Applications of the Monte Carlo method

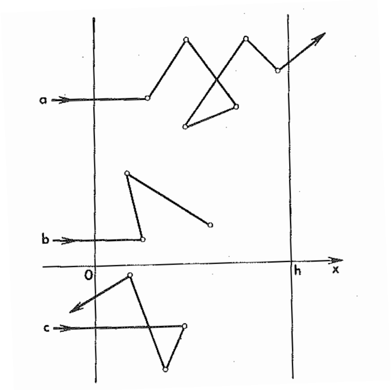
Examples

Karol Kołodziej

Institute of Physics
University of Silesia, Katowice
http://kk.us.edu.pl

Neutron transmission through a plate

The flux of neutrons with energy E_0 is incident on a homogeneous infinite plate $0 \leq x \leq h$. The angle of incidence is 90°. Upon collision with atoms of the plate material neutrons may be either elastically scattered or captured. Possible fates of a neutron are depicted below: (a) it either passes, (b) is captured, or (c) is reflected by the plate.



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We want to calculate the probability of neutron transmission through the plate p^+, the probability of neutron reflection by the plate p^- and the probability of neutron capture inside the plate p^0.

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The physical meaning of these cross sections is as follows: the probability of neutron capture upon collision with an atom is equal to σ_c/σ and the probability of scattering is equal to σ_s/σ.

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Neutron transmission through a plate

The *free path length of a neutron* λ, i.e. the length of the path from one collision to another is a random variable with the probability density

$$p(x) = \sigma e^{-\sigma x}.$$

Let us check the normalization condition, assuming that the macroscopic width of the plate h can be set ∞.

$$\int_0^\infty p(x) dx = \sigma \int_0^\infty e^{-\sigma x} dx == \sigma \left[-\frac{1}{\sigma} e^{-\sigma x} \right]_o^\infty = \sigma \frac{1}{\sigma} e^0 = 1,$$

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Similarly, let us find the expectation value of λ

$$\boldsymbol{M}\lambda = \sigma \int_0^\infty x e^{-\sigma x} dx = \left\{ \begin{array}{lcl} u = x & \Rightarrow & du = dx \\ dv = e^{-\sigma x} dx & \Rightarrow & v = -\frac{1}{\sigma} e^{-\sigma x} \end{array} \right\}$$

$$= \sigma \left[-\frac{x}{\sigma} e^{-\sigma x} \Big|_0^\infty + \frac{1}{\sigma} \int_0^\infty e^{-\sigma x} dx \right] = -\frac{1}{\sigma} e^{-\sigma x} \Big|_o^\infty = \frac{1}{\sigma}.$$

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Neutron transmission through a plate

Let us solve the formula for drawing λ values

$$\sigma \int_0^{\lambda} e^{-\sigma x} dx = \gamma,$$

where γ is the random variable uniformly distributed in the interval $(0, 1)$.

$$\sigma \left[-\frac{1}{\sigma} e^{-\sigma x} \right]_0^{\lambda} = \gamma \quad \Rightarrow \quad -e^{-\sigma\lambda} + 1 = \gamma \quad \Rightarrow \quad e^{-\sigma\lambda} = 1 - \gamma.$$

Hence

$$\lambda = -\frac{1}{\sigma} \ln(1 - \gamma).$$

However, $1 - \gamma$ is also random variable uniformly distributed in the interval $(0, 1)$, the same as γ, therefore we can write

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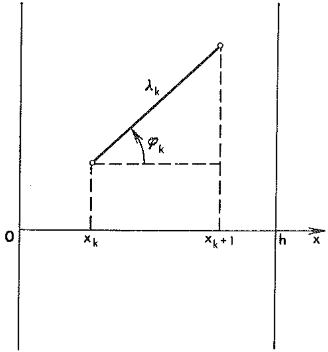
Calculation of a definite integral

We select a random direction of the neutron after scattering. As the problem is symmetric with respect to rotations about the Ox-axis, the neutron direction after k-th scattering inside the plate at the point with abscissa x_k is completely determined by the angle φ_k, as in the figure below.



We are now ready to simulate the trajectory of a neutron.

Neutron transmission through a plate

Actually, we can use the random variable $\mu_k = \cos\varphi_k$ instead, which we assume to be uniformly distributed in the interval $(-1, 1)$. Thus, we generate

$$\mu_k = \cos\varphi_k = [1 - (-1)]\gamma - 1 = 2\gamma - 1.$$

We draw the free path length

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Then we check the condition of neutron transmission through the plate

$$x_{k+1} > h.$$

If it is so, the computation of the trajectory is terminated and 1 is added to the counter of transmitted neutrons.

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Otherwise we check the condition of reflection

$$x_{k+1} < 0.$$

If it is so, the computation of the trajectory is terminated and 1 is added to the counter of reflected neutrons.

If neither of the two conditions are satisfied, i.e.

$$0 \leq x_{k+1} \leq h,$$

which means that the neutron has undergone the $(k+1)$-th collision inside the plate, we choose another value of γ and check the capture condition

$$\gamma < \frac{\sigma_c}{\sigma}.$$

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Neutron transmission through a plate

Obviously, the initial values for each trajectory are

$$x_0 = 0, \qquad \cos\varphi_0 = 1.$$

After N trajectories are sampled we obtain the following results

- N^+ neutrons were transmitted through the plate,
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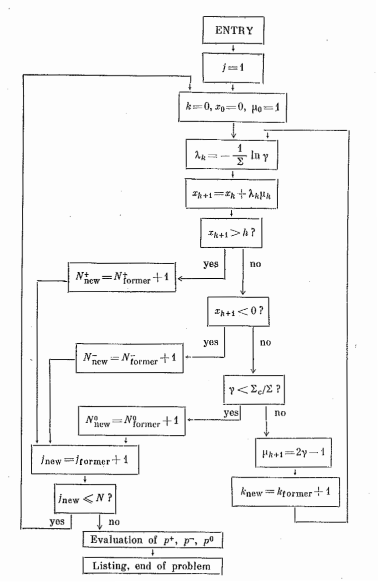
Here is the block scheme of the computer program for this problem



Calculation of a definite integral

Let us consider a function $g(x)$ defined in the interval $a < x < b$. We want to approximate the integral

$$I = \int_a^b g(x)dx.$$

Although this problem is not at all probabilistic, we will apply the Monte Carlo method to solve it.

Let us choose an arbitrary distribution density $p_\xi(x)$ specified in the interval (a, b), i.e. an arbitrary function $p_\xi(x)$ satisfying the conditions

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Calculation of a definite integral

Along with the random variable ξ defined on the interval (a, b) with the density $p_\xi(x)$, we will need another random variable

$$\eta = \frac{g(\xi)}{p_\xi(\xi)}.$$

Let us calculate the expectation value of η

$$\boldsymbol{M}\eta = \int_a^b \left[\frac{g(x)}{p_\xi(x)}\right] p_\xi(x)dx = I.$$

Let us consider now N identical independent random variables $\eta_1, \eta_2, ..., \eta_N$ and apply the central limit theorem to their sum. Then we will obtain the relation

$$\boldsymbol{P}\left\{\left|\frac{1}{N}\sum_{j=1}^{N}\eta_j - I\right| < 3\sqrt{\frac{\boldsymbol{D}\eta}{N}}\right\} \approx 0.997.$$

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$$I \approx \frac{1}{N} \sum_{j=1}^{N} \frac{g(\xi_j)}{p_\xi(\xi_j)}.$$

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However, the variance $\boldsymbol{D}\eta$, and hence the estimated error of our approximation, depends on what specific variable ξ is used. Indeed

$$\boldsymbol{D}\eta = \boldsymbol{M}\eta^2 - I^2 = \int_a^b \left[\frac{g(x)}{p_\xi(x)}\right]^2 p_\xi(x)dx - I^2 = \int_a^b \frac{g^2(x)}{p_\xi(x)}dx - I^2.$$

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The choice of the best ξ

To find the minimum of the variance

$$\boldsymbol{D}\eta = \int_a^b \frac{g^2(x)}{p_\xi(x)}dx - I^2$$

among all possible choices of $p_\xi(x)$ we will use the Schwartz inequality which for real functions $u(x)$ and $v(x)$ integrable with their squared module in the interval (a, b) has the form

$$\left[\int_a^b |u(x)v(x)|dx\right]^2 \leq \int_a^b u^2(x)dx \int_a^b v^2(x)dx.$$

Let us set $u(x) = \frac{g(x)}{\sqrt{p_\xi(x)}}$ and $v(x) = \sqrt{p_\xi(x)}$, then we will obtain

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Hence, for the variance, we will get

$$\boldsymbol{D}\eta = \int_a^b \frac{g^2(x)}{p_\xi(x)} dx - I^2 \geq \left[\int_a^b |g(x)| dx \right]^2 - I^2.$$

Now, let us choose

$$p_\xi(x) = \frac{|g(x)|}{\int_a^b |g(x)| dx}$$

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