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7th Exercise Sheet Advanced Computational Physics

Will be discussed in the week December 1–December 5, 2025.

Exercise 1: Simple Monte Carlo Integration

Compute by means of Monte Carlo integration the integral

$$I = \int_0^6 \exp(-x/2) dx. \tag{1}$$

by :

1. direct integration (analytical/Monte Carlo by exponentially distributed random numbers)
2. Markov chain Monte Carlo. We are now interested in measuring the integrand, not computing the integral. To this end, choose a step size d (wisely), and update the current position x according to the Metropolis algorithm by choosing a random step of maximum length d. Don't forget that in every step you can move to larger or smaller values of x. Show that you satisfy detailed balance and think of a way to normalize your sampling procedure. Take into account that the integrand is a function of a continuous variable x.
3. Modification (advanced). Suppose the following procedure. Suppose you start with moving to the right. If you accept the move, then always choose moving to the right in the next step. If you reject the move, then start moving to the left. So, you keep moving in one direction until you have a rejection (bounce), and then you change the direction and keep moving in this direction until there is another bounce after which you change the direction again. Does this Monte Carlo Markov chain produce the right answer ?

Exercise 2: Classical One-dimensional Ising model

Write a simple Monte Carlo program to simulate the one-dimensional Ising model. Make the implementation generic so that you can easily change it to another lattice in future work. The only update we are going to consider is the single spin flip update, in which is a spin is chosen at random and flipped according to the Metropolis algorithm. Compute the magnetization, energy, spin susceptibility and spin correlation function as a function of temperature and compare with the exact results you have obtained in the first exercise sheet. Do not forget the error bars. You can also check your answer against the ALPS `https://alps.comp-phys.org` or ALPSCore `https://alpscore.org` implementations.