Random processes and Monte Carlo Simulation

- Applications of Monte Carlo simulations.
- Random number generators.

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- Dice: In a large number of throws, the probability of getting a given face is $\frac{1}{6}$.

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- Often need a program that generates a random variable with a given probability distribution.

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- Hardware – external sources of random numbers which are generated by from a physical process.
- Software – source of pseudo random numbers.

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- This is because computers have only a limited number of bits to represent a number.
- It implies that no matter which pseudo random number generator you use – it will always repeat itself (period of the generator).

Good random number generators

Important issues:

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Two basic techniques for RNG

The standard method of generating pseudorandom numbers use modular reduction in congruential relationships:

- Congruential methods.
- Feedback shift register methods

Linear congruent method for RNG

Generates a pseudo random sequence of numbers $\{x_1, x_2, \dots, x_k\}$ of length M over the interval $[0, M-1]$:

$$x_i = \quad \mod (ax_{i-1} + c, M) = \text{remainder}\left(\frac{ax_{i-1} + c}{M}\right)$$

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Note that

$$\mod (b, M) = b - \text{int}(b/M) * M$$

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\begin{aligned}
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$a = 4, c = 1, M = 9, x_1 = 3$ leads to the following sequence:

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x_2 =& 4 \\
x_3 =& 8 \\
x_4 =& 6 \\
x_{5-10} =& 7, 2, 0, 1, 5, 3
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interval:$0 - 8$ i.e. $[0, M - 1]$
Period: 9 i.e. M numbers (then repeat).

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- For $c = 0$ called "Multiplicative congruential generator".

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- Scale results from x_i on $[0, M-1]$ to y_i on $[0, 1]$.

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$$z_i = A + (B-A) * y_i$$

Feedback shift register generator

Simple shift register where the vacated bit is filled with the exclusive-or of two other bits in the shift register.

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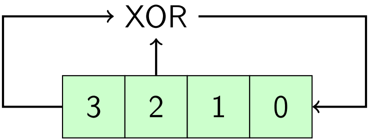

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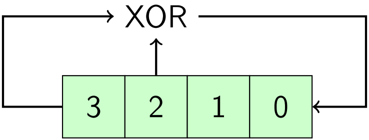

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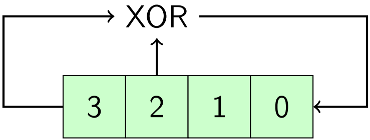

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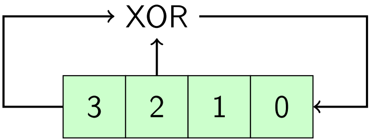

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- The register is shifted 1 step to the left.
- The result of the exclusive-or is entered into bit 0.

4bit shift register PRNG

Here is the pattern of bits, starting with 0001:

0001
0010
0100
1001
0011
0110
1101
1010
0101
1011
0111
1111
1110
1100
1000
0001

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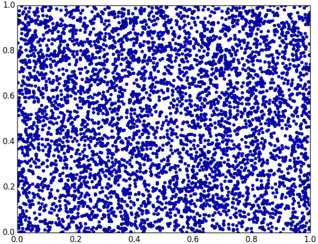
- Implemented in numpy.

How do we check the RNG?

- 2D plot, x_i and y_i from two random sequences (parking lot test).



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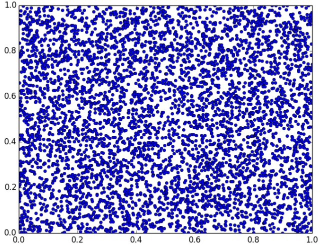

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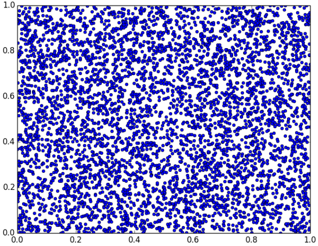
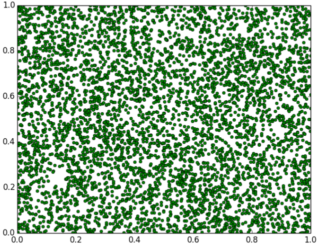


- Plot 3D figure (x_i, y_i, z_i)
- Plot correlation (x_i, x_{i+k})



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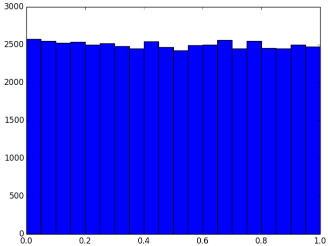
- Near neighbour correlation:

$$\frac{1}{N} \sum_{i=1}^{N} x_i x_{i+k} \approx \frac{1}{4}$$

- Uniformity (50000 random numbers)



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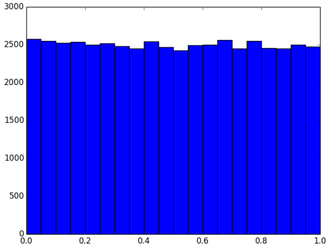

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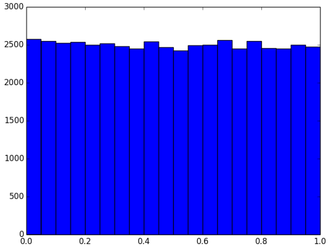

- 4th moment: (50000 random numbers)

$$< x^4 >= 0.1988$$

- near neighbor correlation: (50000 random numbers) $= 0.2478$

Test suites for RNG

Good test suites exist – TestU01 – which can be used to uncover problems in random number generators.

Dont try to invent your own random number generator – unless you know what you are doing. This is very tricky business!!!

- Monte Carlo integration.

Monte Carlo integration – basic idea

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- In principle, we can reverse the argument: we can start with an exact problem – such as the calculation of an integral – and find an approximate solution to it by running a suitable random process on the computer!
- This leads to novel ways of performing integrals..

General idea

Suppose we want to evaluate the integral:

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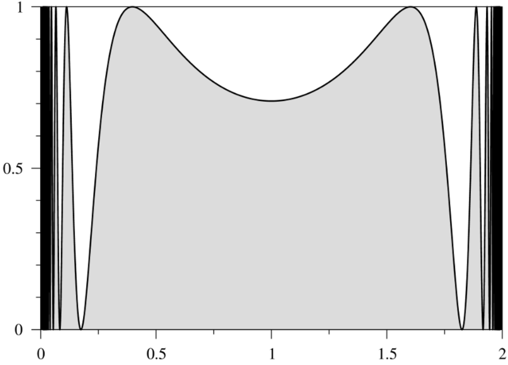

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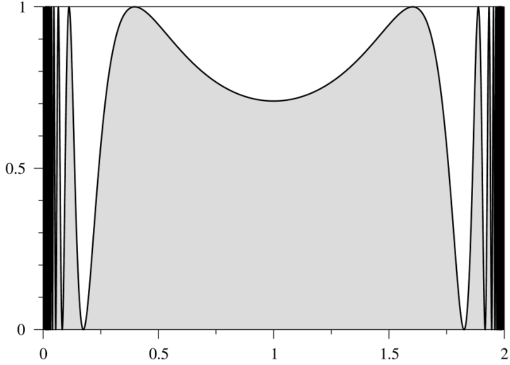

It is perfectly well behaved in the middle of its range – but varies infinitely fast at the edges.

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- Methods such as trapezoidal rule or Simpson's rule or Gaussian quadrature are not likely to work well as they will not capture the infinitely fast variation of the function at the edges.
- Monte carlo integration offers a simple way to tackle this integral.

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- We generate a large number, N, of random points in the bounding rectangle and check each one to see if it is below the curve and keep a count of the number that are – k.
- Then the fraction of points below the curve is k/N. This should be equal to the probabilitly, $p = I/A$

$$I \simeq \frac{kA}{N}$$

Example

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)}\right] dx$$

N	I
10^4	1.4542
10^5	1.45252
10^6	1.452492
10^7	1.4513378
10^8	1.45123546

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But there are $\binom{N}{k}$ ways of choosing k points from a list of N.

Total probability that we get k points below:

$$P(k) = \binom{N}{k} p^k (1 - p)^{N-k}$$

Binomial distribution!

Mean of this distribution:

$$
\begin{aligned}
< k > &= \sum_{k=0}^{N} kP(k) \\
&= \sum_{k=1}^{N} k \binom{N}{k} p^k (1-p)^{N-k} \\
&= Np \sum_{k=1}^{N} \binom{N-1}{k-1} p^{k-1} (1-p)^{(N-1)-(k-1)}
\end{aligned}
$$

$$\text{Subsitute} \quad j = k-1 \quad \& \quad M = N-1$$

$$
\begin{aligned}
&= Np \sum_{j=0}^{M} \binom{M}{j} p^j (1-p)^{M-j} \\
&= Np
\end{aligned}
$$

$< k^2 >$ of this distribution:

$$< k(k-1) > = \sum_{k=0}^{N} k(k-1)P(k)$$

$$= \sum_{k=2}^{N} k(k-1)\binom{N}{k} p^k (1-p)^{N-k}$$

$$= N(N-1)p^2 \sum_{k=2}^{N} \binom{N-2}{k-2} p^{k-2}(1-p)^{(N-2)-(k-2)}$$

$$\text{Subsitute} \quad j = k-2 \quad \& \quad M = N-2$$

$$= N(N-1)p^2 \sum_{j=0}^{M} \binom{M}{j} p^j (1-p)^{M-j}$$

$$= N(N-1)p^2$$

$$< k^2 > = < k(k-1) > + < k > = N(N-1)p^2 + Np$$

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Error in Trapezoidal rule went as $\mathcal{O}(h^2) \sim \frac{1}{N^2}$ and in Simpson's rule as $\mathcal{O}(h^4) \sim \frac{1}{N^4}$ – clearly showing that when we can use the regular methods – we should use them. This method is only good for pathological integrands.

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- A simple way to estimate $\langle f \rangle$ is to just measure $f(x)$ at N points, $x_1, x_2, \ldots, x_N$ chosen uniformly at random between a and b:

$$\langle f \rangle = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

$$I \simeq \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$

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$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

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- Variance on the sum is N times the variance on a single term or $N \mathrm{var} f$.

- Variance of the sum on N independent random numbers is equal to N times the variance of a single one.
- Random numbers in this case are the values $f(x_i)$ and we can estimate the variance of a single one of them $\mathrm{var} f = \langle f^2 \rangle - \langle f \rangle^2$ with:

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- Variance on the sum is N times the variance on a single term or $N \mathrm{var} f$.
- Error/standard deviation on the integral:

$$\sigma = \frac{b-a}{N} \sqrt{N \mathrm{var} f} = (b-a) \frac{\sqrt{\mathrm{var} f}}{\sqrt{N}}$$

which goes as $1/\sqrt{N}$ but the variance is smaller!

Multidimensional integrals

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- For higher dimensions – more than 4/5, Monte carlo method becomes faster than any of the deterministic methods!

Importance Sampling

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- The variance, σ in such cases is very high.
- Importance sampling is a way to get around this problem.

Importance Sampling

- For any general function, $g(x)$, we can define a weighted average over the interval from a to b:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx}$$

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- Setting $g(x) = f(x)/w(x)$ we have:

$$\left\langle \frac{f(x)}{w(x)} \right\rangle_w = \frac{\int_a^b w(x) f(x)/w(x) dx}{\int_a^b w(x) dx} = \frac{I}{\int_a^b w(x) dx}$$

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- Then the average number of sample that fall in this interval are $Np(x)dx$ and so for any function $g(x)$:

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b Np(x)g(x)dx$$

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- So using this the general weighted average is given as:

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- This is useful because it allows us to choose a $w(x)$ that can get rid of the pathologies of $f(x)$.
- The price we pay is that we have to draw our samples from a non-uniform distribution rather than a uniform distribution.

Error Analysis

$$\sigma = \frac{\sqrt{\mathrm{var}_w(f/w)}}{\sqrt{N}} \int_a^b w(x)dx$$

where

$$\mathrm{var}_w g = \langle g^2 \rangle_w - \langle g \rangle_w^2$$