THE UNIVERSITY OF HONGKONG
DEPARTMENT OF PHYSICS

Exercise sheet #4

Course: *Machine Learning in Physics (PHYS3151)* – Professor: *Dr. Ziyang Meng*
Due date: *Apr. 14th, 2022*

1. Background information

1.1. Ising model.

The Ising model is named after Ernst Ising, Ph.D. in Physics (1924) from the University of Hamburg under the supervision of Wilhelm Lenz. Ising solved the one-dimensional (1D) Ising model exactly to find no phase transition. He also provided arguments on why there would not be a phase transition in higher dimensions either. In 1936, Peierls argued that both 2D and 3D Ising models admit phase transitions. The system undergoes a second order phase transition at the critical temperature $T_c \sim 2.269$. For temperatures less than T_c, the system magnetizes, and the state is called the ferromagnetic or the ordered state. This amounts to a globally ordered state due to the presence of local interactions between the spin. For temperatures greater than T_c, the system is in the disordered or the paramagnetic state. In this case, there are no long-range correlations between the spins.

The two dimensional Ising model, as illustrated in Fig.1, consists of a square lattice with a spin S on each site. The spin can only take two values: +1 or -1.

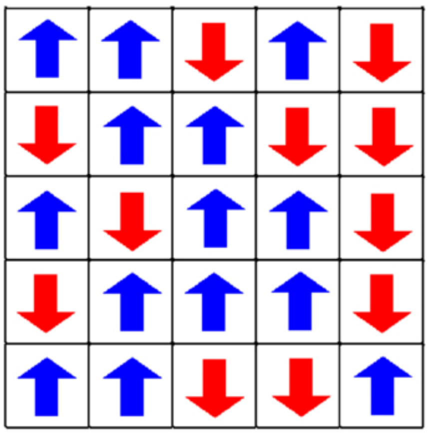

Figure 1: The schematic plot of 2D Ising model

The energy of the whole lattice is defined as the sum of the interactions of the spins with their nearest neighbors.

$$E(C) = -J \sum_{\langle i,j \rangle} S_i S_j \tag{1}$$

C refers to a configuration of the spins on the lattice sites. For a N-site system, $C = \{S_1, S_2, ..., S_N\}$ with $S_i = \pm 1$. J is a constant and here we set $J = 1$.

1.2. Physical observables.
The magnetization of the system for a certain configuration is defined as

$$m(C) = \frac{1}{N}\sum_i S_i \tag{2}$$

where $N = L^2$. After the system is fully thermalized, the expected value for a physical observable A can be evaluated by

$$\langle A \rangle = \frac{1}{K}\sum_{\{C_j\}} A(C_j) \tag{3}$$

where K is total number of configurations. Here we use the standard deviation as the error bar

$$\sigma = \sqrt{\frac{\sum_{i=1}^{M}(A_i - \mu)^2}{M}} \tag{4}$$

where M is the total number of measurements of A. μ is the mean value of A

$$\mu = \frac{1}{M}\sum_{i=1}^{M} A_i \tag{5}$$

From these definitions we can measure the expected value of energy and magnetization of the system. Also, the specific heat C and susceptibility χ can also be evaluated by

$$C = \frac{1}{N}\frac{d\langle E \rangle}{dT} = \frac{1}{NT^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

and

$$\chi = \frac{1}{NT}(\langle M^2 \rangle - \langle |M| \rangle^2) \tag{7}$$

where $M = \sum_i S_i$.

1.3. Monte Carlo Simulation.
The procedure of Metropolis algorithm for Monte Carlo simulation is shown below.

1. Initialize the lattice (randomly generate a configuration among $\{\pm 1, \pm 1, ..., \pm 1\}$ as the initial configuration). Set the lattice size L and the temperature T.
2. Randomly choose a spin. Consider to flip the spin S_i to $-S_i$. Calculate the change of the energy of the system (ΔE) due to the flip.
   - If $\Delta E < 0$, then accept the flip;
   - Else, accept the flip with $P = e^{-\Delta E/T}$
3. Consider $L \times L$ times of step 2 as one Monte Carlo iteration, and monitor the behaviour of physical observable as function of iterations.

2. Project content

Please use the Metropolis algorithm to perform the Monte Carlo simulation of the 2D Ising model and finish the following tasks.

1. Draw the dynamics of any observable you like discussed above (A vs. iterations) at $T = 0.5, 2.27, 4$. For each temperature, please show that the observable converges after certain steps with only a small thermal fluctuation.

2. Draw $\langle|m|\rangle$,$\langle m^2\rangle$, $\langle E\rangle/N$, $\langle C\rangle$, $\langle\chi\rangle$ versus the temperature from $T = 0.25$ to 4 with 0.25 as footstep with errorbars for $4 \times 4, 6 \times 6, 8 \times 8, 10 \times 10$ systems.

3. According to the $M(T)$ curve of 10×10 system you obtained in the last question, generate 5000 random spin configurations at each temperature (total 8×10^4 configurations) and make sure the configuration has the same M as your previous $M(T)$ curve. Then randomly choose 5000 spin configurations from these 8×10^4 configurations, and perform PCA on these faked configurations and compare with the one in *Ising model PCA.ipynb*, what is the difference and why there is the difference?

3. Reference Materials

Some useful materials:

- The basic concept of Monte Carlo simulation, including the statistical mechanics, importance sampling, detailed balance, and the Metropolis algorithm for the Ising model:
  http://physics.bu.edu/ py502/lect5/mc.pdf

- Classical Monte Carlo and the Metropolis algorithm for 2D Ising model:
  https://www.phas.ubc.ca/berciu/TEACHING/PHYS503/PROJECTS/05dominic.pdf