Introduction to Computational Physics SS2018

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Exercise 10 from June 26, 2019
Return by noon of July 12, 2019 (added one more week)

1 Monte Carlo Integration – Importance Sampling

In the lecture Monte Carlo integration will be presented. For a function f we compute the expectation value $\langle f \rangle_p$ over a probability density function (PDF) $p(x)$:

$$\langle f \rangle_p = \int f(x)p(x)dx \approx \frac{1}{N}\sum_i^N f(x_i) \tag{1.1}$$

where the set of numbers x_i ($x_i = 1 \ldots N$) is distributed according to $p(x)$. The simple case is to use equally distributed random numbers (RN) with $p(x) \equiv 1$, but the use of suitable non-trivial PDF's $p(x)$ may provide faster convergence (see below importance sampling).

Write a program using equally distributed random numbers to do definite numerical integrations of standard functions (e.g. x^2, x^3, $\sin(x)$, $\exp(x)$, in [0,1]). Use two input parameters N and x_0 (i.e. the total number of RN's to be used, and the initial seed).

Compute the difference (the error) between your Monte Carlo result and the mathematically known result. Plot it as a function of N (log scales); also plot the variance (variation using different seeds but same N) as a function of N.

We will compare the simple Monte Carlo integration with another one using "importance sampling". This is the introduction of a new PDF $g(x)$, and use

$$\langle f \rangle = \int f(x)dx \equiv \int [f(x)/g(x)]g(x)dx \tag{1.2}$$

If $g(x)$ is small where $f(x)/g(x)$ is small and vice versa it means we are "sampling" the function $f(x)/g(x)$ preferrably where the integrand delivers significant contributions, and the error could be smaller than in the standard case (for same N). The clever choice of $g(x)$ is important for success. A simple example is, if $f(x) = \exp(-x^2)$, we use $g(x) = \exp(-x^2/2)$.

2 Importance Sampling and Random Walk (Homework)

1. Importance Sampling (10 points)

Compute the integral

$$I = \frac{1}{\pi} \int_{-\infty}^{\infty} \exp(-y_1^2 - y_2^2) dy_1 dy_2$$

numerically with Monte Carlo methods; compare equally distributed RN's again with an appropriate importance sampling.

Hints:

- first use equally distributed RN's in $[-5, +5]$
- second use importance sampling with a suitable function. Hint: use the function provided in the Box Muller algorithm* as given in the lecture.

2. Random Walk (10 points)

Construct a stochastic process, which has the probability density function

$$g(y_1, y_2) = \frac{1}{2\pi} \exp(-(y_1^2/2) - (y_2^2/2))$$

as an equilibrium distribution (Metropolis method). After an initial phase of i random walk steps store the sequence of k pairs of numbers y_1, y_2; the sequence y_1, y_2 is a stochastic representation of the underlying equilibrium distribution. For each sequence a "measurement" of the value of the integral is obtained, and the expectation value is the average of many such measurements.

Create $N = 100, 1000, 10000$ of such sequences y_1, y_2 and determine the integral as average of all measurements, and plot the error as function of N.

What is a good choice for the number of initial steps i? Just check for convergence of the result.

$\star$:

$$y_1 = \sqrt{-2 \ln x_1} \cos(2\pi x_2) \quad (2.3)$$

$$y_2 = \sqrt{-2 \ln x_1} \sin(2\pi x_2) \quad (2.4)$$

with $x_1, x_2 \in [0, 1]$.