Magnetism: Part 1

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We work with the Ising model in two dimensions. In practice, this means that you have a square lattice of $N = L \times L$ spins. For a configuration of spins

$$S = (s_1, \ldots, s_N)\,, \tag{1}$$

the energy is given by

$$\boxed{E(S) = -\frac{1}{2} J \sum_{i=1}^{N} \sum_{j \in \text{neighbors of } i} s_i s_j - B \sum_{i=1}^{N} s_i}\,, \tag{2}$$

with $s_i = \pm 1$, J the exchange interaction, and B an external field.

If the total number of configurations is K, the thermal average of a quantity $A(S)$ is

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{K} A(S_i) e^{-\beta E(S_i)} \tag{3}$$

with the partition function $Z = \sum_{i=1}^{K} e^{-\beta E(S_i)}$. The free energy of the system is given by[1]

$$F = E - TS = -\frac{1}{\beta} \ln(Z) \tag{4}$$

The value of the total magnetization for a configuration S is given by $M(S) = \sum_{i=1}^{N} s_i$ and its average value

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{K} M(S_i) e^{-\beta E(S_i)}\,. \tag{5}$$

You will often work with the mean magnetization per site $m = \langle M \rangle / N$.

1. Derive some equalities needed in your computations.

[1] Do not confuse the entropy S in the expression of F with the spin configuration.

a) Show that the magnetization (at constant temperature) can be obtained as

$$\langle M \rangle = -\frac{\partial F}{\partial B} \,. \tag{6}$$

The magnetization is the order parameter of the model, characterizing its different phases (Figs. 4 and 5 of the lecture notes). For $T < T_c$, M is discontinuous crossing the $B = 0$ line, so this phase transition is "first order" (discontinuity in the first derivative of the free energy). Through the critical point, M is continuous, so the transition is also named "continuous".

b) The magnetic susceptibility (at constant temperature) is the response of the magnetization to a change in the external magnetic field and is defined as

$$\chi = \frac{\partial \langle M \rangle}{\partial B} \,. \tag{7}$$

Show that χ can be expressed in terms of the fluctuations of the magnetization as

$$\chi = \beta \left[\langle M^2 \rangle - \langle M \rangle^2 \right] \,. \tag{8}$$

Hint: Simply take the derivative in Eq. 7 and think how B couples to M in $E(S)$.

2. In the Ising model with N spins, how many spin configurations S are there? If a computer can perform the sums in the averages above with a timing of one billion configurations S per second, how much time do you need for $L = 5$? And for $L = 10$?
For a realistic system, summing over all configurations is not an option! We use Monte Carlo sampling to obtain the most thermally relevant configurations in the averages.

3. A few simple questions about Monte Carlo and the Metropolis algorithm, which is summarized in Section 2.5 of the lecture notes.

You want a sequence of spin configurations $\{S_0, S_1, \ldots\}$ distributed as $P(S) = e^{-\beta E(S)}/Z$.

If you move through space with a transition probability $W(S \to S')$ that satisfies "detailed balance":

$$\boxed{P(S)W(S \to S') = P(S')W(S' \to S)} \tag{9}$$

and if the process is ergodic (i.e. you can explore all space), then, the sequence

$$S_1 \xrightarrow{W} S_2 \xrightarrow{W} \ldots \xrightarrow{W} S_{N_{\mathrm{MC}}} \tag{10}$$

will be asymptotically distributed like $P(S)$ and you can compute your averages as

$$\boxed{\langle A \rangle \approx \frac{1}{N_{\mathrm{MC}}} \sum_{i=1}^{N_{\mathrm{MC}}} A(S_i) \,.} \tag{11}$$

To this aim, you factorize W in a probability of updating and of accepting the move:

$$W(S \to S') = T(S \to S')A(S \to S') \,. \tag{12}$$

In your code, you choose $T(S \to S')$ (e.g. flip the spin) and determine $A(S \to S')$ so that Eq. 9 is satisfied.

a) If you propose a move $S \to S'$ by flipping a spin chosen randomly on the lattice, is your transition probability T symmetric, namely, is $T(S \to S') = T(S' \to S)$? Explain.

b) Show that the original choice of A by Metropolis (valid for a symmetric T),

$$A(S \to S') = \min\left\{1, \frac{P(S')}{P(S)}\right\}, \tag{13}$$

satisfies detailed balance (Eq. 9).

c) If the move is rejected, do you need to add the current value of $M(S)$ a second time in your average of the magnetization? Explain why.

4. You will begin your simulations with a **paramagnet**. Therefore, set $\boxed{J = 0}$.

To avoid doing any brute force programming, try to think about the problem and the form of $E(S)$. Answering the questions a), b), and c) should help you.

a) At each step, you need to compute $E(S') - E(S)$ to accept/reject the move where S' and S only differ by one spin flip. How can we compute this energy efficiently?

Hint: Write out the two energies and compute the difference.

b) How can you use the answer to question a) to compute efficiently $M(S')$ if you know $M(S)$ at the previous step?

c) If we want to plot and analyze $m(S) = M(S)/N$ over the sequence (or other averages), do you need to store the spin configurations of the whole sequence $\{S_0, S_1, \dots\}$?

Discuss the answers to 4.a), 4.b), and 4.c) with us before starting to program.

Note: There are two variables in your problem, the temperature (or the inverse temperature β) and the magnetic field B. However, only the product βB enters in $\beta E(S)$. For simplicity, set $\beta = 1$ and only use B as free parameter.

5. For the paramagnet, choose $L = 10$ and start with one value of B (e.g. $B = 0.5$).

Recall that the exact result for the average magnetization per spin is:

$$m = \tanh(\beta B)\,. \tag{14}$$

a) Perform a few Monte Carlo simulations and plot $m(S_k) = M(S_k)/N$ for the different runs. Does the behavior of $m(S)$ change significantly from one run to the other?

Hint: To begin, use $N_{\mathrm{MC}} = 2000$, so the run takes a few seconds and not minutes!

b) It will take some Monte Carlo steps (κ) before the system is equilibrated. How long is your equilibration time κ if you start from a random configuration?

Note: These first κ configurations will not be included in the averages.

c) Compute the average magnetization discarding the equilibration steps. Give an estimate of the error on the average magnetization computed with $N_{\mathrm{MC}} = 2000$.

Hint: You cannot estimate the error from just one measurement of the average: Comparing with the exact value is not a good measure (you might have been lucky).

d) If the data are independent, one can compute the error on the average magnetization per site as

$$\Delta_m = \sqrt{\frac{\langle m^2 \rangle - \langle m \rangle^2}{N_{\rm MC} - 1}} \tag{15}$$

If you compare to what you have found in c), is Δ_m a good estimate of the error on the average?

If the answer is positive, your data are probably reasonably decorrelated (nearly independent samples). If the answer is negative, your data are correlated and you have an effective smaller number of data points which are independent.

e) What is the impact of the choice of L on your simulation? Explain your findings as regards κ, the length of the run, the average magnetization, and the fluctuations of the magnetization around the average.

Hint: Perform the calculations with $L = 5$ and $L = 15$.

6. Since from one step to the next you only vary one spin, it is better to establish a simulation "time" unit so that a Monte Carlo step corresponds to $N = L \times L$ attempts of random spin flips. In this way, the probability of a given spin having been selected after a time unit should be N independent.

   a) Modify the code and store $m(S)$ only after each "unit" Monte Carlo step (i.e. after $N = L \times L$ spin flips).

   b) What is the equilibration time κ? How does it relate to the value you had obtained in point (5)?

   c) Compute the error on the magnetization per site, Δ_m, using the magnetization values computed only after each "unit" step. Is this a good estimate of the error on the average magnetization?

7. Perform the simulations for different values of B between -2 and $+2$. Compute the magnetization and compare with the exact values. Produce a plot of $m(B)$.

   Hint: Make a function (dependent on B) of the previous program.

8. For the paramagnet, compute the susceptibility in the interval $-2 \leq B \leq 2$.

   a) Use the formula in terms of the fluctuations of the magnetization (Eq. 8).[2] Compare your results with the analytical solution

$$\frac{\chi}{N} = \beta \frac{1}{\cosh^2(\beta B)} \,. \tag{16}$$

   b) You could also compute χ by finite differences as a derivative of $\langle M \rangle$ (Eq. 7). Select $B = 1$ and investigate what is the effect of changing the small displacement ΔB in the computation of χ as a derivative. Can you explain your result?

[2] Note that $\chi = N^2 \beta [\langle m^2 \rangle - \langle m \rangle^2] = N \beta [\langle s^2 \rangle - \langle s \rangle^2]$. To have a quantity independent on the size of the system, plot $\chi/N = N\beta[\langle m^2 \rangle - \langle m \rangle^2]$.

9. **Optional exercise on blocking analysis**. In a Monte Carlo run with the Metropolis algorithm, the data are correlated. This means that if you perform $N_{\rm MC}$ steps to compute m, you have a smaller effective number of independent steps $N_{\rm eff} = N_{\rm MC}/T_c$, where T_c is the correlation time for the quantity you are averaging. Therefore, your error should be be proportional to $\sigma_m/\sqrt{N_{\rm eff}}$ and, consequently, larger than what you obtain by treating all samples as independent.

   A way to analyze the correlation time and to estimate the error is to perform a so-called blocking analysis. The idea is that you divide your data in blocks of $N_{\rm steps}$ so that $N_{\rm steps} \times N_{\rm blocks} \approx N_{\rm MC}$ (Fig. 1). You then compute the average for each block (over the $N_{\rm steps}$) and you treat these averages as your data points. You evaluate the error for this reduced number $N_{\rm blocks}$ of data points.

   Plot this errorbar as a function of $N_{\rm step}$ ranging from 1 (no blocking) to a value $< N_{\rm MC}$. The plateau should give you an estimate of the error and of the correlation time (from the value of $N_{\rm step}$ where you reach the plateau).

   Hint: Compare a run where you compute $m(S)$ after each spin flip with a run where you compute $m(S)$ after every N spin flips.

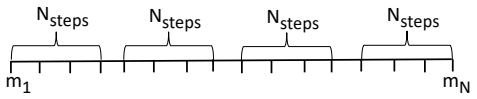

Figure 1: The data are blocked over $N_{\rm steps} = 4$.