Computational Assignment 5: The Two-Dimensional Ising Model

Philip Cherian

November 2, 2023

In this computational exercise, you will learn a very powerful Monte Carlo procedure for simulating systems that exchange energy with a heat-bath at a some fixed temperature T, known as the Metropolis Algorithm. Since we can only sample a finite number n of the total number of microstates, if we want to estimate a physical quantity A we would need to approximate

$$\langle A\rangle \approx A_n = \frac{\sum_{s=1}^{n} A_s e^{-\beta E_s}}{\sum_{s=1}^{n} e^{-\beta E_s}}, \tag{1}$$

where A_s is the value of the physical quantity A in the microstate s. In principle, we could use Equation (1) to estimate $\langle A\rangle$, but it is very inefficient since our randomly chosen microstates will usually be highly improbable and will therefore have a negligible contribution to $\langle A\rangle$. To solve this, we choose to generate our microstates from some probability distribution π_s, which makes certain microstates "more" likely than others. However, if we do this, we have a biased sample and if we wish to average over such a sample generated according to π_s, we also need to weight each microstate by $1/\pi_s$ to eliminate the bias. Now, in principle, any form of π_s could be used, but a reasonable choice of π_s is the Boltzmann probability itself, i.e. we could choose

$$\pi_s = \frac{e^{-\beta E_s}}{\sum_{s=1}^{n} e^{-\beta E_s}}. \tag{2}$$

Using this definition, it should be trivial to show that

$$\langle A\rangle \approx A_n = \frac{1}{n}\sum_{s=1}^{n} A_s. \tag{3}$$

Thus, instead of choosing the configurations randomly and then weighting them with $\exp(-\beta E)$, this method *chooses* configurations with a probability $\exp(-\beta E)$ and weights them evenly.[1] The algorithm to do this is as follows:

- Begin by establishing your system in an initial, arbitrary, microstate.
- Choose a spin at random and try to flip it (i.e. try changing $\sigma_i \to -\sigma_i$).
- Compute the change in energy that this flip would cause:

$$\Delta E = E_{\text{trial}} - E_{\text{old}}.$$

[1] The exact mechanics of this method are a little complex, so don't worry if you don't understand it completely. Just follow the algorithm exactly.

- If $\Delta E \leq 0$, the trial is always accepted. If not, it is accepted with a probability $e^{-\beta\Delta E}$. To enforce this:
  - Compute the quantity $w = e^{-\beta\Delta E}$.
  - Generate a uniform random number r between 0 and 1.
  - If $r \leq w$, accept this flip, otherwise do nothing.

  This method makes sure that microstates are chosen with a probability given by the Boltzman distribution.
- Determine the values of desired physical quantities (like the system's energy, or its magnetisation).
- Repeat this process a large number of times to sample a sufficient number of microstates.
- After a sufficiently large number of microstates have been sampled, start averaging the physical quantities.

We will apply this problem to the two-dimensional Ising model whose energy (in the absence of an external magnetic field) is given by:

$$E = -J \sum_{<p,q>} \sigma_p \sigma_q, \tag{4}$$

where p and q are points on a lattice, and $< p, q >$ represents a sum over nearest neighbours. For a two-dimensional square lattice of length L, this sum can be written explicitly as

$$E = -\frac{J}{2} \sum_{i=1}^{L} \sum_{j=1}^{L} \sigma_{i,j} \left(\sigma_{i,j+1} + \sigma_{i,j-1} + \sigma_{i+1,j} + \sigma_{i-1,j} \right), \tag{5}$$

where $\sigma_{i,j}$ is the value of the spin at lattice-point (i, j). (The factor of half occurs because performing independent sums over i and j lead to each nearest-neighbour's contribution being counted twice.) We also assume periodic boundary conditions.

(a) In the code file provided, complete the `oneMCS` and `simulate` functions. In one Monte-Carlo step per spin – a *sweep* – N spins are chosen at random for trial changes. It is convenient to set $J = 1$, which means that we are measuring temperature in units of J.

We will be working with a square lattice of length L, meaning that the number of spins $N = L^2$. This implies that your array of `spins` must be a 2D array of dimensions $L \times L$. The contribution of each spin $\sigma_{i,j}$ to the total energy is given by

$$E_{i,j} = -J\sigma_{i,j} \left(\sigma_{i,j+1} + \sigma_{i,j-1} + \sigma_{i+1,j} + \sigma_{i-1,j} \right),$$

where the term in the parentheses is called the "nearest-neighbour sum". Remember to enforce periodic boundary conditions! [3]

(b) If you've written your `oneMCS` function correctly, you should be able to run the `animate` function for a 32×32 lattice. The `animate` function requires only an initial spin configuration and β to run. Choose all spins to be randomly oriented initially, and choose a high temperature (say, $T = 10$, i.e. $\beta = 0.1$) and look at the animation. Do all the spins remain randomly oriented? Show a snapshot of the typical configuration. [2]

(c) Next, repeat part for a low temperature (say $T = 0.5$, $\beta = 2$). Is there a preferred direction? The magnetic susceptibility for our system (in the absence of an external field) is given by

$$\chi = \beta \left(\langle M^2 \rangle - \langle |M| \rangle^2 \right). \tag{6}$$

Show numerically that $\langle M \rangle \neq 0$ at low temperatures, and $\langle M \rangle \approx 0$ for high temperatures, meaning that there is some intermediate temperature where $\langle M \rangle$ is first zero. Can you estimate roughly what this temperature is? [2]

(d) You will now try to look for indicators of something called a phase transition. Start by completing the `comparingLattices` function which accepts a list of lengths (say, `Ls = [4,8,16]`, but you will get better answers for larger lattices) and simulates the 2D Ising model for each of these lattice lengths, and plots the average energy per spin, C_V per spin, $\langle |M| \rangle$ per spin, and χ (defined in part (c)). Describe these graphs. In the case of the specific heat (per spin), you should see that it has a broad maximum. What happens to this maximum as L increases? What can you infer about C_V in the thermodynamic limit $N \to \infty$? Does the graph for $\langle E \rangle$ show any indication of something special happening at some temperature? What about χ?[2] In 1942, Lars Onsager showed that for an infinite lattice $T_c = 2J/\ln\left(1+\sqrt{2}\right) = 2.269J$. Find T_c from your simulations on finite lattices, and comment on these values. [3]

[2] These graphs themselves are not enough to infer anything with any confidence, you actually need to do a detailed analysis called "finite-size scaling" before you can rigorously prove anything; the purpose of this exercise is just to show you how simulations with small lattices can still tell you about what happens in the thermodynamic limit.