Particle Methods
Spring Semester 2025

Homework 1

Due date: 12.03.2025

Create a program for a Monte Carlo simulation, designed to address the complexities of the two-dimensional Ising Model on a square lattice ($L \times L$) with periodic boundary conditions. As the lattice size extends towards infinity ($L \to \infty$), the system experiences a phase transition at the critical temperature $T_c \approx 2.269 J/k_B$. Execute the single-spin flip Metropolis-Hastings algorithm for sampling, initiating a repetitive sequence of steps to generate a Markov chain of states.

Part 1

Given the Hamiltonian

$$E = \mathcal{H}(\{\sigma\}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j,$$

which is the total energy of the system in a given configuration, compute $\Delta E = E(X) - E(Y)$, where $E(Y)$ is the same as $E(X)$ except for one spin i that changed sign. Here J is a coupling constant between neighbor spins, only 4 nearest neighbor spins are coupled (up, down, left, right). Provide the full steps derivation.
Hint: $\Delta E = 2J\sigma_i h_i$ where $h_i = \sum_{\langle i,j \rangle} \sigma_j$ is the neighbor field of spin σ_i.

Part 2

Implement the Ising Model in a 2D Lattice (of size $L \times L$) with periodic boundary conditions.

- Choose a site i;
- Calculate $\Delta E = 2J\sigma_i h_i$;
- Generate the next configuration in the Markov chain by flipping spin σ_i with probability $\min\left[1, e^{-\frac{\Delta E}{k_B T}}\right]$.

For simplicity, choose $J = 1$ and $k_B = 1$.
In order to speedup the code you can avoid unnecessary re-evaluations of the exponential function. To achieve this, use an array to store the possible spin-flip acceptance probabilities.

Part 3

The average magnetization of the system in a given configuration is defined as a sum over all spin states divided by the number of spins,

$$M = \frac{1}{L \cdot L} \sum_i \sigma_i.$$

To estimate the time average of some quantity Q, use the formula

$$\langle Q \rangle = \frac{1}{N} \sum_{k=0}^{N-1} Q_k,$$

where N is the length of the sampled Markov chain and Q_k is the value of Q in the k-th state of the chain. Measure and plot energy, $\langle E \rangle$, and absolute average magnetization, $\langle |M| \rangle$, at different temperatures T.
Before shifting to a different temperature, it is crucial to attain system equilibrium. This is achieved by running a number of iterations (N_{therm}) after the initial random initialization. To normalize the impact of system size, updates are measured in units of sweeps, with one sweep equivalent to $N_{subsweep} = L \cdot L$ single-spin updates.

For your implementation, consider the following pseudo-code:

```
Random Initialization
for N_therm do
    Metropolis-Ising algorithm
end for
for N_sample do
    for N_subsweep do
        Metropolis-Ising algorithm
    end for
    Measure quantity Q
end for
Measure average Q in time
Measure standard deviation Q in time
```

a) Determine the critical temperature T_c.
b) Study how your results depend on the system size. Consider $L = 5$, $L = 10$ and $L = 15$.
c) Plot the dependence of M on the simulation time at temperature $T < T_c$. For small systems you should be able to observe sign-flips in average magnetization M.

Parameters:

$L = 10$
$J = 1$
$k_B = 1$
Temperatures to test: [0.0, 1.0, 1.5, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5, 3.0]
$N_{therm} = 100000$
$N_{sample} = 5000$
$N_{subsweep} = L \cdot L$