Random Number Generation (RNG)

read "Numerical Recipes" on random numbers and the chi-squared test.

Today we discuss how to generate and test random numbers.

What is a random number?

- A single number is not random. Only an infinite sequence can be described as random.
- Random means the absence of order. (Negative property).
- Can an intelligent gambler make money by betting on the next numbers that will turn up?
- All subsequences are equally distributed. This is the property that MC uses to do integrals and that you will test for in homework.

"Anyone who considers arithmetical methods of random digits is, of course, in a state of sin." *John von Neumann (1951)*

"Random numbers should not be chosen at random." Knuth (1986)

Random numbers on a computer

- Truly Random - the result of a physical process such as timing clocks, circuit noise, Geiger counts, bad memory
  - Too slow (we need 10^{10}/sec) and expensive
  - Low quality
  - Not reproducible
- Pseudo-random. *prng* (pseudo means *fake*)
  - Deterministic sequence with a repeat period but with the appearance of randomness (if you don’t know the algorithm).
- Quasi-random (quasi means *almost random*)
  - “half way” between random and a uniform grid.
  - Meant to fill space with max. distance between space to fill “holes” sequentially (e.g., [0,100] as 0,1,2,3,…,100).

If doing a low-D integral, QRNG gives up correlation so the sequence will be more uniform than PRNG and converge to mean value quicker than $N^{-1/2}$.

Desired Properties of RNG on a computer

- **Deterministic:** easy to debug (repeatable simulations).

- **Long Periods:** cycle length is long.

- **Uniformity:** RN generated in space evenly.
  - Go through complete cycle, all integers occur once!
  - TEST: N occurrences of x. The no. in (a,b) is equal to

    $N(b-a) \pm [N(b-a)]^{-1/2}$

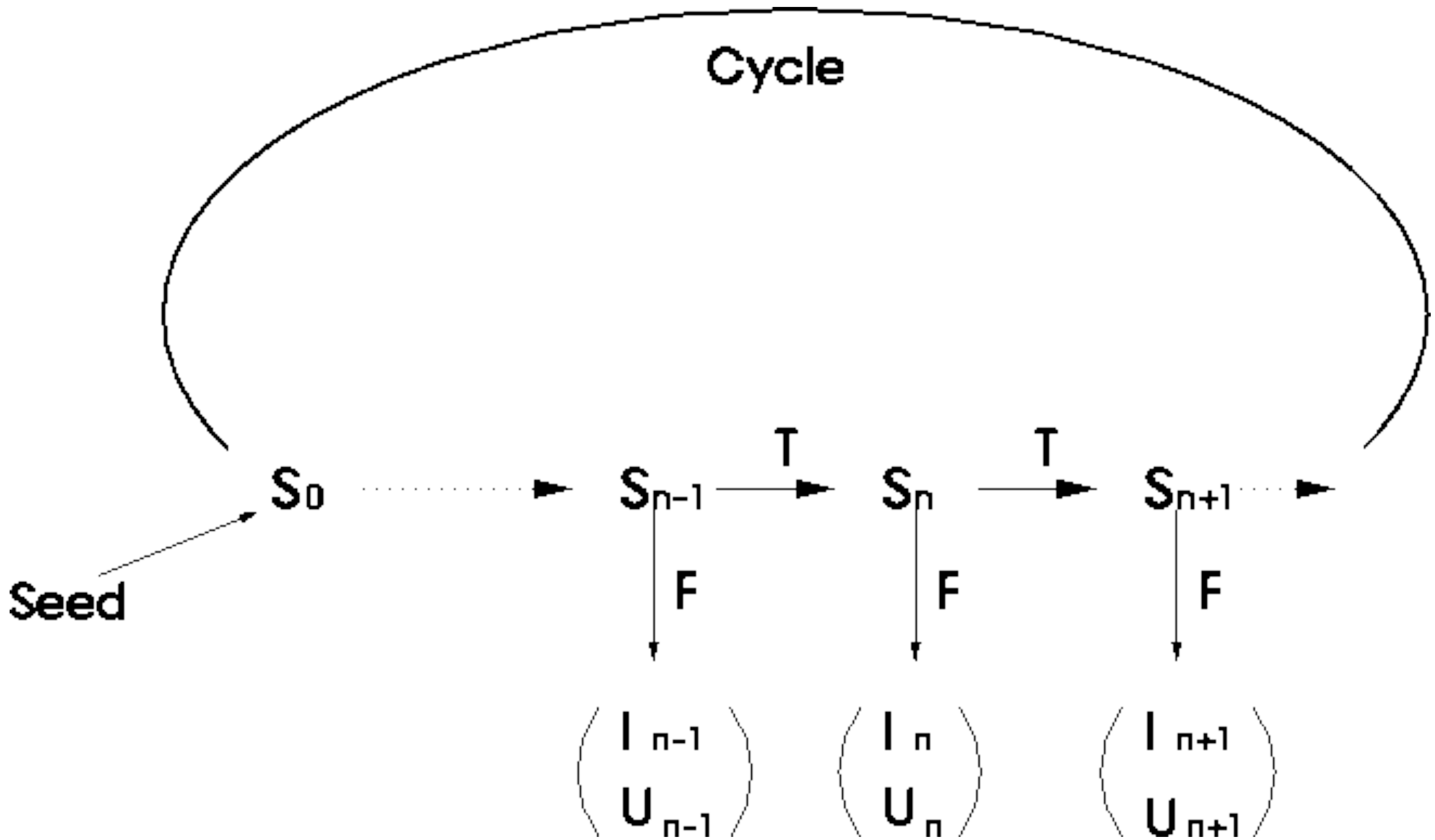
- **Uncorrelated Sequences**:

  $<f_1(x_{i+1})\ldots f_k(x_{i+k})> = <f_1(x_{i+1})>\ldots<f_k(x_{i+k})>$

  Monte Carlo can be very sensitive to such correlations, especially for large k.

- **Efficiency:** Needs to be fast.

Pseudo Random Sequence



S: State and initial seed.

T: Iteration process,

F: Mapping from state to integer RN (I) or real RN (U).

Period or Cycle Length (L)

- If internal state has M bits, total state space is 2^M values.
- If mapping is 1-1, space divides into a finite no. of cycles.
- Best case is a single cycle of length 2^M, otherwise $2^M/L$.
- It is easy to achieve very long cycle length: 32 or 24 bit generators are not long enough!
- Entire period of the RNG is exhausted in:

• rand (1 processor)	~ 100 second
• drand48 (1 processor)	~ 1 year
• drand48 (100 processor)	~ 3 days
• SPRNG LFG (10^5 procs)	~ 10^{375} years

Assuming 10^7 RN/sec per processor

e.g., In 1997, computer has ~10^8 RN/proc/sec (or 2^{26}).
Hence, it takes 1 sec to exhaust generator with 26 bits and 1 year for 2^{51} states.
e.g., consider 1024x1024 sites (spins) on a lattice. With MC, sweep 10^7 times to get averages.
You need to generate 10^{13} RN. A 32-bit RNG from 1980's dangerous on today's computers.

Common PRNG Generators

Linear Congruential Generator (LCG)   modulo (mod) is remainder after division

64-bit word (or 2 32-bit LCG) give a period of ~10^{18}.

• Multiplicative Lagged Fibonacci • Modified Lagged Fibonacci	$z_n = z_{n-k} * z_{n-l}$ $z_n = z_{n-k} + z_{n-l}$ (modulo 2^m)	vary initialization
• 48 bit LCG • 64 bit LCG • Prime Modulus LCG	$z_n = a*z_{n-1} + p$ (modulo m)	vary p vary a
• Combined Multiple Recursive	$z_n = a_{n-1}*z_{n-1} + ...+ a_{n-k}*z_{n-k}$ + LCG	vary LCG
	Recurrence	Parallelization

Uniformity

- Output consists of taking **N bits from state and making an integer in $(0,2^N-1)$ "I_k".**
- One gets a **uniform real "U_k" by multiplying by 2^{-N}**.
- We will study next time how to get other distributions.
- If there is a single cycle, then **integers must be uniform in the range $(0,2^N-1)$.**
- Uniformity of numbers taken 1 at a time is usually easy to guarantee. What we need is higher dimensional uniformity!

Example of LCG: linear congruent generator

Example of LCG(a,c,m,I_0).

e.g., LCG(5,1,16,1): $I_{n+1} = a\, I_n + c \mod(m)$

- I_0 is seed to initiate sequence. (Allows repeatable runs.)
- Sequence is determined by values of (a,c,m,I_0).
- mod(m) is leftover from multiples of m from LCG.

- I_{n+1} are RNG integers.
- Real RNG are created by

$R_n = I_n$ /float(m) for [0,1)

or $R_n = I_n$ /float(m-1) for [0,1]

For uniformity on [0,1), what is desired average and variance of R?

Example of LCG: $I_{n+1} = a\, I_n + c$

e.g., LCG(5,1,16,0) where $a = 5$, $c = 1$, $m = 16$ and $I_0 = 0$

- Choosing udrn: $R_n = I_n$ /float(m) for [0,1).

Thus,

LCG	mod(m)	Integer	Binary	Real
I_0: 0 + 1 = 1	- 0x16	1	0001	1/16 = 0.0625
I_1: 5x1 + 1 = 6	- 0x16	6	0110	6/16 = 0.3750
I_2: 5x6 + 1 = 31	- 1x16	15	1111	15/16 = 0.9375
I_3: 5x15 + 1 = 76	- 4x16	12	1100	12/16 = 0.7500
I_4: 5x12 + 1 = 61	- 3x16	13	1101	13/16 = 0.8125
…				
I_{15}: 5x3 + 1 = 16	- 1x16	0	0000	0/16 = 0.0000

Note: period is $P=2^M$.

Here P=16, where M=Log(m)/base2 = ln(16)/ln(2) = 4

For LCG(5,1,16,0): $I_{n+1} = 5\,I_n + 1$

For LCG(5,1,16,0): $I_{n+1} = a\,I_n + c$ mod(m)

- We have a period P =16, which is the longest it can be.

	Integer	Binary	Real
I_0:	1	0001	1/16 = 0.0625
I_1:	6	0110	6/16 = 0.3750
I_2:	15	1111	15/16 = 0.9375
I_3:	12	1100	12/16 = 0.7500
I_4:	13	1101	13/16 = 0.8125
I_5:	2	0010	2/16 = 0.1250
I_6:	11	1011	11/16 = 0.6875
I_7:	8	1000	8/16 = 0.5000
I_8:	9	1001	9/16 = 0.5625
I_9:	14	1110	14/16 = 0.8750
I_{10}:	7	0111	7/16 = 0.4375
I_{11}:	4	0100	4/16 = 0.2500
I_{12}:	5	0101	5/16 = 0.3125
I_{13}:	10	1010	10/16 = 0.6275
I_{14}:	3	0011	3/16 = 0.1875
I_{15}:	0	0000	0/16 = 0.0000

However, there is correlation in the most significant binary digit!

…1010101…

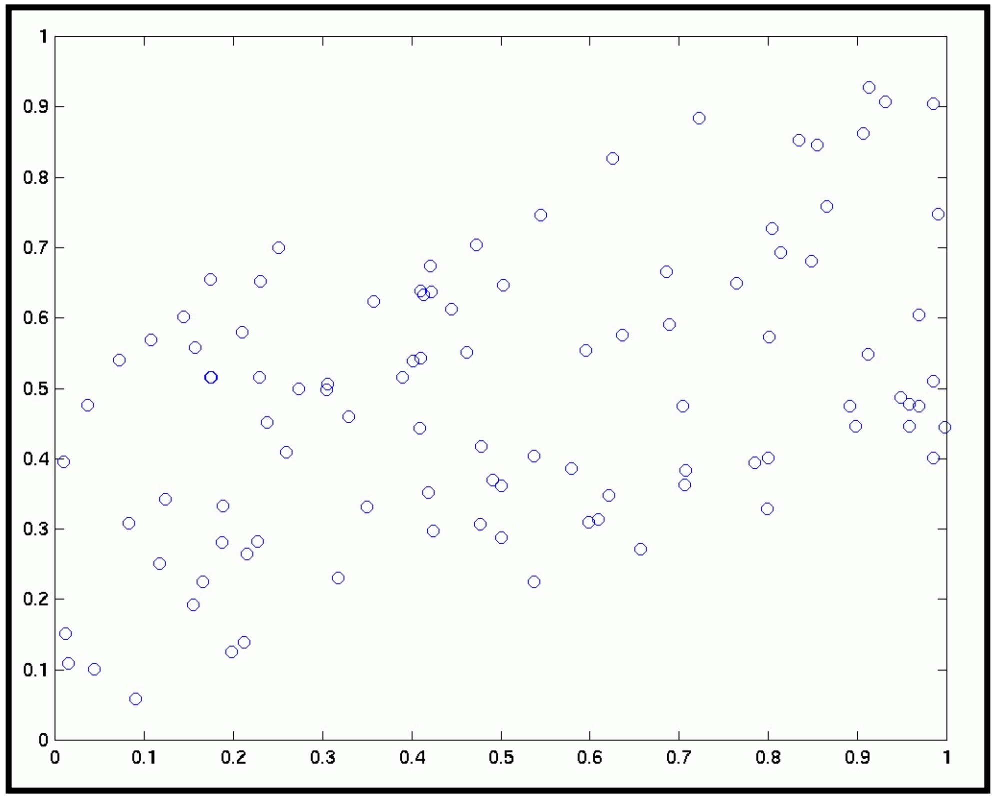
Show analytically that
$\langle R \rangle = 1/2$
$\langle (R - \langle R \rangle)^2 \rangle = 1/12.$

Try it!

Sequential RNG Problems

- Correlations → non-uniformity in higher dimensions

Uniform in 1-D but non-uniform in 2-D



This is the important property to guarantee:

$$\langle f_1(x_{i+1}) f_2(x_{i+2}) \rangle = \langle f_1(x_{i+1}) \rangle \langle f_2(x_{i+2}) \rangle$$

MC uses numbers many at a time--they need to be uniform.

e.g., 128 atom MC moving 3N coords. at random needs 4 PRNG (x,y,z, i) or

128 x 4=1024. So every 1024 moves may be correlated!

Compare error for each PRNG, if similar OK. (Use χ^2-test.)

LCG Numbers fall in planes.

Good LCG generators have the planes close together.

For a k-bit generator, do not use them more than k/2 together.

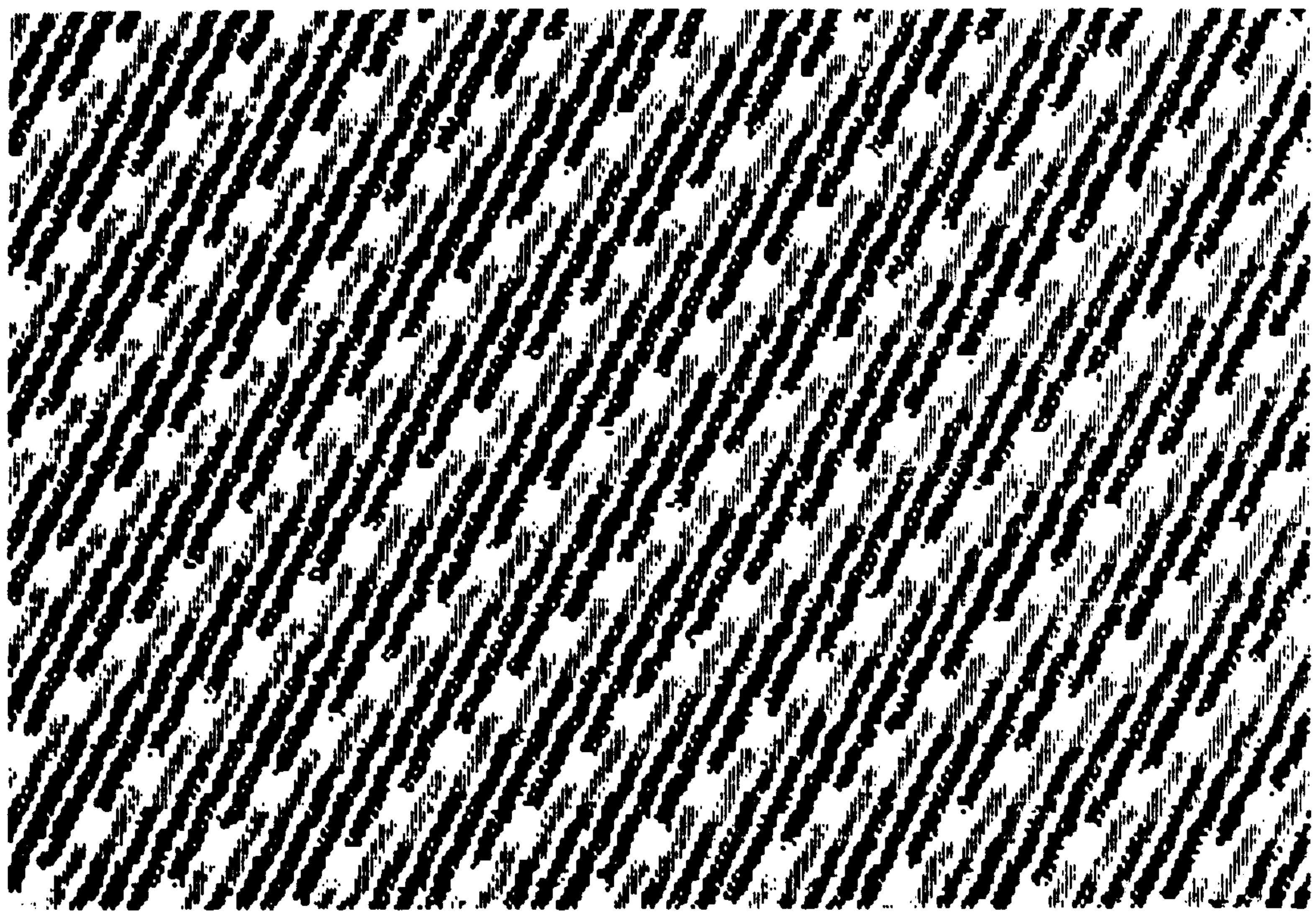


Fig. 8.2 Correlation between the triplets of points $\vec{r}_n$ $\{x_{3n}, x_{3n+1}, x_{3n+2}\}$ generated by a pseudorandom number generator. Th value of the third coordinate is represented by the intensity of the point.

SPRNG: originally a NCSA project

- A library of *many* well tested *excellent parallel* PRNGs
- Callable from FORTRAN, C, C++, and JAVA
- Ported to popular parallel and serial platforms

SPRNG Functions

- int ****init_sprng***(int streamnum, int nstreams, int seed, int param)
- double ***sprng***(int *stream)
- int ***isprng***(int *stream)
- int ***print_sprng***(int *stream)
- int ***make_sprng_seed***()
- int ***pack_sprng***(int *stream, char **buffer)
- int ****unpack_sprng***(char *buffer)
- int ***free_sprng***(int *stream)
- int ***spawn_sprng***(int *stream, int nspawned, int ***newstreams)

What is a chisquare test

- Suppose $\{x_1, x_2, \ldots.\}$ are N Gaussian random numbers mean 0, variance 1
- What is the distribution of $y = \sum_{k=1}^{N} x_k^2$?
- $Q(\chi^2 | N)$ is the probability that $y > \chi^2$
- The mean value of y is N, its variance is 2N.
- We use it to test hypotheses. Is the fluctuation we see, what we expect?

$$\chi^2 = \sum_{k=1}^{N} \left(\frac{x_k - x_k^{(0)}}{\sigma_k} \right)^2$$

- Roughly speaking we should have $N - \sqrt{2N} < \chi^2 < N + \sqrt{2N}$
- More precisely look up value of $Q(\chi^2 | N)$

Chi-squared test of randomness

- HW exercise: do test of several generators
  - Divide up “cube” into “N” bins.
  - Sample many “P” triplets.
  - Number/bin should be $n = P/N \pm (P/N)^{1/2}$

    In example: expected $n = 10 \pm (10)^{1/2}$

N=100

P=1000

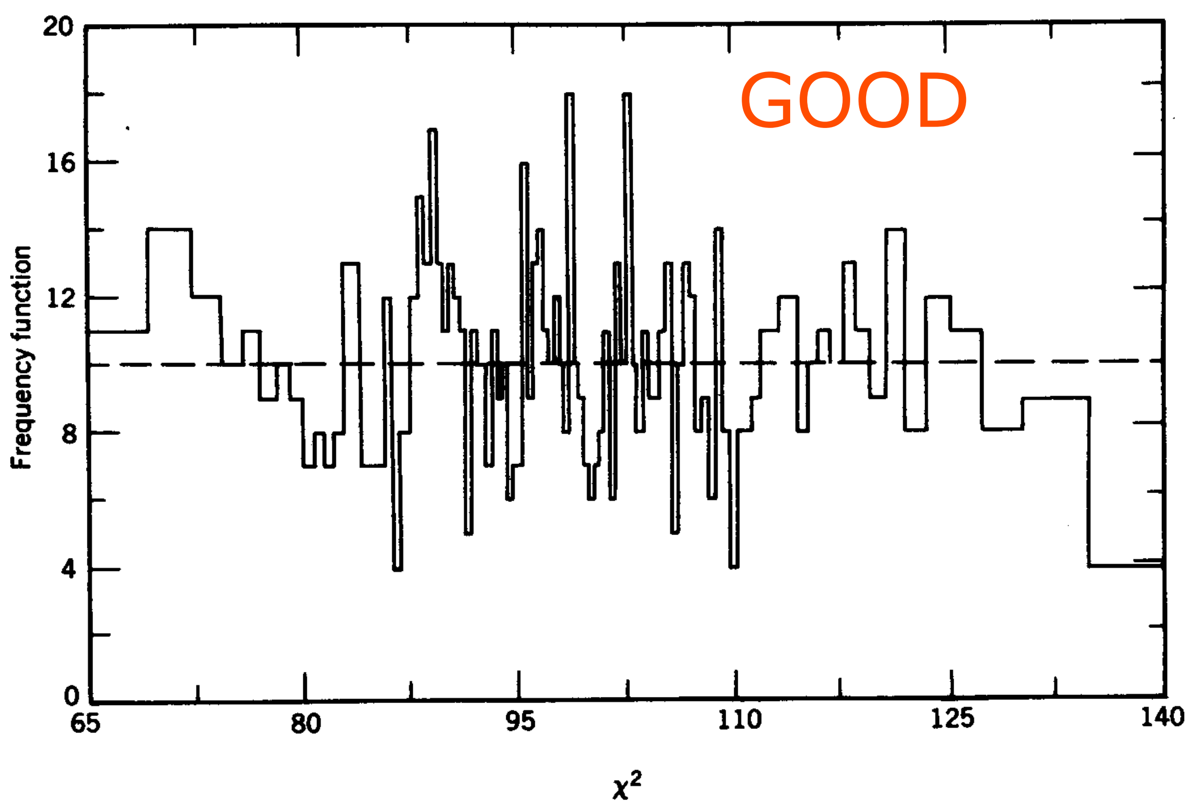


Figure A.1. The frequency function of observed values of χ^2 after 1000 samples. The bins are equally probable intervals where the expected number of χ^2 in each bin is 10. The pseudorandom number generator was Eq. (A.13).

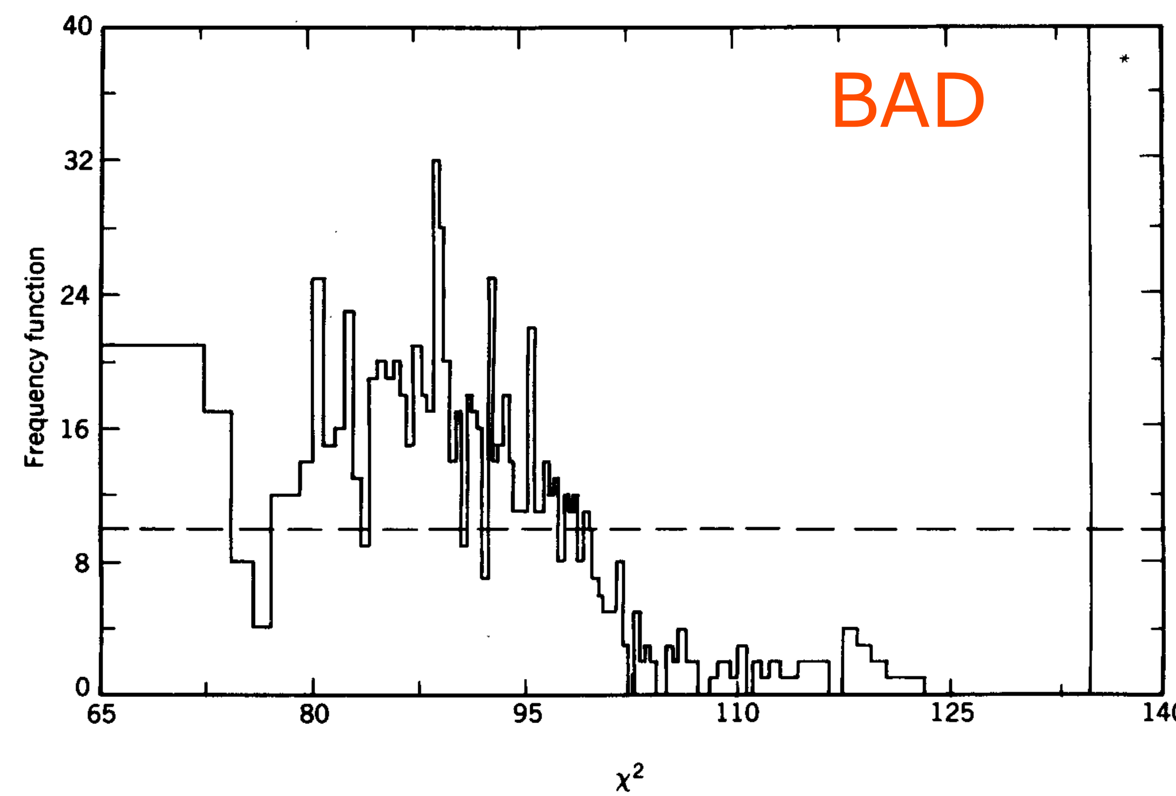


Figure A.2. The frequency function of observed values of χ^2 after 1000 samples using prn generator Eq. (A.14). The expected number of χ^2 in each bin is 10. The value of the bin indicated by (*) is offscale.

See "Numerical Recipes" on reserve or on-line (link on class webpages)

- **Chi-squared statistic** is $\chi^2 = \sum_i \frac{(N_i - n_i)^2}{n_i}$
  - **n_i (N_i) is the expected (observed) number in bin i.**
  - N_i is an integer! (Omit terms with $0 = n_i = N_i$)
  - Term with $n_i = 0$ and $N_i \neq 0$, correctly give $\chi^2 = \infty$.)
  - Large values of χ^2 indicate the "null" hypothesis, i.e. unlikely.
- The ***chi-squared probability*** is $Q(\chi^2 \mid N\text{-}1)$

  (N-1) because of "sum rule".

  The incomplete Γ-fct
  N.R. Sec. 6.2 and 14.3
- Table may help with interpreting the ***chi-squared probability***.

Probability	Interpretation
<1%	reject
1-5%	suspect
5-10%	almost suspect
10-90%	pass
90-95%	almost suspect
95-99%	suspect
>99%	reject

Recommendation: For careful work use several generators!

- For most real-life MC simulations, *passing existing statistical tests is necessary but not sufficient*.

- Random number generators are still a ***black art***.

- ***Rerun with different generators***, since *algorithm may be sensitive to different RNG correlations*.

- **Computational effort is not wasted**, since results can be *combined to lower error bars*.

- In SPRNG, relinking is sufficient to change RNGs.

Parallel Simulations

- Parallel Monte Carlo is easy? Or is it?

- Two methods for easy parallel MC:
  - **Cloning**: same serial run, different random numbers.
  - **Scanning**: different physical parameters (density,…).

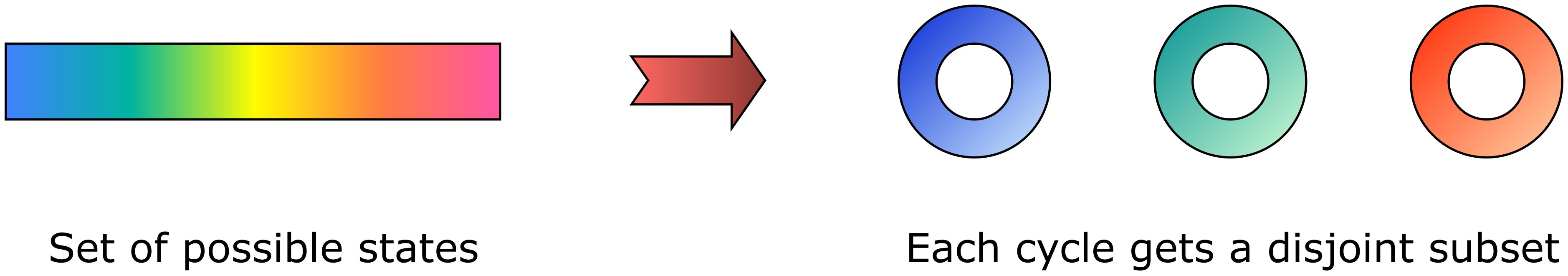
- Any parallel method (MPI, ..) can be used.

- Problems:
  - Big systems require excessive wall clock time.
  - Excessive amounts of output data generated.
  - Random number correlation?

Parallelization of RNGs

- Cycle Division: Leapfrog or Partition. Correlation problems

- Cycle Parameterization: If PRNG has several cycles, assign different cycles to each stream



- Iteration Parameterization: Assign a different iteration function to each stream

Examples of Parallel MC codes and Problems

- Embarrassingly parallel simulations. Each processor has its own simulation. Scanning and cloning.

  Unlikely to lead to problems unless they stay in phase.

- Lots of integrals in parallel (e.g. thousands of Feynman diagrams each to an accuracy of 10^{-6}).

  Problem if cycle length is exhausted.

- Particle splitting with new particles forking off new processes. Need lots of generators.

  Problem if generators are correlated initially.

- Space-time partitioning. Give each local region a processor and a generator.

  Problem if generators are correlated.