2D Ising model simulation

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The objective of this simulation was to explore the physics of a phase transition in a 2d Ising model. The Metropolis Monte Carlo algorithm was used to update the system. The Monte Carlo algorithm, in the context of the simulation works as follows.

- An NxN lattice is generated as a numpy array
- A site, S, is chosen either randomly or by sequencing through the lattice and dE, the change in energy of the lattice from flipping the spin on S, is calculated
- Only if dE is less than zero or a random number in [0,1] is less than exp(dE/kT), the spin is flipped
- Steps 2 and 3 are repeated for as long as desired.

Enough iterations of the MMC algorithm will equilibrate the lattice. Values for energy and magnetization can be acquired by averaging over the lattice after an iteration of the MMC algorithm enough times to obtain an average.

Magnetization vs temperature

The first exercise was to investigate the critical temperature of the lattice by determining the magnetization as a function of temperature. When not in a magnetic field, the magnetization of the lattice should remain at saturation when above the critical temperature. When the temperature is below the critical temperature, magnetization should oscillate around zero when above the critical temperature. The magnetization of the lattice can be determined by simply summing the total spins of the system. This can be done using np.sum for the array holding the system. Shown below is the magnetization of the lattice versus temperature.

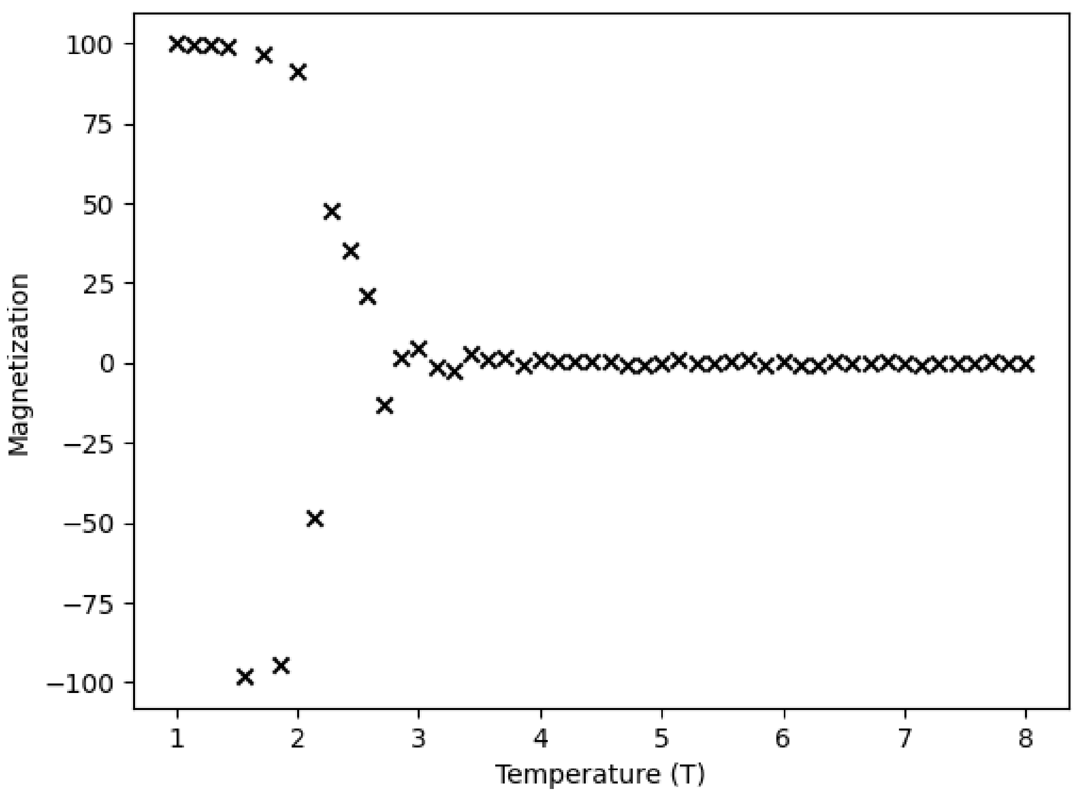

Figure 1: Magnetization versus temperature for a 10x10 lattice in the absence of a magnetic field

From the graph, the critical temperature of the lattice is 2.278. After this point the magnetization drops and begins to oscillate around zero. A temperature range of 1 to 8 was used and 50 values were plotted. Below the critical temperature, the lattice behaves as a ferromagnet with innate magnetization. Above the critical temperature, the lattice acts as a paramagnet with little or no magnetization unless placed in a magnetic field.

When the initial state is changed so that 75% of the sites are set to have a positive spin, the lattices equilibrate to have a positive net magnetization.

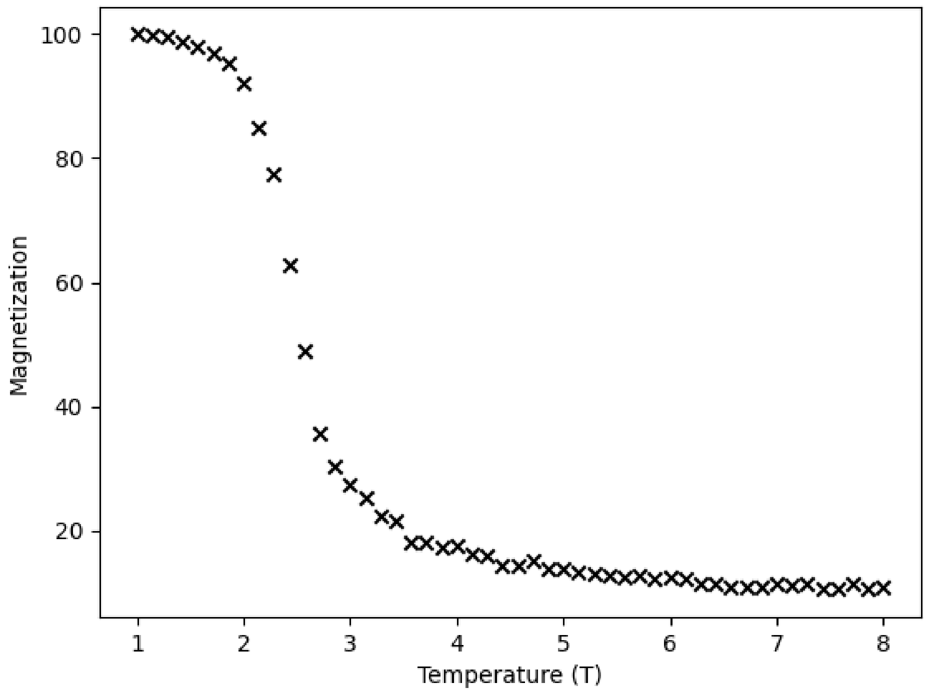

Figure 2: Magnetization versus temperature for a 10x10 lattice with a 75% positive initial state in the absence of a magnetic field

Energy as a function of temperature

Then the energy of the lattice was found as a function of temperature.

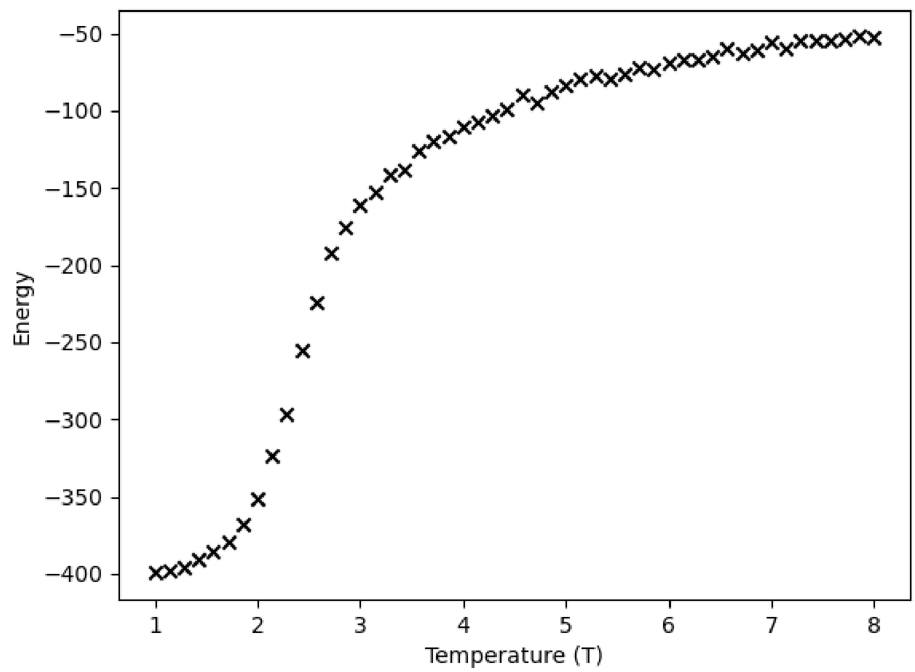

Figure 2: Energy versus temperature for a 10x10 lattice in the absence of a magnetic field

The energy of the lattice increases in a non-linear way with temperature and a substantial increase in energy is seen at the critical temperature. 50 values for energy were found with temperature ranging from 1 to 8.

Magnetization as function of magnetic field

The magnetization of the lattice at a constant temperature in a magnetic field was then investigated. The temperature was held constant at T = 3. This was to ensure the lattice was acting as a paramagnet. The magnetic field ranged from -5 to 5 and 30 points were plotted.

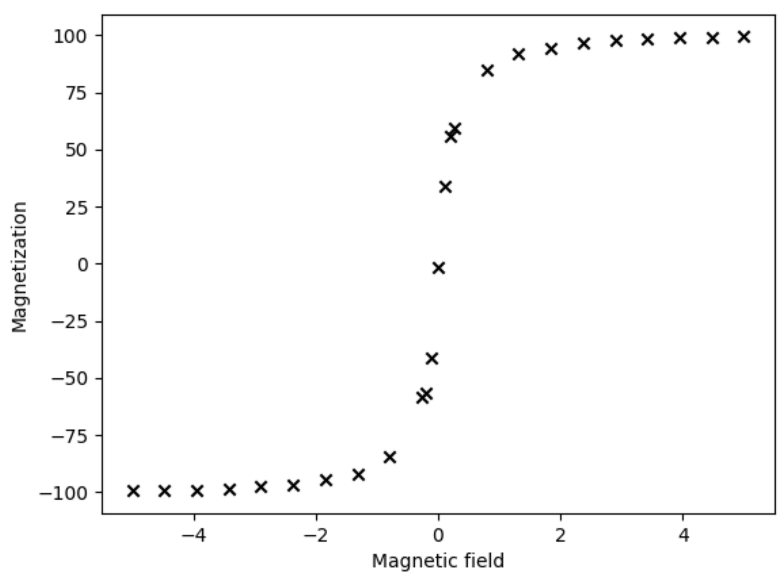

Figure 3: Magnetization verse magnetic field strength for a 10x10 lattice

The magnetization behaves as a paramagnet. Magnetization reaches saturation (+/-100 as there are 100 sites) for high enough magnetic fields and sharply decreases towards zero magnetization in no magnetic field before reversing direction. Furthermore, the absolute maximum magnetization is proportional to the square of the system size (proportional to the number of sites).

$$|M| \propto N^2$$

Heat capacity vs temperature

The heat capacity of the lattice was then graphed against temperature. The heat capacity is proportional to the standard deviation of the energy times the inverse of the temperature squared.

$$C = 1/T^2 * \sigma e$$

The standard deviation of the energy was determined using the std function for numpy arrays. The graph is given below for temperature ranging from 1 to 8 with 50 data points.

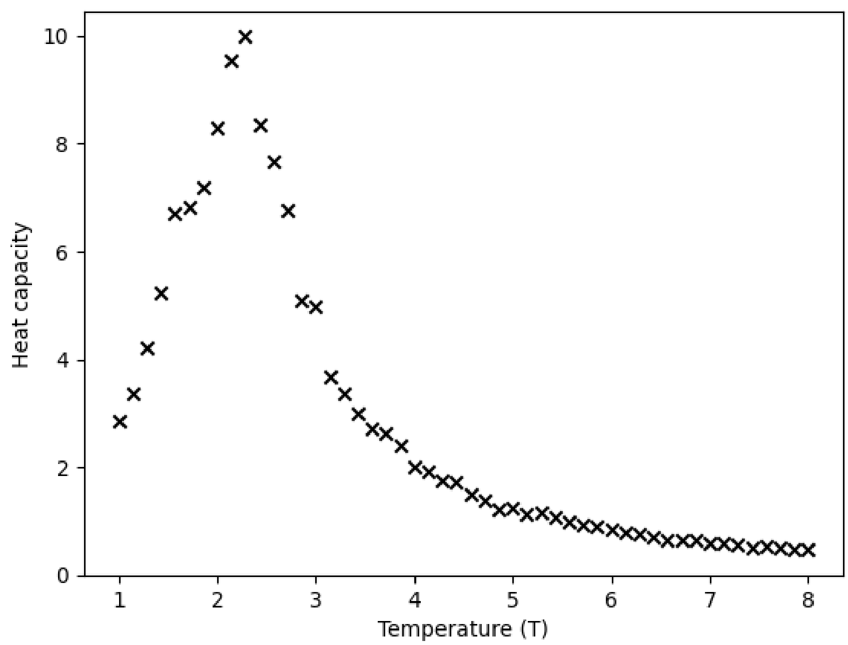

Figure 4: Heat capacity vs temperature for a 10x10 lattice

As can be seen from the graph, the heat capacity reaches a maximum at the critical temperature of the lattice and exponentially decreases towards zero as temperature goes beyond critical.

Low metropolis sample size

The metropolis algorithm is iterated over to equilibrate the lattice and iterated over again to return the lattice in multiple states to average over for more accurate measurements of energy and magnetization. The above graphs used 200 cycles of the MMC algorithm to equilibrate the lattice and 500 cycles to average over for energy and magnetization values. Shown below are the graphs for magnetization versus temperature and energy versus temperature for only 5 cycles to equilibrate and 5 cycles to average over.

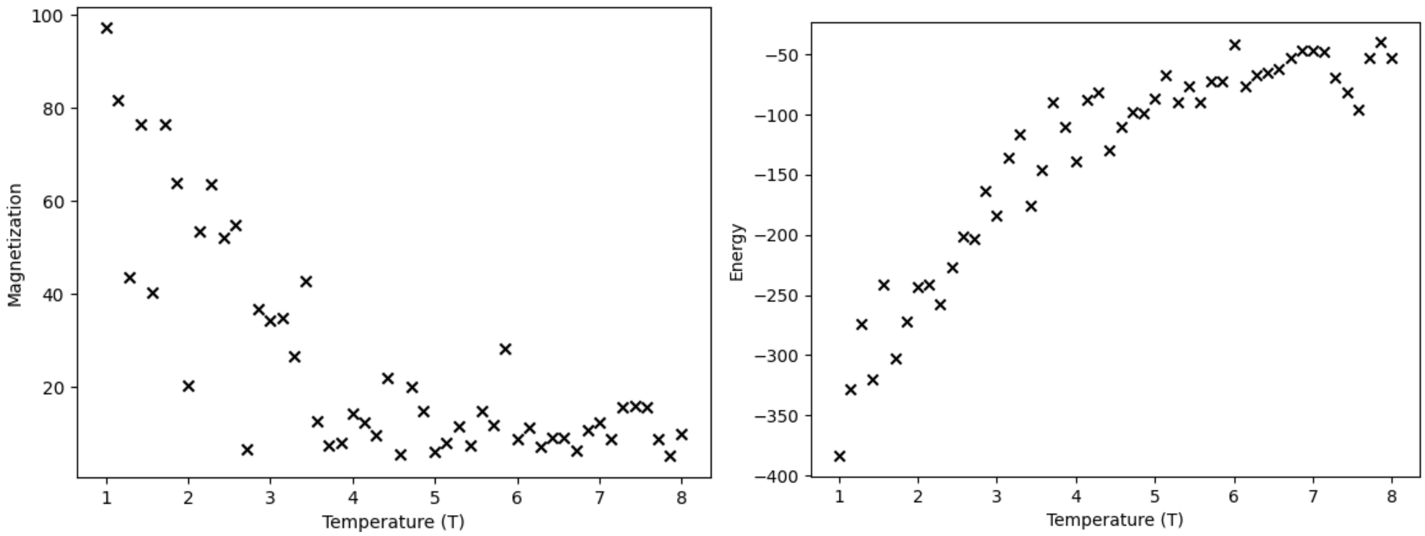

Figure 5: Magnetization (left) and energy (right) both graphed against temperature

When number of iterations of the MMC algorithm is decreased, the accuracy of the results is significantly impacted. The energy and magnetization have a much greater variance and no longer demonstrate the behaviour of the Ising model.

Heat capacity versus system size

The heat capacity of the lattice was then graphed against system size for the lattice at constant temperature. System size was ranged from 1 to 50. The heat capacity can be determined by the standard deviation of the energy of the lattice.

$$C = 1/T^2 * \sigma e$$

The graph is shown below.

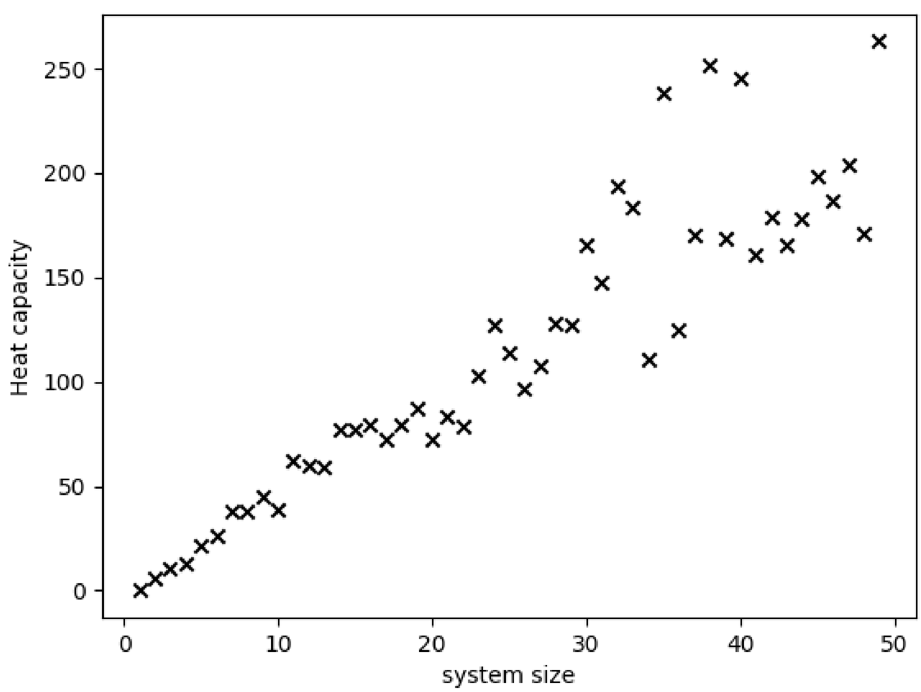

Figure 6: Heat capacity versus system size

The heat capacity increases with system size. The fluctuation of values increases as the system size increases. However, the MMC algorithm can be changed so that the site chosen to update is chosen sequentially rather than randomly. This decreases the fluctuation in heat capacity, as shown below.

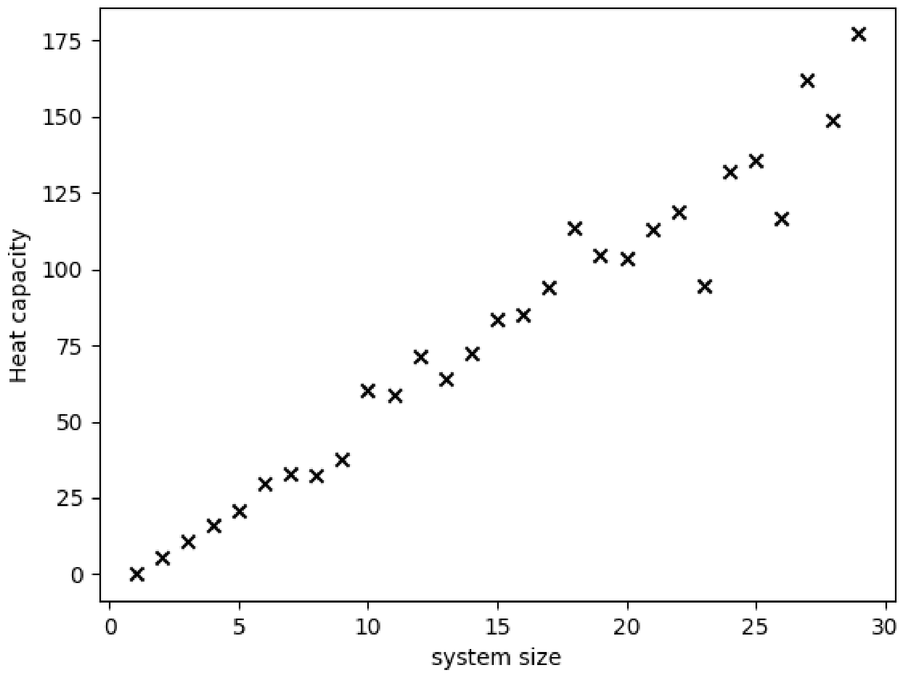

Figure 7: Heat capacity versus system size for sequential updating