Lisa Larrimore
Physics 114 - Seminar 14

Monte Carlo Simulation of the 2D Ising Model

The Metropolis Algorithm

We know that the expectation value of an observable A can be written as

$$\langle A \rangle = \frac{\sum_r A_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}, \tag{1}$$

where A_r is the value of A for the state r. So given a system that has a discrete number of states, we could, using a computer, calculate A for each state and weight these values by their Boltzman factors to find the average A. This might be feasible for a system with a small number of states, but if we have a 20×20 spin lattice interacting via the Ising model, there are 2^{400} states, so we cannot possibly examine all of them.

What if we decide to just sample some of the states? How would we decide which ones? This is where the "Monte Carlo" part comes in. Named for the Mediterranean casino town, a Monte Carlo method is any algorithm that involves a pseudorandom number generator.

One (bad) way of using random numbers would be to randomly pick a lot of states, measure A for each of them, and weight these values of A by their Boltzman factors. We might get close to the right answer if we sampled a lot of states, but we would spend a lot of time calculating A for states that contribute very little to the final result (an Ising lattice at very high temperature is unlike to be in the state with all spins pointing in one direction).

Instead of sampling (measuring parameters like A for) a lot of states and then weighting them by their Boltzman factors, it makes more sense to *choose states based on their Boltzman factors* and to then weight them equally. This is known as the Metropolis algorithm, which is an *importance sampling* technique. One pass through the algorithm is described here:

1. A trial configuration is made by randomly choosing one spin.
2. The energy difference of the trial state relative to the present state, δE, is calculated.
3. If $\delta E \leq 0$, the trial state is energetically favorable and thus accepted. Otherwise, a random number $0 \leq \eta \leq 1$ is generated, and the new state is only accepted if $\exp(-\beta \delta E) > \eta$. This condition can be rewritten as $-\beta \delta E > \log \eta$, which is what I used in the code.

Calculating Observables

We can obtain some qualitative information about our simulation by watching the spin array during a simulation. I have written an IDL program, `see_spins.pro`, that allows us to do this. For high temperatures, the spins remain randomly aligned after long periods of equilibration, whereas for low temperatures, the spins end up pointing in mostly the same direction.

To get more quantitative results, we can measure the energy and the magnetization at each step of the routine. Before we start taking statistics, we should allow the system to equilibrate for a long time (my code equilibrates for `nequil` passes). We can then measure the magnetization by taking the sum of all the spins in the lattice, and we can calculate the energy by determining the energy for each spin and dividing by two for double counting.

What about the specific heat or susceptibility? There isn't a good way to claculate a derivative of the partition function in our code, but it turns out that the specific heat can also be written in terms of the variance of the energy:

$$\begin{aligned} C_V =& \frac{\partial \langle E \rangle}{\partial T} \\ =& -\frac{\beta}{T} \frac{\partial \langle E \rangle}{\partial \beta} \\ =& \frac{\beta}{T} \frac{\partial^2 \ln Z}{\partial \beta^2} \\ =& \frac{\beta}{T} \frac{\partial}{\partial \beta} \left(\frac{1}{Z} \frac{\partial Z}{\partial \beta} \right) \\ =& \frac{\beta}{T} \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2} \left(\frac{\partial Z}{\partial \beta} \right)^2 \right] \\ =& \frac{\beta}{T} \left[\left\langle E^2 \right\rangle - \langle E \rangle^2 \right]. \end{aligned} \tag{2}$$

Incidentally, this is known as the Fluctuation Dissipation Theorem.

Similarly, the magnetic susceptibility, χ, can be written in terms of the variance in the magnetization:

$$\begin{aligned} \chi =& \frac{\partial \langle M \rangle}{\partial H} \\ =& \beta \left[\left\langle M^2 \right\rangle - \langle M \rangle^2 \right]. \end{aligned} \tag{3}$$

So by keeping statistics on E, E^2, M, and M^2, we can plot the energy, the magnetization, the specific heat, and the magnetic susceptibility. On each of these graphs, each circle represents an independent run of $100,000$ steps of equilibration and $100,000$ more steps of data taking.

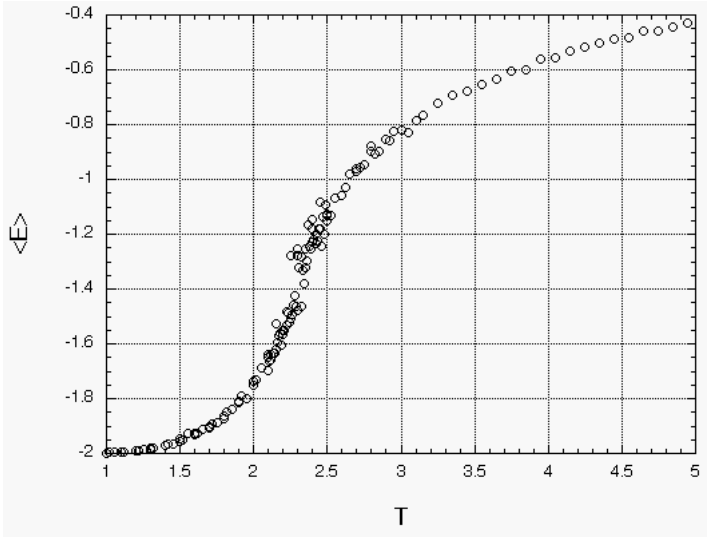

Figure 1: The energy is a continuous function of temperature, which, as we expect, increases as a function of T.

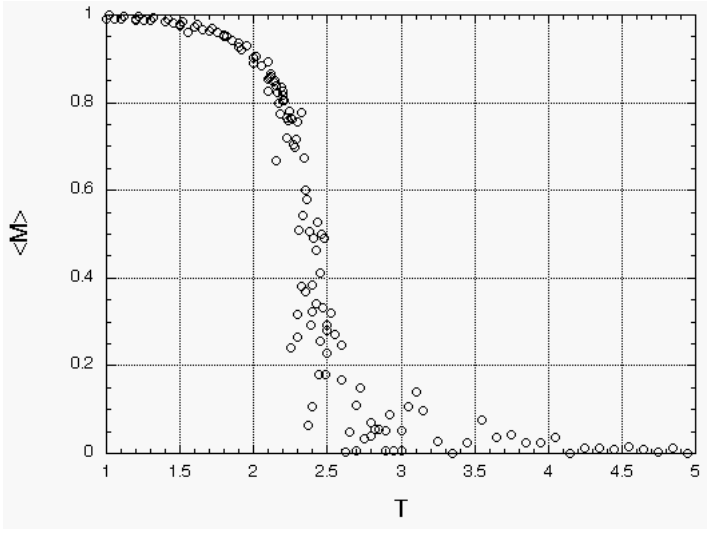

Figure 2: The magnetization drops off sharply near the critical temperature, which, in our units where $k = J = 1$, is approximately 2.3.

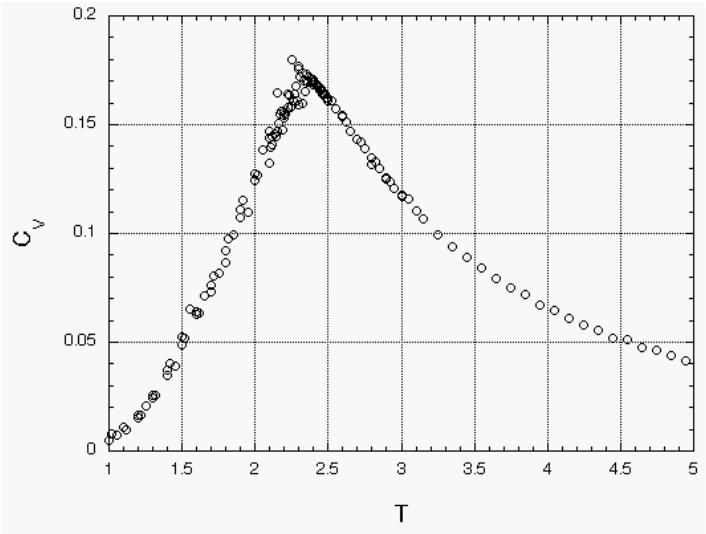

Figure 3: The specific heat has a peak at the critical temperature.

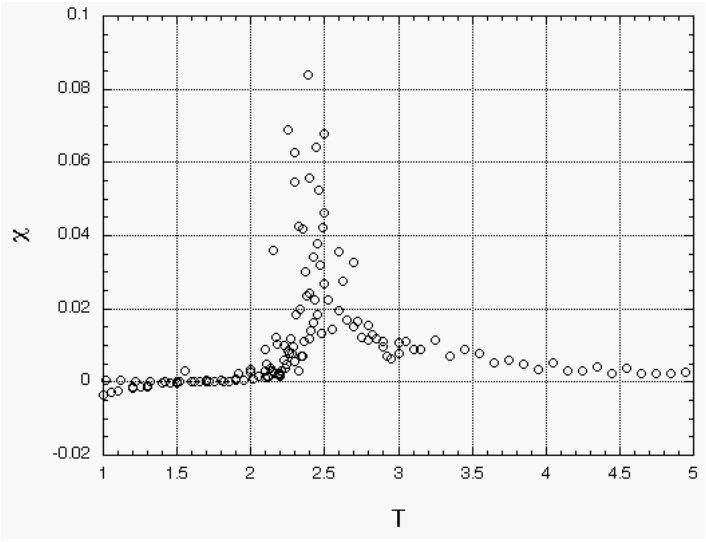

Figure 4: The magnetic susceptibility has a sharp jump at the critical temperature.