Magnetisation of the Ising Model

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In this report we produce a simulation of the Ising model using the Metropolis Monte-Carlo method. We investigate the effect of temperature and magnetic field strength on the magnetisation of the system.

1 Ising Model

The model we investigate is made of L^2 particles, each with a spin of $+1$ or -1 with coordinate s_i. The particles sit in a square lattice and interact with their 4 horizontal and vertical neighbours.

The Hamiltonian of this system is given:

$$H(s) = -H\sum_{i}^{L^2} s_i - J\sum_{\langle i,j\rangle} s_i s_j \tag{1}$$

such that the sum over the pair $\langle i,j\rangle$ is over the pairs of adjacent particles. Here, H is the magnetic field strength and J is the interaction energy, which we set to 1.

1.1 Magnetisation

It will be useful to know the maximum and minimum possible magnetisation of our system when analysing results. The magnetisation of our model is given by a summation over the spins:

$$M = \sum_{i}^{L^2} s_i \tag{2}$$

We can then evaluate the maximum magnetisation as the magnetisation of the state with all spins of $+1$, which is L^2. Similarly, with spins of -1, the minimum magnetisation is $-L^2$.

2 Monte-Carlo Simulation

To estimate the average magnetisation $\langle M\rangle$ for a given temperature and field strength, we produce configurations of atoms with the Metropolis algorithm. Trial moves are generated randomly, either flipping all spins (with probability $\frac{1}{L^2+1}$) or flipping the spin of a single particle, chosen randomly.

To estimate an error for our magnetisations we use block averaging once the particle has reached equilibrium. We must first chech how many iterations of the algorithm the particle takes to reach equilibrium, and that the equilibrium is constant.

We can plot the magnetisation of the particle over a short period - to inspect closely the equilibrium time - and a longer period - to ensure the model reaches a constant equilibrium.

Figure 1 shows that the system reaches an equilibrium around 500 timesteps. In further simulations, we will ignore the first 1000 to avoid the equilibriation period affecting our averages.

Figure 2 shows us that the system reaches a constant equilibrium over the course of our simulation.

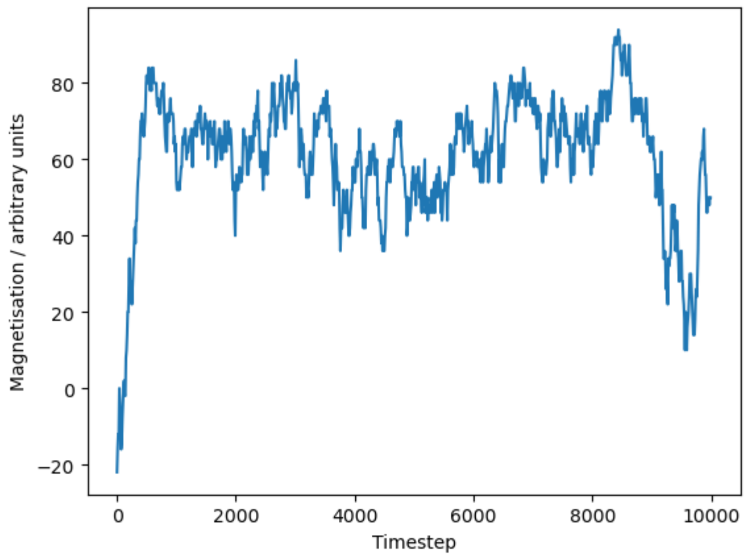

Figure 1: The magnetisation of the Ising model with 100 particles, a field strength $H = 1$ and a temperature of $t = 4$ in a Metropolis Monte-Carlo simulation of 10 000 timesteps. We can see that the magnetisation oscillates about equilibrium after around 500 simulation steps.

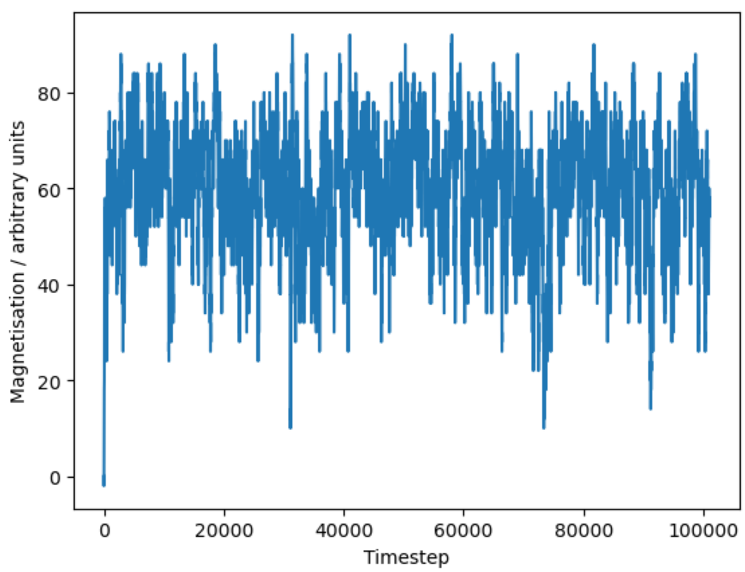

Figure 2: The magnetisation of the Ising model with 100 particles, a field strength $H = 1$ and a temperature of $t = 4$ in a Metropolis Monte-Carlo simulation of 100 000 timesteps. We can see that the magnetisation oscillates about a constant equilibrium for this timescale.

2.1 Estimating Error

When taking block-averages to calculate ensemble averages and errors, we must ensure we do not underreport the error with blocksizes which are too small. In figure 3 we compare the errors for a range of block sizes and see that a block size of 250 correctly reports the maximum errors. We wil use a blcok size of 250 for averaging in this report.

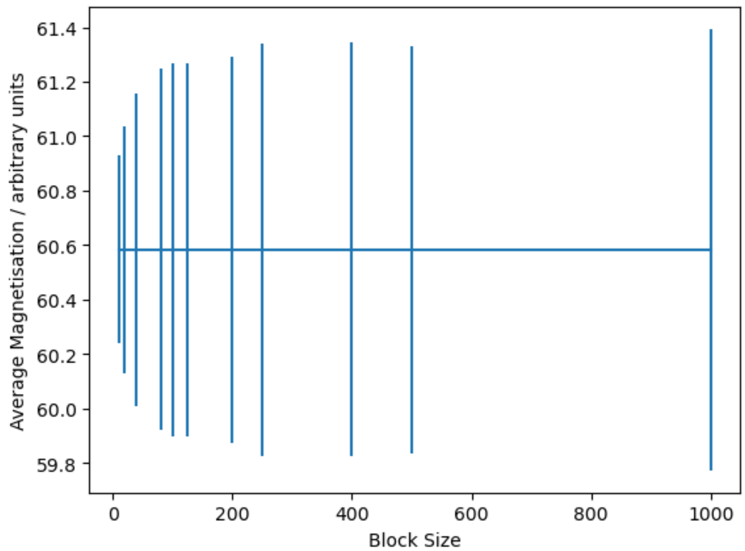

Figure 3: The dependance of the estimates for the magnetisation of 100 particles in the Ising model on the size of the blocks they were calculated from with a Monte-Carlo simulation. Error estimates are shown with the vertical bars. The error calculations were performed using 10 000 data points. Error is underestimated with a small block size.

3 Results

Plotting the magnetisation for temperatures $t = 2, 4$ and 8 over a range of magnetic field strengths gives us figure 4.

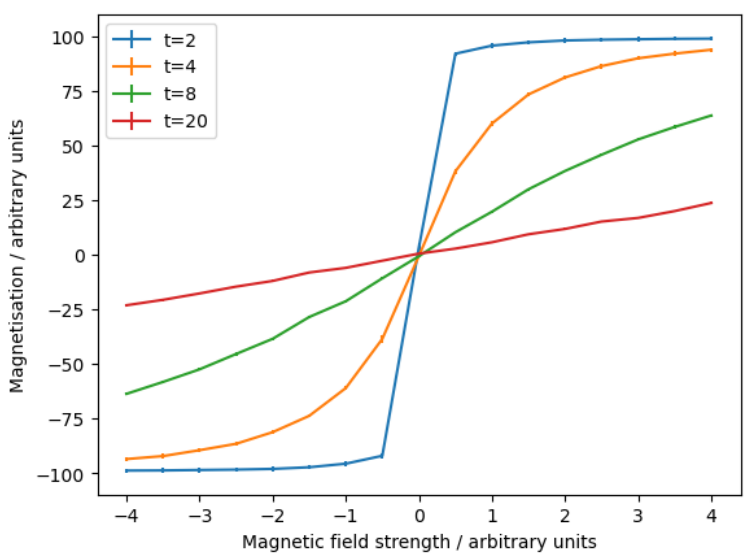

Figure 4: The dependence of the magnetisation of a system of particles in the Ising model on the magnetic field strength. These results were calculated using a Metropolis Monte-Carlo simulation with 100 000 timesteps. Error bars are reported on the graph, although they are often obscured by the thickness of the lines.

3.1 Interpretation

We can see that at the extremes of magnetic field strength the magnetisation approaches the maximum and minimum we calculated in section 1.1, where most of the spins are aligned with the field. The effect of temperature is also clear - at low temperatures, when the polarity is flipped the particles respond by flipping, even for a weak magnetic field. At higher temperatures, the polarity of the particles depends less strongly on the magnetic field, approaching a random distribution around zero, with a small linear correlation with field strength.