right)_{n=0}^{N-1}$$

EXAMPLES

$N = 2^{31} - 1$, dimension $d = 2$, zoom into the unit interval



$a = 950706376$



$a = 16807$

LINEAR CONGRUENTIAL GENERATOR (LCG)

(D.H. Lehmer, 1949)

DEFINITION

m ... modulus
a ... multiplier
b ... additive constant
y_0 ... initial value

$$y_{n+1} \equiv a \cdot y_n + b \pmod{m}, \quad n \geq 0,$$

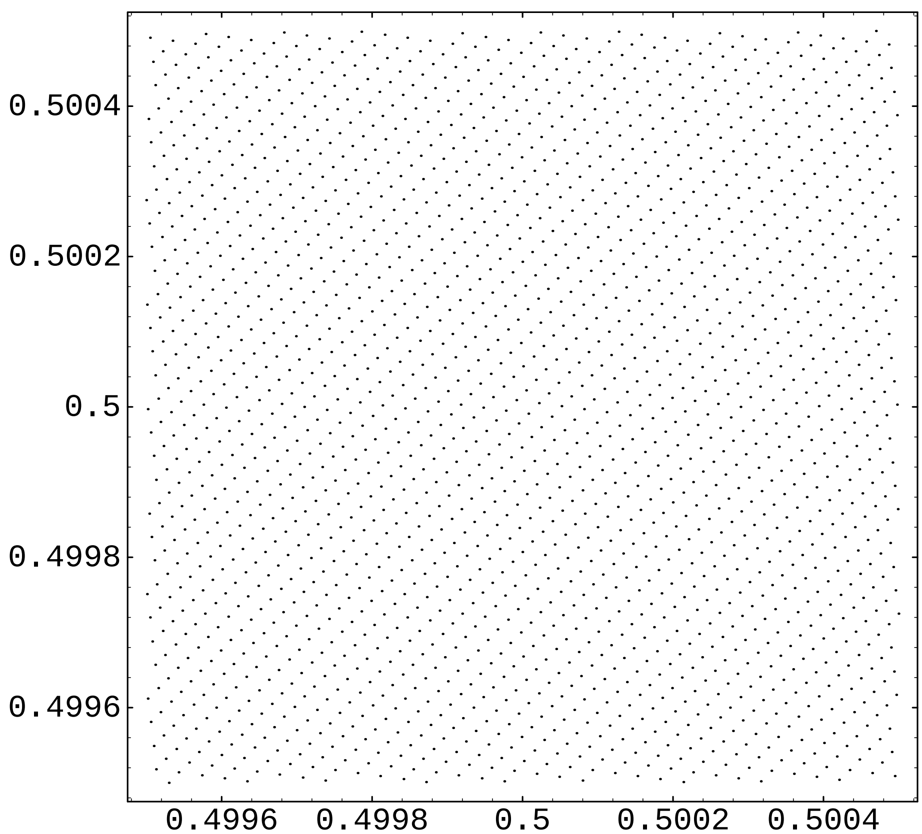
NOTATION

LCG(m, a, b, y_0)

OUTPUT STREAM

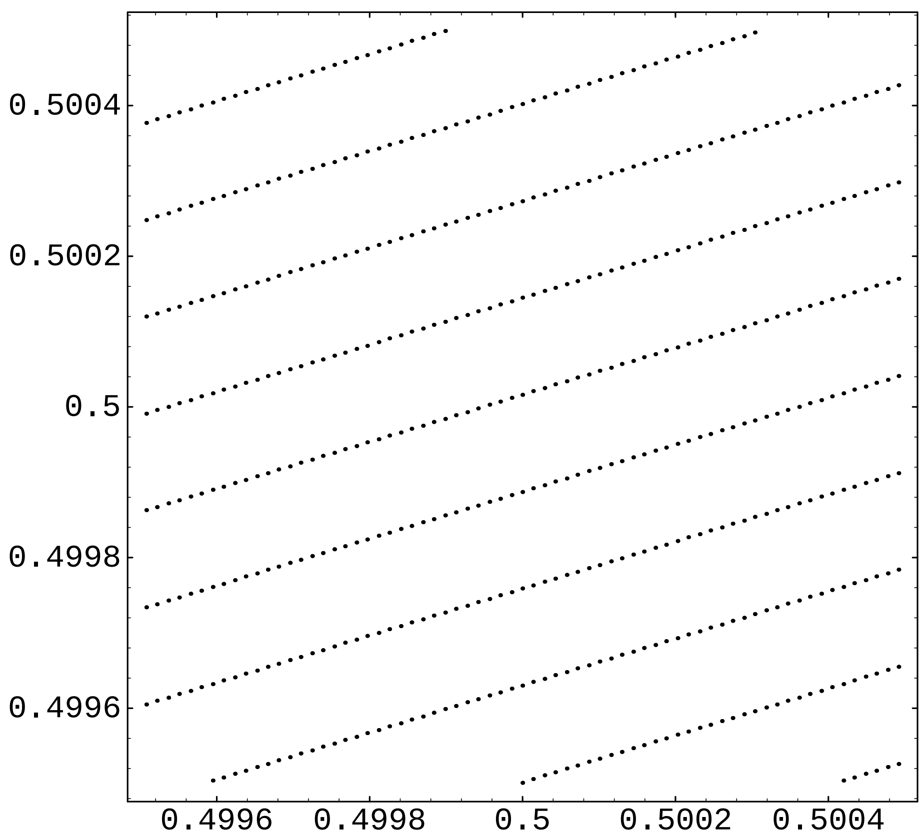
$$x_n := \frac{y_n}{m} \in [0, 1[, \quad n = 0, 1, \ldots$$

THE POINTS OF A SIMSCRIPT LCG



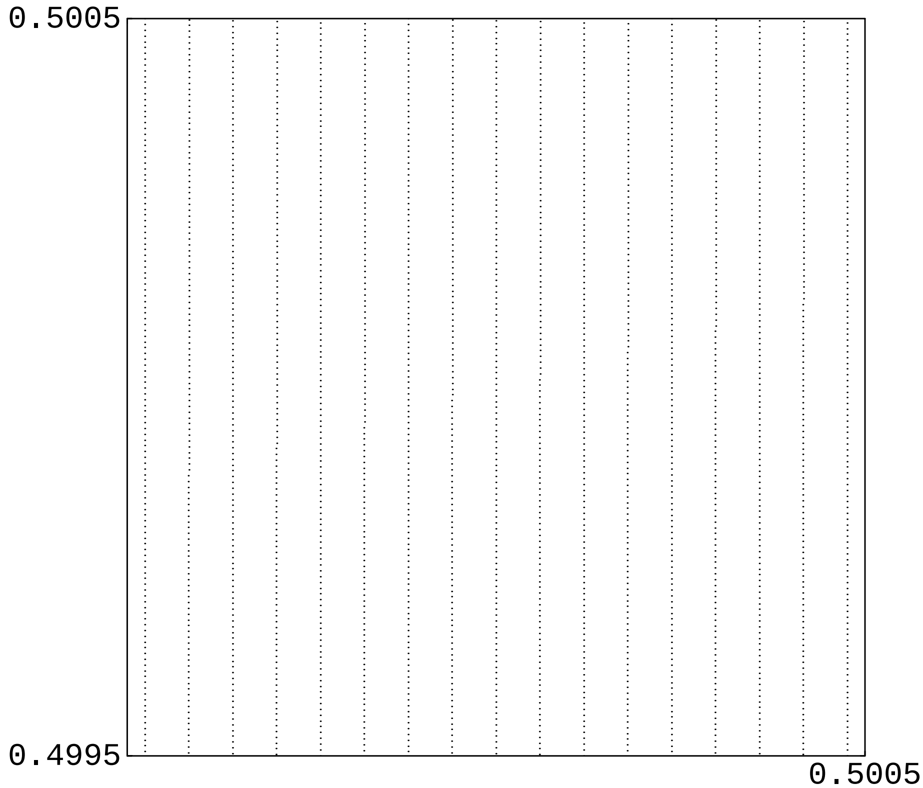
Point Structure: LCG($2^{31}-1$,630360016,0,1)
(nonoverlapping pairs, all possible points)

THE POINTS OF SUPER-DUPER



Point Structure: LCG(2^{32}, 69069, 0,1)
(nonoverlapping pairs, all possible points)

THE POINTS OF MINSTND



Point Structure: LCG($2^{31} - 1$, 16807, 0, 1)
(nonoverlapping pairs, all possible points)

INVERSIVE CONGRUENTIAL GENERATOR (ICG)

(J. Eichenauer und J. Lehn, 1986)

DEFINITION

m	...	modulus, $m = p$ prime
a	...	multiplier
b	...	additive constant
y_0	...	initial value

$$y_{n+1} \equiv a \cdot \overline{y_n} + b \pmod{m}, \quad n \geq 0,$$

where ($\overline{c} \in \mathbf{Z}_p$)

$$\overline{c} := \begin{cases} c^{-1} & \text{if} \quad c \neq 0 \\ 0 & \text{if} \quad c = 0. \end{cases}$$

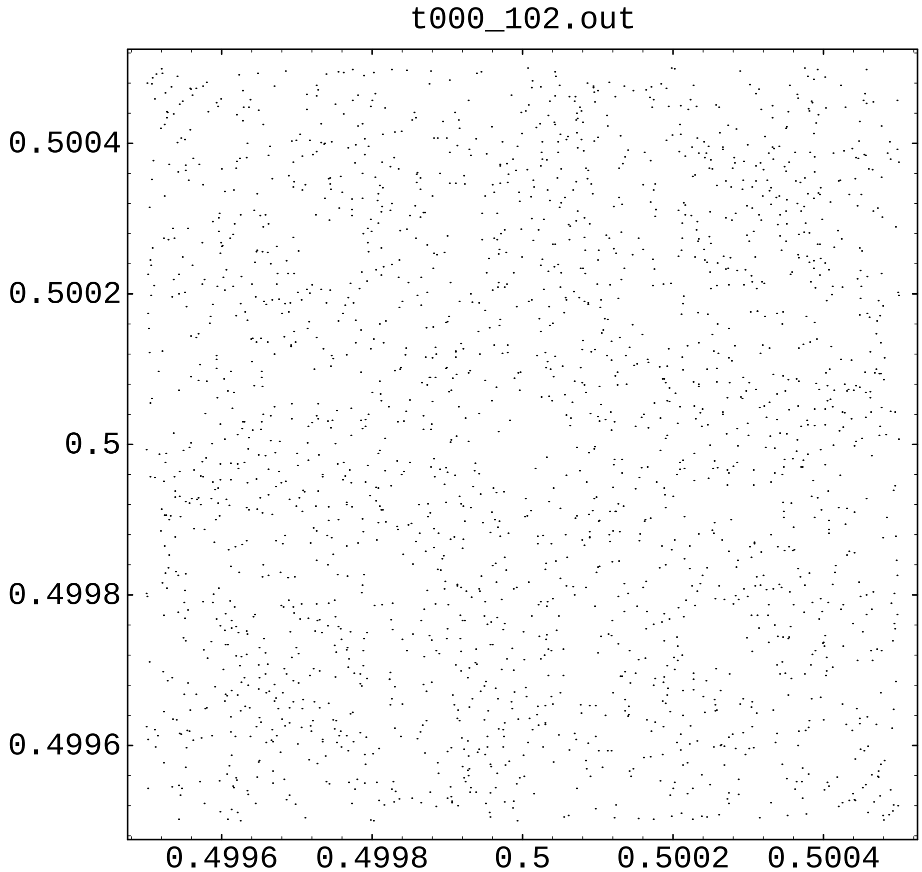
NOTATION

ICG(m, a, b, y_0)

OUTPUT STREAM

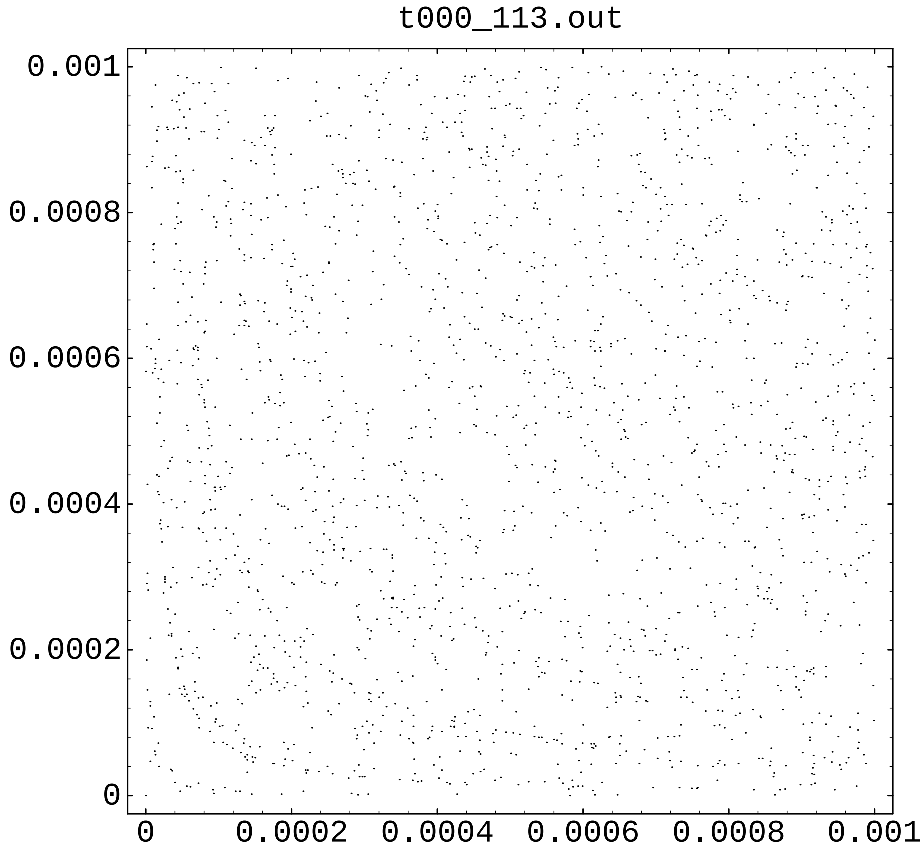
$$x_n := \frac{y_n}{m} \in [0, 1[, \quad n = 0, 1, \ldots$$

THE POINTS OF AN ICG "MOTHER"



Point structure: ICG($2^{31} - 1$, 1288490188, 1, 1),
(nonoverlapping pairs, all points, the region near (0.5, 0.5))

THE POINTS OF AN ICG "MOTHER"



Point Structure: ICG($2^{31} - 1$, 1288490188, 1, 1),
(nonoverlapping pairs, all points, the region near (0.0, 0.0))

EXPLICIT-INVERSIVE CONGRUENTIAL GENERATOR (EICG)

(J. Eichenauer -Herrmann, 1993)

DEFINITION

m ... modulus, $m = p$ prime
a ... multiplier
b ... additive constant
n_0 ... initial value

$$y_n \equiv \overline{an + b} \pmod{m}, \quad n \geq n_0,$$

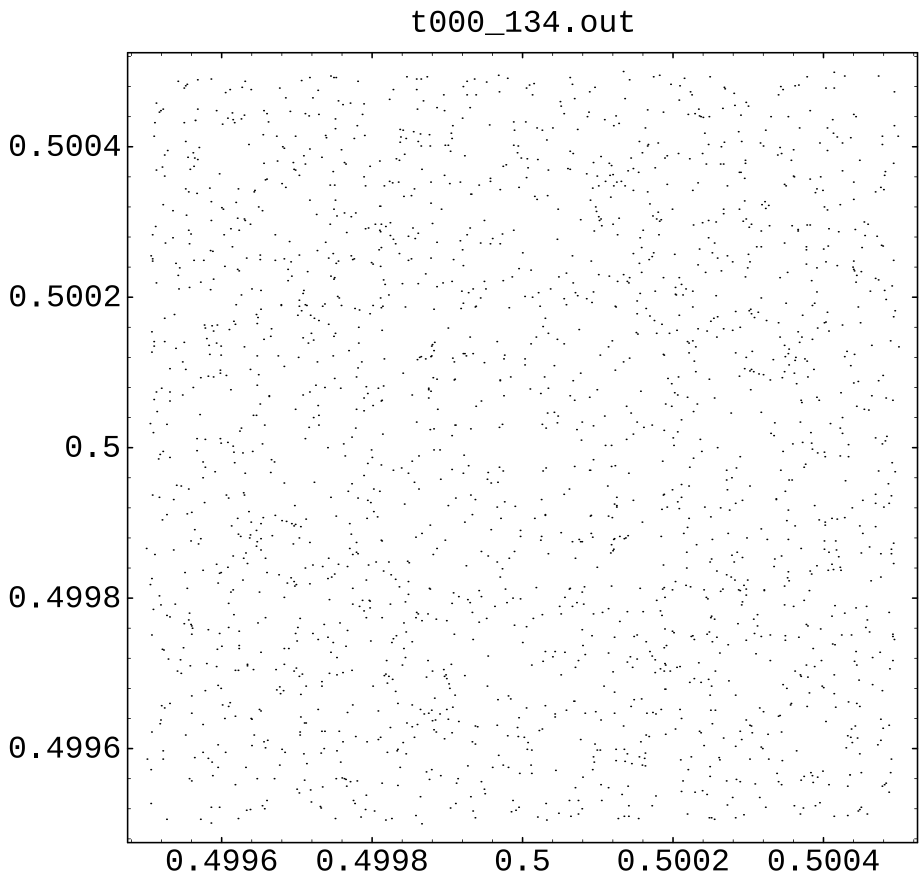
NOTATION

EICG(m, a, b, n_0)

OUTPUT STREAM

$$x_n := \frac{y_n}{m} \in [0, 1[, \quad n = n_0, n_0 + 1, \ldots$$

THE POINTS OF AN EICG



Point structure: EICG($2^{31}-1$, 1288490188, 1, 0),
(nonoverlapping pairs, all points, the region near(0.5, 0.5))

TT800

Matsumoto and Kurita(1992, 1994)

TYPE OF ALGORITHM: tGFSR

Generate w-bit integers $\mathbf{x}_n$, $n \geq 0$, by the rule

$$\mathbf{x}_{n+p} = \mathbf{x}_{n+q} \oplus \mathbf{x}_n A, \quad n \geq 0,$$

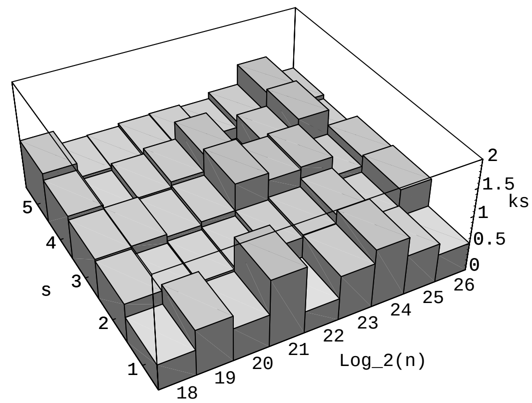
$\oplus$: XOR
A: binary matrix

PROPERTIES

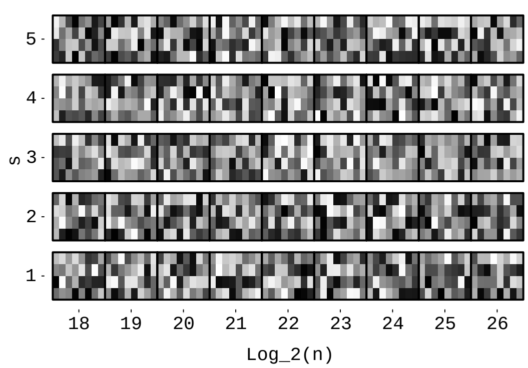
Parameters	initial values not all zero
	$(w, p, q, A) = (32, 25, 7,$ see paper$)$
Period length	2^{800}
Correlation analysis	k-distribution
	$k(16) = 50,\ k(24) = k(32) = 25$

THE M-TUPLE TEST: TT800

LOAD TEST
Dimension $d = 1$ to 5, first four digits



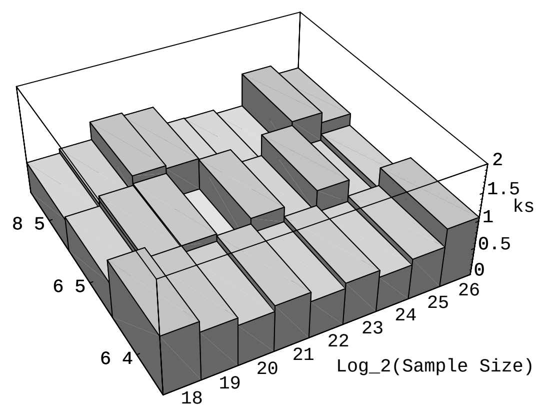
LOAD TEST: KS Values



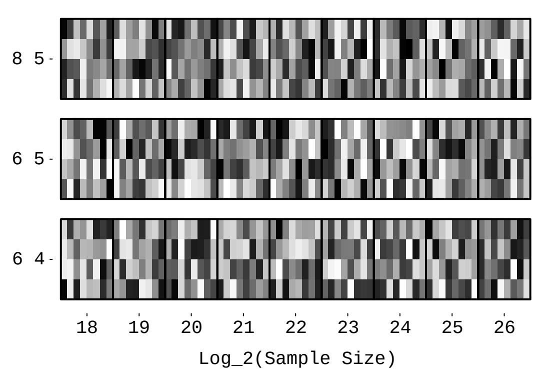
LOAD TEST: Upper Tail Probabilities

THE M-TUPLE TEST: TT800

Dimension $d = 4, 5$
No. of blocks $r = 6, 8$, four digits each



TT800: KS Values



TT800: Upper Tail Probabilities

PARALLEL STREAMS OF RANDOM NUMBERS

QUESTION

How to produce uncorrelated streams of random numbers on L parallel processors?

APPROACH 1

Employ many (small) RNGs,
use different RNGs for different processors,
i.e.
RNG #1 on processor #1,
RNG #2 on processor #2,
...

APPROACH 2

Employ one (big) RNG,
use different subsequences for different processors
i.e.
subsequence #1 on processor #1,
subsequence #2 on processor #2,
...

Approach 2a: Leap-Frog Method
Approach 2b: Sequence Splitting Method

LEAP FROG

ORIGINAL RNG

$$x_0, x_1, \dots, x_{L-1}, x_L, x_{L+1}, \dots, x_{2L-1}, x_{2L}, x_{2L+1}, \dots$$

LEAP-FROG SUBSEQUENCES

Partition original stream $(x_n)_{n\geq 0}$ into L subsequences

$$(x_{Ln+j})_{n\geq 0}, \quad 0 \leq j < L,$$

$$\boxed{x_0}, x_1, \dots, x_{L-1}, \boxed{x_L}, x_{L+1}, \dots, x_{2L-1}, \boxed{x_{2L}}, x_{2L+1}, \dots$$

i.e. first subsequence is

$$x_0, x_L, x_{2L}, x_{3L}, \dots, x_{nL}, \dots$$

second subsequence is

$$x_1, x_{L+1}, x_{2L+1}, x_{3L+1}, \dots, x_{nL+1}, \dots$$

L: lag (i.e. # of processors)
j: index

REQUIREMENTS

- Need to jump ahead (by L steps)
- Need good subsequences:
  intra-correlations
  inter-correlations

LEAP FROG: EXAMPLE

ORIGINAL RNG

$$\mathrm{LCG}(m, a, 0, y_0)$$

PRECOMPUTING

$$\begin{aligned} y_n &\equiv a\, y_{n-1} \pmod m, \quad n = 0, 1, \ldots \\ \Rightarrow y_n &\equiv a^n\, y_0 \pmod m \\ \Rightarrow y_{nL+j} &\equiv (a^L)^n\, y_j \pmod m, \quad n = 0, 1, \ldots \end{aligned}$$

This is

$$\mathrm{LCG}(m, a^L, 0, y_j)$$

QUESTION

If a is good, will a^L also be a good multiplier?

ANSWER

Not necessarily!

SEQUENCE SPLITTING

ORIGINAL RNG

$$x_0, x_1, \ldots, x_{P-1}, x_P, x_{P+1}, \ldots, x_{2P-1}, x_{2P}, x_{2P+1}, \ldots, x_{3P-1}, \ldots$$

SUBSEQUENCES

Split original stream $(x_n)_{n\geq 0}$ into L blocks

$$(x_{jP+n})_{n=0}^{P-1}, \quad 0 \leq j < L,$$

$$\boxed{x_0, x_1, \ldots, x_{P-1}}, \boxed{x_P, x_{P+1}, \ldots, x_{2P-1}}, \boxed{x_{2P}, x_{2P+1}, \ldots, x_{3P-1}}, \ldots$$

i.e. first subsequence is

$$x_0, x_1, x_2, \ldots, x_{P-1},$$

second subsequence is

$$x_P, x_{P+1}, x_{P+2}, \ldots, x_{2P-1}.$$

REQUIREMENTS

- Need to jump ahead (to x_P, x_{2P}, ...)
- Need uncorrelated subsequences:
  inter-correlations = *long-range* correlations

SEQUENCE SPLITTING: EXAMPLE

ORIGINAL RNG

$$\mathrm{LCG}(m, a, 0, y_0)$$

PRECOMPUTING

$$\begin{aligned} y_n &\equiv a\, y_{n-1} \pmod{m}, \quad n = 0, 1, \ldots \\ \Rightarrow y_{jP} &\equiv a^{jP}\, y_0 \pmod{m} \\ \Rightarrow y_{jP+n} &\equiv a^n\, y_{jP} \pmod{m}, \quad n = 0, 1, \ldots \end{aligned}$$

This is

$$\mathrm{LCG}(m, a, 0, y_{jP})$$

QUESTION

Will there be correlations between such blocks?

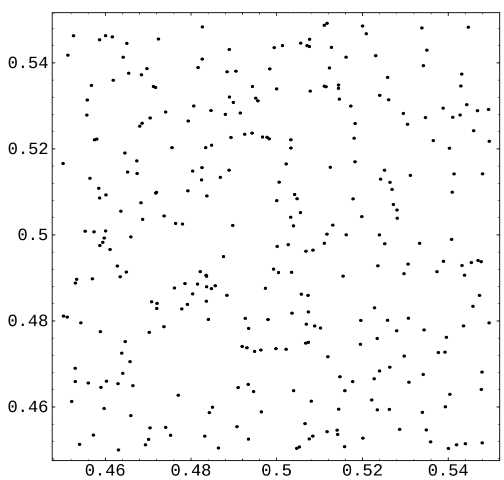
ANSWER

Such *long-range correlations* may be extremely strong!

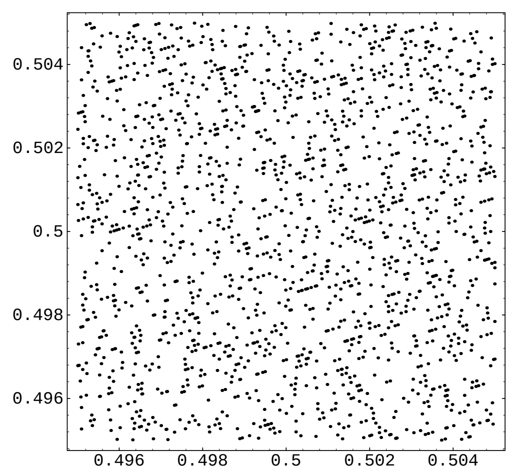
INCREASING THE SAMPLE SIZE

SETUP

- RNG: LCG(2^{32}, 69069, 0, 1)
- Dimension: $d = 2$
- Produce nonoverlapping pairs $(x_{2n}, x_{2n+1}) \in [0, 1[^2$



2^{15} Points



2^{25} Points

OBSERVATION

The regularities of the RNG begin to appear.

QUESTION

What is the influence on our simulations?

DISCUSSION

QUESTION

Given an RNG with period length τ:
Which sample sizes N are safe?

ANSWER

A general answer is impossible.

EMPIRICAL EVIDENCE

- Linear methods (LCG, MRG, ...)

$$N < \sqrt{\tau}$$

- Inversive methods (ICG, EICG, ...)

$$N < \tau^{3/4}$$

WARNING

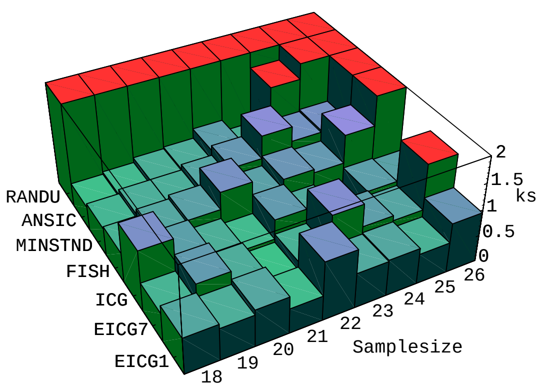
For particular simulations, the bounds for N may be smaller.

INCREASING THE DIMENSION

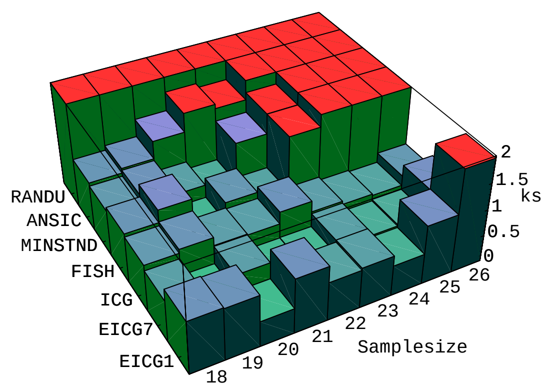
SETUP

- RNG: a fixed set (i.e. RANDU, MINSTND, ANSIC,...)
- Dimension: $d = 3, 4$
- Test statistics: overlapping serial test (first four digits)
- Plot KS-test (bar chart) and values (pattern plot)

Dimension 3



Dimension 4



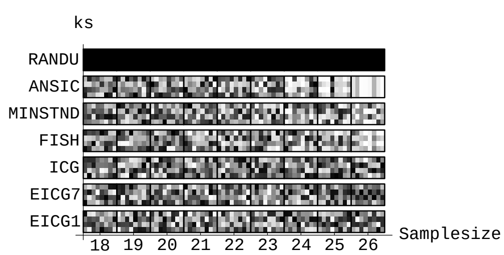
KS Test Values

INCREASING THE DIMENSION

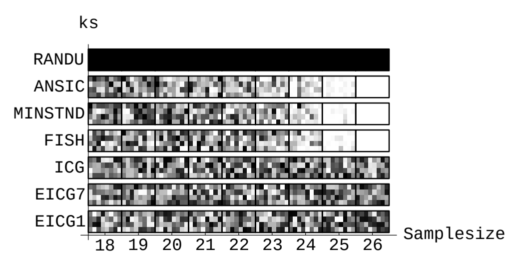
SETUP

- RNG: a fixed set (i.e. RANDU, MINSTND, ANSIC,. . .)
- Dimension: $d = 3, 4$
- Test statistics: overlapping serial test (first four digits)
- Plot KS-test (bar chart) and values (pattern plot)

Dimension 3



Dimension 4

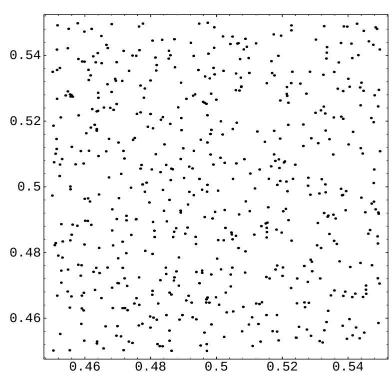


Upper Tail Probabilities

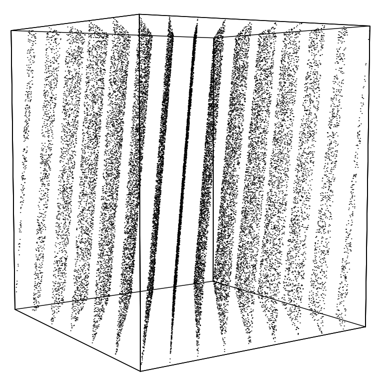
INCREASING THE DIMENSION

SETUP

- RNG: LCG(2^{31}, 65539, 0, 1), i.e. RANDU
- Dimension: $d = 2, 3$
- Sample size: $N = 2^{16}$
- Plot nonoverlapping pairs (x_{2n}, x_{2n+1}) and triples $(x_{3n}, x_{3n+1}, x_{3n+2})$, $0 \leq n < N$.



Dimension 2: A Zoom



Dimension 3: The Unit Cube

QUESTION

How to prevent such *unpleasant surprises*?

DISCUSSION

QUESTION

Given an RNG with period length τ:
Which dimensions d are safe?

ANSWER

A general answer is impossible.

THEORETICAL PREDICTION

- RNGs with lattice structure: check with spectral test
- RNGs without lattice structure: check with discrepancy
- RNGs without theoretical support: avoid them!

WARNING

Theoretical support is *no guarantee*, only a very reliable prediction.

A FISHMAN GENERATOR

SETTING

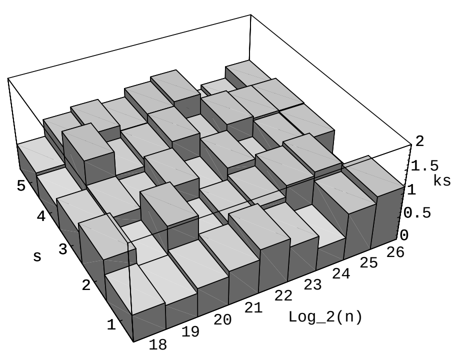
$$\mathrm{RNG} = \mathrm{LCG}(2^{48}, 55151000561141, 0, 1)$$

SPECTRAL TEST

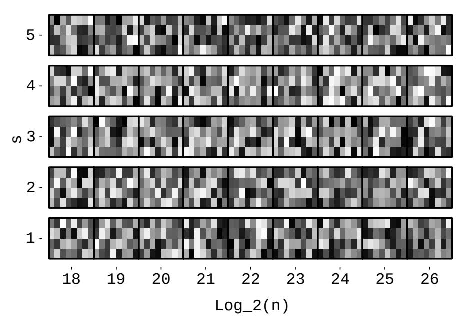
2	3	4	5	6	7	8
0.9246	0.8170	0.9240	0.8278	0.8394	0.6274	0.4471

Spectral Test for Dimensions 2 to 8

LOAD TEST



KS Values



Upper Tail Probabilities

A FISHMAN GENERATOR: LAG 23

SETTING

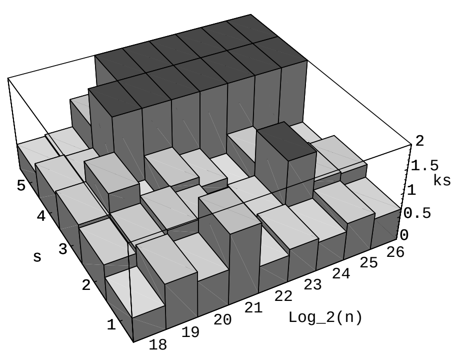
RNG = LCG(2^{48}, 55151000561141, 0, 1)

SPECTRAL TEST FOR THE SUBSEQUENCE $(x_{23n})_{n\geq 0}$

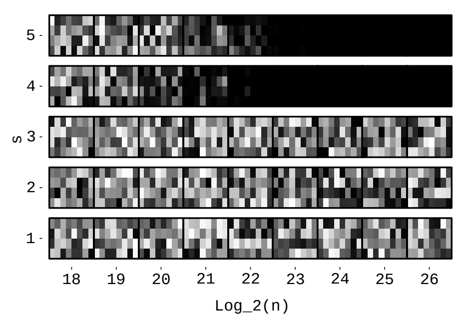
2	3	4	5	6	7	8
0.2562	**0.0600**	**0.0114**	**0.0462**	0.1275	0.2031	0.2077

Spectral Test for Dimensions 2 to 8

LOAD TEST FOR THE SUBSEQUENCE $(x_{23n})_{n\geq 0}$



KS Values



Upper Tail Probabilities

MONTE CARLO INTEGRATION

SETUP

- Test function

$$f(\mathbf{x}) = \prod_{i=1}^{d} g(x_i), \quad \mathbf{x} = (x_1, \ldots, x_d) \in [0,1]^d,$$
$$g : [0,1] \to \mathbb{R}.$$

- Node set ω produced by an RNG

$$\omega = (\mathbf{x}_n)_{n=0}^{N-1} \text{ in } [0,1[^d,$$

- Monte Carlo integration error

$$R_N(f,\omega) := \int_{[0,1]^d} f(\mathbf{x})\, d\mathbf{x} - \frac{1}{N} \sum_{n=0}^{N-1} f(\mathbf{x}_n)$$

QUESTION

What is the influence of the RNG?

STATISTICAL BACKGROUND

SETTING

- Choose integrand f with integral zero
- Dimension d is fixed

For a given sample size N:

- Generate 64 independent samples $\omega_1, \ldots, \omega_{64}$
  (hence, $\omega_k \in [0,1[^d$)
- Compute the 64 errors $R_N(f, \omega_k)$, $1 \leq k \leq 64$
  (hence, $R_N(f, \omega_k)$ has normal distribution)
- Compute the sample mean $\hat{\mu}$ and variance $\hat{\sigma}$ of the 64 errors
  (hence, $\hat{\mu}$ is Student t-distributed, $\sqrt{64}\,\hat{\mu}/\hat{\sigma} \sim t_{63}$)
- Compute the 99% confidence interval for Student t-distribution:

$$]\hat{\mu} - 0.332\hat{\sigma}, \hat{\mu} + 0.332\hat{\sigma}[$$

- Compare with expected value of sample mean: 0.

MC INTEGRATION: DETAILS

SETTING

- Test function

$$f(\mathbf{x}) = \prod_{i=1}^{d} (x_i^5 - 1/6)$$

- Dimension $d = 6$
- RNG = LCG(2^{48}, 44485709377909, 0, 1)
- Sample size $N = 2^{20}, 2^{21}, \ldots, 2^{27}$
- Number of replications for each N: 64
- Independent node sets ω_k, $1 \leq k \leq 64$, constructed from nonoverlapping d-tuples of random numbers

TEST STATISTICS

- For each N, compute the 64 integration errors

$$R_N(f, \omega_k), \quad 1 \leq k \leq 64.$$

- Compute the sample mean $\hat{\mu}$ and variance $\hat{\sigma}$ of the 64 errors
- Compute the 99% confidence interval for Student t-distribution:

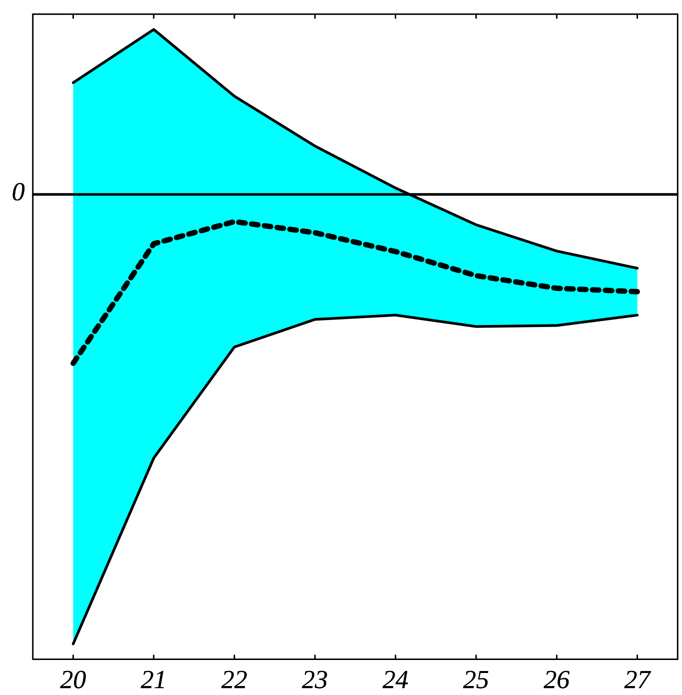
$$]\hat{\mu} - 0.332\hat{\sigma}, \hat{\mu} + 0.332\hat{\sigma}[$$

- Compare experimental value $\hat{\mu}$ with expected value 0
(see plots)

MC INTEGRATION: EXAMPLE

SETTING

1. Take first string of Nd consecutive random numbers, take out lag 128-index 0 numbers, construct nonoverlapping d-tuples from them: Get first "small" node set $\omega_1^{(1)}$
2. Repeat procedure with lag 128-index 1 numbers, get second "small" node set $\omega_1^{(2)}$, and so on (i.e., for each index, hence 128 times).
3. Construct the union of these 128 small node sets to get the first node set ω_1.
4. Repeat 1. to 3. with second string of Nd consecutive random numbers to get second node set ω_2, and so on (i.e. 64 times)

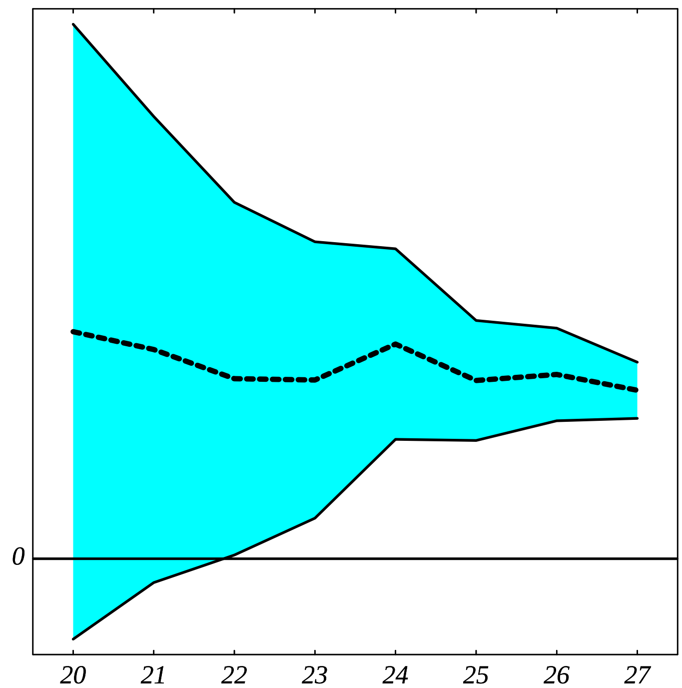


Mean Integration Error, Union Of Leap Frog Streams

MC INTEGRATION: EXAMPLE

SETTING

1. Take first string of Nd consecutive random numbers with lag 128 and index 0, construct nonoverlapping d-tuples from them: Get first node set ω_1
2. Repeat procedure 1. with second string of Nd consecutive lag 128-index 0 random numbers to get second node set ω_2, and so on (in total, 64 times).



Mean Integration Error, Leap Frog Stream
(lag = 128, index = 0)

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