Homework 9

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1 Problem1: Volume of hypersphere using MC

1.1 problem description

The interior of a d-dimensional hypersphere of unit radius is defined by the condition $x_1^2 + x_2^2 + \cdots + x_d^2 \leq 1$. Write a program that finds the volume of a hypersphere using a Monte Carlo method. Test your program for d=2 and d=3 and then calculate the volume for d=4 and d=5, compare your results with the exact results.

1.2 algorithm description

First generate uniform random points in $[-1, 1)$ for each dimension x_i with Linear Congruential Generator.

$$M_i = (aM_{i-1} + c) \mod m \tag{1}$$

we simply choose a initial M_0, and then generate a sequence of pseudo-random integers M_i. The parameters are chosen such that m is a large prime number, a is a small integer, and c is an integer relatively prime to m. The random number in $[0, 1)$ can be obtained by dividing M_i by m.

Then get $x_i = 2Y_i - 1 \in [-1, 1)$ from the uniform distribution $Y_i \in [0, 1)$,check if the point lies within the hypersphere by evaluating the condition $x_1^2 + x_2^2 + \cdots + x_d^2 \leq 1$. Count the number of points that satisfy this condition and divide it by the total number of points generated.

The exact volume V_d of a d-dimensional hypersphere of radius r is given by the formula:

$$V_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2} + 1)} r^d \tag{2}$$

where Γ is the Gamma function. In my code, I use `math.gamma()` to calculate the Gamma function value.

1.3 output

run `problem1.py`

Dim	MC Volume	Exact Volume	Error (%)
2	3.14042	3.14159	0.04
3	4.18901	4.18879	0.01
4	4.94266	4.93480	0.16
5	5.28381	5.26379	0.38

Figure 1: Volume of hypersphere

2 Problem2: 3D Heisenberg model MC

2.1 problem description

Write a MC code for a 3D Face-Centered Cubic lattice using the Heisenberg spin model (adopt periodic boundary condition and only consider nearest neighbour interaction). Estimate the ferromagnetic Curie temperature T_c.

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \quad J = 1, \quad |\vec{S}_i| = 1 \tag{3}$$

2.2 algorithm description

Metropolis algorithm is used to simulate the Heisenberg model on a 3D Face-Centered Cubic (FCC) lattice. The key steps of the algorithm are as follows:

- **Lattice Initialization:** Create a 3D supercell FCC lattice of size $L \times L \times L$ with periodic boundary conditions. Each lattice site contains a spin vector $\vec{S}_i$ initialized randomly on the unit sphere with uniform distribution.

- **Monte Carlo Steps:** For each Monte Carlo step, randomly select a lattice site and propose a new spin orientation by generating a random vector on the unit sphere.Calculate the change in energy ΔE due to the proposed spin change using the Hamiltonian:

$$\Delta E = -J \sum_{\langle ij \rangle} (\vec{S}_i' - \vec{S}_i) \cdot \vec{S}_j \tag{4}$$

  where $\vec{S}_i'$ is the proposed new spin and the sum is over nearest neighbors, 12 in total.

- **Acceptance Criterion:** Accept the proposed spin change with probability:

$$P = \min\{u, e^{-\Delta E / k_B T}\} \tag{5}$$

  where k_B is the Boltzmann constant and T is the temperature.u is a uniform random number in $[0, 1)$.

- **Measurement:** After reaching equilibrium, measure physical quantities such as magnetization, specific heat C_v, and magnetic susceptibility χ by sampling over many Monte Carlo steps. Repeat the above steps for a range of temperatures to observe phase transitions and estimate the Curie temperature T_c.

2.3 output

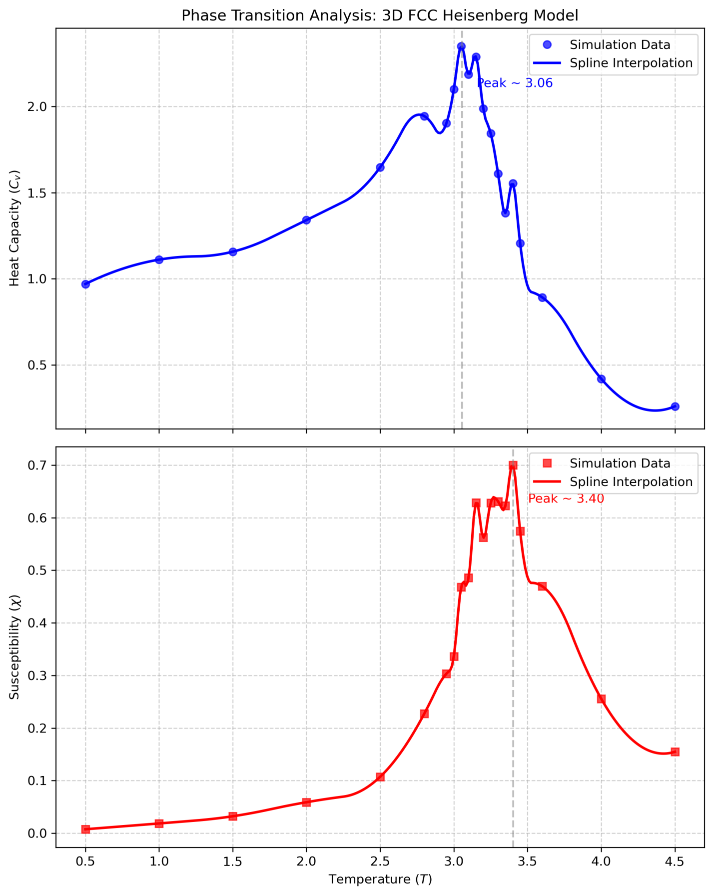

Figure 2: C_v and Magnetic susceptibility χ vs Temperature

It can be seen from the figure that C_v and χ both show a unstable peak at around $T = 3.1$, indicating the transition temperature $T_c \approx 3.1 k_B^{-1}$.