Homework 4

Due date: 07/11/2021

Monte Carlo simulation: Importance sampling

The details can be found in the uploaded lecture notes under the subtitle "Importance sampling and Metropolis algorithm".

Instead of choosing configurations (states) randomly, then weighting them with $\exp(-E/k_B T)$, we choose configurations with a probability $\exp(-E/k_B T)$ and then weight them evenly.

Consider a particle moving in the one-dimensional space under a potential $U = \frac{1}{2}kx^2$. The probability density function for the particle position x is given by $f(x) = ae^{-U(x)/k_B T}$ in which a is a normalization constant for $\int_{-\infty}^{\infty} f(x)dx = 1$. For simplicity, we set $k_B T/k = 1$ for computational purpose.

(a) Use the Metropolis algorithm to generate a sequence of states (i.e. a sequence of particle position x, also called a Markov chain) according to the PDF $f(x) \propto \exp\left(-\frac{1}{2}x^2\right)$ and evaluate the expectation values (mean values) of x, x^2, x^3, and x^4.

(b) Plot the histogram of the x values in the sequence and compare it with the PDF $f(x)$.

Long runs are necessary for obtaining good results: (i) We must wait for a sufficiently long time to let the sequence reach equilibrium distribution; (ii) The sequence for averaging must be long enough to reduce statistical fluctuations.

Note that you can use any computer language to carry out the numerical computation.

Please submit both the computer program and the plots.