Problem Set 4

In this assignment you will learn how to perform Monte Carlo simulations using Metropolis algorithm. Submit your solution using the iNTULearn site.

Q1. is compulsory for everyone. Q2. is for PAP723 students.

1. 2D ISING MODEL

Consider the 2D Ising model with $N = L \times L$ spins arranged in a square lattice. Let S_i denote the spin at site i, which can have the value +1 or -1. The system state is specified by the values of all the spins, $\{ S_i \}$. The total energy is

$$E = -J \sum_{\langle ij \rangle} S_i S_j, \quad J > 0$$

where J is the inter-spin coupling strength. In the sum, $\langle ij \rangle$ denotes pairs of nearest-neighbour i and j sites; pairs should not be double-counted. The average uniform magnetization per site is

$$m = \frac{1}{N} \sum_i S_i.$$

We will take periodic boundary conditions. For example, if the lattice has L sites in the x direction, each spin at $x = 0$ is a neighbour of the spin at $x = L - 1$ in the same row. We shall implement the Metropolis algorithm to simulate the Ising model on a square lattice of size $L \times L$.

Define the following simulation parameters

Simulation parameters	
`J`, `T`	The Ising model parameters J and the temperature T (set $J = 1$).
`L`	Number of lattice points in the x and y directions.
`nequil`	The number of Monte Carlo steps to perform for equilibration.
`nbins`	The number of bins for the measurement MC steps.
`mstep`	The number of MC steps in each bin.

Define the system variables

System variables	
`spn`	The configuratio of the system (spin at each lattice site).
`pacc`	The acceptance probabilities for a single spin flip. Pre-calculate the probabilities for all the possibilities of the initial state of the chosen spin and the state of its neighbours.
`nbor`	(optional) The nearest neighbours of each site.

Define the measurement variables

Measurement variables	
`enr`	A 1D array of length `nbins`, recording the energy per spin, E for each bin, averaged over the measurements after each MC step.
`mag`	A 1D array of length `nbins`, recording the average magnetisation M for each bin, averaged over the measurements after each MC step.
`enr2`	A 1D array of length `nbins`, recording E^2 for each bin, averaged over the measurements after each MC step.
`mag`	A 1D array of length `nbins`, recording M^2 for each bin, averaged over the measurements after each MC step.
`be`,`bm`,`be2`,`bm2`	local variables in a bin to record the energy, magnetisation and their squared values.

Initialise the `spn` array to a random initial state.

Create the `pacc` array of probabilities.

Write a function `metropolis` that uses the Metropolis algorithm to update the configuration. Choose a spin at random and flip it using the Metropolis algorithm. Do not recalculate the total energy of the configuration at each step - instead use the `pacc` array. Repeat the process N times. Remember to use periodic boundary conditions for determining the nearest neighbours of each site. This constitutes a single MC step.

Write a function `measure` to calculate the energy, magnetisation and their squared values.

Write a function `average1` to calculate the bin averages of the energy and magnetisation and the error bars using

$$\langle \mathcal{O} \rangle = \frac{1}{N_{bins}} \sum_b \mathcal{O}[b]$$
$$\Delta \mathcal{O} = \sqrt{\frac{1}{N_{bins}-1} \sum_b \left[(\mathcal{O}[b])^2 - \langle \mathcal{O} \rangle^2 \right]}$$

Write a function `average2` to calculate the bin-averaged specific heat using

$$C_v = \frac{1}{NT^2} \left[\langle E^2 \rangle - \langle E \rangle^2 \right].$$

Using all of the above, write a function `simulation` that does the following:

- Initialise the system to a random configuration.
- Calculate the acceptance probabilities.
- Equilibrate the system by performing `nequil` MC steps.
- Start the measurement runs: Create a bin and perform `mstep` MC steps. After each MC step, run `measure` to calculate the measurement variables and add them to the bin variables.
- At the end of each bin, calculate the average values of the measured observables and record them in the `enr`, etc. arrays.
- Repeat the process for `nbins` bins.
- After completing `nbins`, average the measured quantities over the bin values and the associated error bars.

For all the functions use appropriate arguments and output variables as you deem fit.

Write a program, which runs the Ising model simulation for several different values of $T (0.1 < T < 4.0)$, and plots the following equilibrium thermodynamic variables as a function of T:

- The absolute value of the magnetization $\langle |m| \rangle$
- The specific heat $C_v = \frac{1}{NT^2} \Big[\langle E^2 \rangle - \langle E \rangle^2 \Big]$.
- The magnetic susceptibility $\chi_m = \frac{N}{T} \langle |m|^2 \rangle - \langle |m| \rangle^2$.

Choose $J = 1.0$ and a lattice of size $N = L \times L = 16 \times 16$. Choose `nequil` = `mstep` = 10000 and `nbins` = 10. When calculating M, C_v and χ_m, include only values after the system has reached equilibrium.

You should be able to observe a ferromagnetic-to-paramagnetic transition: at high temperatures ($T > T_c$) the magnetisation is small. As the critical temperature is approached, the magnetisation grows rapidly and saturates to a constant value at low temperatures. What is the value of the critical temperature? What is the behaviour of the other observables across the transition?

Repeat the simulation for multiple system sizes to check the effects of finite size lattices.

2. AUTOCORRELATION IN THE 2D ISING MODEL

Using the codes developed for the previous problem, write a program to calculate the autocorrelation in the magnetisation for the 2D Ising model simulation using the metropolis algorithm. For this problem, use a single bin with 1000 MC states. Calculate the autocorrelation for $\tau = 0, \ldots, 100$ MC steps for different temperatures and show that the autocorrelation gets longer as $T \to T_c$.