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Computational Physics II
SS 2018

Deadline: 16. May 2018
Please turn in a written documentation of your results and submit the programs to Jonathan Prexl at *jonathan.prexl@physik.uni-marburg.de*

4.1. Importance sampling for Monte Carlo integration

Determine the indefinite integrals

$$I_1 = \int_0^\infty x e^{-x} dx \tag{1}$$

$$I_2 = \int_0^\infty \sin(\pi x) e^{-x} dx \tag{2}$$

by introducing suitably distributed new variables.

Hint: the exact result are $I_1 = 1$ and $I_2 = \pi/(1+\pi^2)$.

4.2. Markov Chain dynamics

Simulate the 2-state Markov process with transition probabilities $w_{12} = \beta$ and $w_{21} = \alpha$ for different values of the parameters. Program the dynamics so that it follows N realizations determines the probabilities to be in either state.

The evolution of probabilities follows the rule

$$p_1(n+1) = (1-\alpha)p_1(n) + \beta p_2(n) \tag{3}$$

$$p_2(n+1) = \alpha p_2(n) + (1-\beta)p_2(n) \tag{4}$$

What is the invariant distribution $p_i(n+1) = p_i(n)$ and how quickly does it relax to this invariant distribution?

Compare the analytical results with the numerical ones for the case when all random walks start initially in state 1.

4.3. One-dimensional Ising dynamics

The 1d Ising model on a ring has N spins that can be either up or down with Hamiltonian

$$H = -J \sum_i s_i s_{i+1} \tag{5}$$

The Boltzmann weights of a certain state $\{s_i\}$ of the spin chain is given by $p = \exp(-\beta H)$, where $\beta = 1/(kT)$.

Write a program that simulates this chain and determines the mean and variance of the magnetiziation $M = \sum_i s_i$ for various temperatures $\tilde{\beta} = J/(kT)$.