Ising Model & Monte Carlo method

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Ising Model:

1. Hamiltonian of the system:

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_j \sigma_j$$
$$\xlongequal{h=0} -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

   h is the external magnetic field (for simplicity we now consider $h = 0$), and $J > 0$ which means it's ferromagnetic. (And it's reasonable to consider the lowest energy state is when the spins are all $+1$.)

2. Total Energy at configuration $\{\sigma_i\}$:

$$E_{\{\sigma_i\}} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_j \sigma_j$$

3. Spin state σ_i is differed by

$$\sigma_i = \begin{cases} +1 \\ -1 \end{cases}$$

4. Configuration probability:

$$P_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta}$$

   where $\beta = (k_B T)^{-1}$ and Z_β is the partition function.

5. Partition function:

$$Z_\beta = \sum_\sigma e^{-\beta H(\sigma)}$$

Mento Carlo Method (Metropolis Method):

Given L^d lattice point. (For instance $d = 1$, which means 1-d Ising model.)

(1) Generate a initial state (let's call it state one) by pseudo random number;

(2) Flip over a single point to generate a new state (let's call it state two);

(3) If $E_1 > E_2$, the energy of the whole system decreases, $W(1 \to 2) = 1$, the system goes to state two;

(4) If $E_1 < E_2$, to make the whole system obey Boltzman distribution, generate a random number between 0 and 1 to compare with $W(1 \to 2) = e^{-\beta \Delta E}$, where $\Delta E = E_2 - E_1$; if the random number is smaller than W, the system goes to state two, otherwise, it remains in state one;

(5) Now we call the current state state one and go back to step 2, repeat it for sufficient many times to reach equilibrium;

(6) Calculate the magnetization at the current temperature;

(7) Move to the next temperature and go back to step one till a certain temperature;

(8) Plot magnetization versus temperature and obtain the critical temperature. (However, the magnetization isn't exactly accurate, so the accuracy of critical temperature is somehow unsatisfying. The analytic result is around 2.26 with my parameters, but the result I have is near 2.0.)

Note that my results are based on the simplification that spin has the values of only +1 and -1. Simple modification can expand it to vector (which obviously make it harder to calculate). But there's another complication: the spin state cannot be simply filp over.

All my codes and results can be found in https://github.com/Turgon-Aran-Gondolin/C_Primer_Files/tree/master/Monte_Carlo/2-d_Ising_Model.