Modelling of Complex Systems

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Project 4

Phase transition in the Ising model

Part 1 — Ising model on the ring

The energy of the Ising model on a ring is

$$E = -J\sum_{n=1}^{N}\sigma_n\sigma_{n+1} - H\sum_{n=1}^{N}\sigma_n, \qquad (1)$$

where $\sigma_n = \pm 1$ and $\sigma_{N+1} \equiv \sigma_1$. The contribution of the interactions of spin σ_n with its nearest-neighbouring spins and with the external field H to the system's energy is

$$E_n(\sigma_n) = -J\sigma_n(\sigma_{n-1} + \sigma_{n+1}) - H\sigma_n \qquad (2)$$

We can choose $J = 1$ as the coupling constant. Use the Metropolis algorithm and find the dependence of the mean magnetic moment with the temperature.
Compare with the exact result:

$$\langle m\rangle(H,T) = \frac{\sinh(H/T)}{\sqrt{\sinh^2(H/T) + e^{-4J/T}}}. \qquad (3)$$

Plot $m(H,T)$ as a function of T at a fixed H.

Metropolis algorithm.

In the context of the simulation of a system of spins, the Metropolis algorithm can be summarized as follows.

1. Generate the initial microstate. It may be convenient to use all spins up ($\sigma = 1$) for the initial state since it takes less computational time. One also can use a state when spins take at random the values ± 1.
2. Choose a spin at random and flip it, i.e., ${\sigma_n}^{(new)} = -{\sigma_n}^{(old)}$.
3. At given T and H compute the change in the energy of the system due to the flipping of spin n:

$$\Delta E_n = E_n\left({\sigma_n}^{(new)}\right) - E_n\left({\sigma_n}^{(old)}\right). \qquad (4)$$

4. If ΔE_n is less than or equal to zero, accept the new microstate (set $\sigma_n = {\sigma_n}^{(new)}$), and go to step 8.
5. If ΔE_n is positive, compute the quantity $w = e^{-\Delta E_n/T}$.
6. Generate a random number r in the unit interval [0, 1).
7. If $r < w$, accept the new microstate ($\sigma_n = {\sigma_n}^{(new)}$); otherwise keep the system in the previous microstate ($\sigma_n = {\sigma_n}^{(old)}$). The quantity w is the probability of accepting a new microstate with a higher energy than the previous microstate.
8. Determine the value of the desired physical quantities. We are interested in the magnetization per spin

$$m^{(a)} = \frac{1}{N}\sum_{n=1}^{N}{\sigma_n}^{(a)}, \qquad (5)$$

where the index a labels the microstates.
9. Repeat steps (2) through (8) many times to obtain a large number of microstates.
10. Periodically (once every 100 microstates) compute averages over the microstates. Skip first 100 microstates because the system is very far from equilibrium.

$$\langle m \rangle = \frac{1}{t} \sum_{a=1}^{t} m^{(a)} \qquad (6)$$

Here t is the total number of microstates. Analyse how $\langle m \rangle$ depends on t. In order words, calculate $\langle m \rangle$ after the first 100 microstates (summation from $a = 1$ to $a = 100$), then after 200 microstates (summation from $a = 1$ to $a = 200$), then after 300 microstates and so on (summation from $a = 1$ to $a = 100 \times k$). You will get $\langle m \rangle(k)$ where $k = 1,2,3, \ldots$. Plot $\langle m \rangle(k)$ versus $t = 100 \times k$. This plot will show how $\langle m \rangle$ tends to the equilibrium value over time.

Parameters for simulations:
Number of spins: $N = 1000$,
Number of generated microstates: $t = 100\,000$,
Temperature range: $T = [0.1, 10]$,
Temperature step: $\Delta T = 0.05$,
Magnetic field: $H = 0.1$.

Part 2 — Ising model with all-to-all interaction (long-ranged interaction)

The energy of the Ising model with the long-ranged interaction is

$$E = -\frac{J}{N} \sum_{n=1}^{N-1} \sum_{n'=n+1}^{N} \sigma_n \sigma_{n'} - H \sum_{n=1}^{N} \sigma_n, \qquad (7)$$

where $\sigma_n = \pm 1$. The contribution to the system's energy of the interactions of spin σ_n with the other spins and with the external field H is

$$E_n(\sigma_n) = -\frac{J}{N} \sigma_n \sum_{n' \neq n} \sigma_{n'} - H \sigma_n \qquad (8)$$

We can choose $J = 1$ for the coupling constant.
Use the Metropolis algorithm and calculate the magnetization per spin in the microstate a

$$m^{(a)} = \frac{1}{N} \sum_{n=1}^{N} \sigma_n{}^{(a)}, \qquad (9)$$

Then, calculate the averaged magnetization and susceptibility:

$$\langle m \rangle = \frac{1}{t} \sum_{a=1}^{t} m^{(a)}, \qquad (10)$$

$$\chi = \frac{N}{T} \left[\frac{1}{t} \sum_{a=1}^{t} \left(m^{(a)} \right)^2 - \langle m \rangle^2 \right], \qquad (11)$$

where t is the total number of microstates. Compare the results of simulations with the exact results for $\langle m \rangle$ and χ given by the following equations:

$$\langle m \rangle = \tanh(J\langle m \rangle/T + H/T), \qquad (12)$$

$$\chi = \frac{1}{T \cosh^2\left(\frac{J\langle m \rangle}{T} + H/T\right) - J/T}. \qquad (13)$$

Plot $\langle m \rangle$ and χ versus T. Analyse a temperature dependence of $\langle m \rangle$ and χ near the critical point $T_c = J$.

Parameters for simulations:
Number of spins: $N = 100$,
Number of generated microstates: $t = 50\,000$,
Temperature range: $T = [0.1, 10]$,
Temperature step: $\Delta T = 0.05$,

Magnetic field: $H = 0$ and $H = 0.001$.