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Computer Simulations in Statistical Physics

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Problem set 2

Proseminar

Problem 2.1 *Pseudo-Random Numbers*

Maybe the most basic pseudo-random number generator is the linear congruential generator (LCG). This generator creates a sequence of random numbers, X_n, using the recursive relation:

$$X_{n+1} = (aX_n + c) \bmod m, \tag{1}$$

with the constants

- modulus m
- multiplier $a < m$
- increment $c < m$
- “seed” $X_0 < m$.

a) Illustrate the basic properties of the sequence by setting the modulus $m = 9$ and varying the constants a, c and X_0 (pen and paper).

b) Generate a list of pairs of pseudo-random numbers, (X_{2n}, X_{2n+1}) with $n = 1, ..., 100.000$, using the LCG with constants $\{m_1 = 9,\ a_1 = 4,\ c_1 = 1\}$. Repeat for $\{m_2 = 521,\ a_2 = 364,\ c_2 = 3\}$ and then for $\{m_3 = 2^{32},\ a_3 = 1664525,\ c_3 = 1013904223\}$. Rescale the random numbers to the interval $[0, 1]$ and plot the first 1000 pairs in a 2D graph. What do you observe? Subsequently, plot the whole list.

c) Repeat the previous task with Marsaglia’s quasi-random number generator (see code-snippet).

Problem 2.2 *Box–Muller transform*

The Box–Muller transform, by G.E.P. Box and M.E. Muller is a pseudo-random number sampling method for generating pairs of independent, standard, normally distributed (zero expectation, unit variance) random numbers, given a source of uniformly distributed random numbers in the interval $[0, 1]$.

Suppose that u_1 and u_2 are independent samples chosen from the uniform distribution on the unit inteval $[0, 1]$. Then,

$$\begin{aligned} z_1 &= \sqrt{-2\ln u_1}\cos(2\pi u_2) \\ z_2 &= \sqrt{-2\ln u_1}\sin(2\pi u_2) \end{aligned} \tag{2}$$

are two independent random variables with a standard normal distribution ($\mu = 0$ and $\sigma = 1$).

a) Using the Box-Muller transform, generate a sequence of $N = 10^3$ gaussian random number with standard deviation $\sigma = 2.5$ and mean $\mu = 1$.

b) Plot an hystogram of the data.

c) Compute numerically their average value

$$\langle x \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i \ , \tag{3}$$

and their variance

$$\langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{N}\sum_{i=1}^{N} x_i^2 - \langle x \rangle^2 \ , \tag{4}$$

and compare them with the expected average μ and variance σ^2.

d) Plot the autocorrelation function

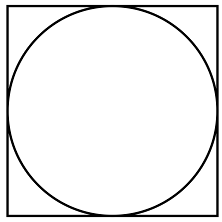
$$C_n = \frac{\langle (x_i - \mu) \cdot (x_{i+n} - \mu) \rangle}{\sigma^2} \ , \tag{5}$$

for $n = 0, 1, \ldots, N-1$ (in the previous expression the average $\langle \cdot \rangle$, is over all possible values of i: $i = 1, 2, \ldots, N-n$).

e) Repeat for $N = 10^4$.

Problem 2.3 *How To Integrate By Drawing Random Numbers*

Imagine a game in which children are randomly throwing pebbles into a square. Each pebble falling inside the square constitutes a trial, and pebbles inside the circle which is inscribed into the square are counted as "hit". This procedure is called direct sampling.



a) Construct an algorithm which enables the determination of π using this children's game. This algorithm calculates an estimator for π, called $\hat{\pi}(X)$, with random numbers $X = (x, y)$. Write down the the function for the estimator explicitly.

b) Implement the algorithm. Draw enough random numbers $X_n = (x_n, y_n)$ such that the standard error of the mean $\Delta\hat{\pi}$ is smaller than 0.0001[1]. Use a LCG with constants m_3, a_3, c_3 (see last problem).

c) Repeat the same procedure for a LCG with constants m_1, c_1, a_1.

d) Integrate the function $f(x) = x^2$ over the interval $I = [0.0, 1.0]$ using a modification of the above algorithm.

[1]As you know, the mean is calculated as $\langle\hat{\pi}\rangle = \frac{1}{N}\sum_{n=1}^{N}\hat{\pi}(X_n)$. If you do not remember how the standard error of the mean is determined, please do a short research in the literature.