FYS3150 Project 4

Markus Borud Pettersen

November 19, 2019

Abstract

We explore the two-dimensional Ising model numerically, using the Metropolis algorithm. Considering the case of a square lattice of spins interacting magnetically without an applied magnetic field, we first find analytical expectation values for a 2×2 lattice of spins, which are used to test a c++ implementation of the Ising model. A 20×20 model was then simulated for 10^6 Monte Carlo cycles, and at a low scaled temperature, $\hat{T} = 1.0$, the equilibration time for the average scaled energy per spin was found to be approximately 1000 cycles using an ordered spin configuration, and roughly 4000 for a random initialization. For a higher scaled temperature $\hat{T} = 2.4$ the randomly initialized system equilibrated more quickly than an equivalent system with an ordered initialization. By examining the relative frequency of energies during this simulation, it was revealed that the higher temperature case also carried a wider distribution of energies (final average energy variance $\sigma_E^2 = 8.09$) than the corresponding distribution at low temperature ($\sigma_E^2 = 0.03$). Finally, the critical temperature for an infinite spin lattice was estimated using the average, simulated critical temperatures of models of lattice size 40×40, 60×60, 80×80, and 100×100, with the critical temperature estimated to be $\hat{T}_C(\infty) = 2.245 \pm 0.016$, which almost contains the exact value of 2.269.

1 Introduction

Many systems in nature can be modelled as being binary, in the sense that the individual components that make up the system can assume one of two states. For example, neuronal activity in the brain can be modelled by imagining that each "neuron" can be either on, or off. However, it is by allowing these simple components to interact, that interesting behaviour emerges. For the neuronal example, an interaction can be that different nodes in a network excite each other, causing spike trains of activity. In this text, we will explore the so-called Ising model, which is typically used to describe a system of particles on a lattice. Each of these particles has so-called spin, either up or down, and interact magnetically. For all its simplicity, the Ising model still manages to capture some of the complex properties of real magnetic materials, such as phase transitions.

We will begin our investigation by outlining the Ising model for spins on a lattice interacting magnetically, and consider the specific case of a 2×2 lattice. Using the Boltzmann distribution, and some statistical physics, we arrive at analytical expressions for the expected values for the absolute magnetization, energy, heat capacity at constant volume, and magnetic susceptibility in the 2×2 case. After describing the Ising model, we move on to the Metropolis Algorithm, a Monte Carlo simulation strategy for computing the behaviour of the Ising model over time, at different temperatures. We then address how to implement the Metropolis algorithm as part of a Monte Carlo simulation of the Ising model.

2 Theory

2.1 The Ising Model

While usually used to model the magnetization of simple solids in terms of particle spins [1], the Ising model can in general be said to describe a system of particles on a lattice, where each particle can take on one of two values. The particles are coupled by some interaction, and may also interact with their environment. For the magnetic case, these values are taken to be the dimensionless particle spins, which can be either up

(1), or down (-1), and the external interaction may be in the form of an applied magnetic field. As each particle in a way acts like a small bar magnet, they also interact magnetically with each other, the effect of which depends on the material we wish to investigate. In this text, we will consider the simplest case, in which only nearest neighbours interact, and there is no applied magnetic field. In that case, the total energy of a configuration of spins is given by

$$E = -J \sum_{<k,l>} s_k s_l, \tag{1}$$

where s is the spin of a particular particle, while the indices $\langle k, l \rangle$ indicate that we only sum over nearest neighbours. J is a coupling constant reflecting the strength of particle-particle interactions, with units of energy. The actual value of J depends on the situation we are modelling. Note also that we have to sum over the entire lattice in order to obtain the total energy.

When modelling materials, spins can for example tend to interact in such a way that they align, and strengthen an applied magnetic field. As a famous example, *ferromagnetic* iron not only strengthens any magnetic field it is exposed to, it also retains its magnetization for some time afterward[2]. From (1) we can see that a positive value of J implies that the energy is minimized when spins align. For this simple reason, our model will be mimicking the behaviour ferromagnetic materials, as we will only consider the $J > 0$. However, we will not apply a magnetic field, we will only consider *spontaneous* magnetization.

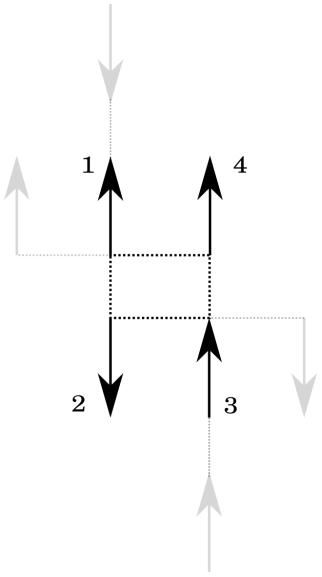

Figure 1: Illustrated 2×2 lattice of spins, with periodic boundary conditions.

As stated previously, we will only sum over nearest neighbours, and we will also only count a contribution to the energy once. What this, and (1) in essence leads to, is that we count the number of *bonds* in the lattice. To see how this works in practice, and also find some useful analytical expressions, we are going to consider a grid of only 2×2 spins. We will also limit ourselves to so-called periodic boundary conditions, where we say that the spins along the boundaries, actually "sees" a spin outside the boundary, whose spin value is taken to be equal to the that of the spin on the opposite side of the lattice. By doing so, we can create a slightly more realistic dynamic in our system, as opposed to just having free ends, and neglecting possible boundary effects. Note that for large system, and certainly in the thermodynamic limit when the number of spins go to infinity, there is little or no distinction between these two types of boundary conditions.

In order to visualize how we may find the energy of a finite grid of spins, Fig. 1 shows 2×2 spins arranged on a square grid. We treat the particles as distinguishable, as they can be identified by their position, and denote the particles with subscripts 1 through 4, going counterclockwise. We have also attempted to illustrate the periodic boundary conditions, shown as shaded spins outside the actual lattice. Note how these spins take on the spin value of the particle on the other side of the lattice.

To find the energy associated with the configuration in Fig. 1, and guarantee that we don't count terms twice, we can position ourselves at spin sites 1 and 3 (or 2 and 4), and simply follow the prescription in (1). Doing so, we find that the total energy is

$$E = -2J(s_1 s_2 + s_1 s_4 + s_3 s_2 + s_3 s_4), \tag{2}$$

where s denotes a spin value, and the factor two comes from the periodic boundary conditions. It should be pointed out that this not only tells us the energy of the specific configuration in Fig. 1, it gives us a way of finding the energy for *any* 2×2 spin configuration. Plugging in $s_1 = s_3 = s_4 = 1$, and $s_2 = -1$, we find $E = 0$ for the case in Fig. 1.

As we are going to simulate our Ising model using a Monte Carlo method, it would be very useful to know the *expected* behaviour of the simplest case, our 2×2 grid. To determine any expectation values for the system, we first need to know that it actually follows a probability distribution, and if so, which one. As it turns out, we can model this system as a collection of particles in thermal equilibrium with their surroundings. From thermodynamics, such systems tend to obey the Boltzmann distribution

$$P_i(E_i) = \frac{1}{z} e^{-\beta E_i}, \tag{3}$$

where z is the so-called partition function of the system, while E is the energy associated with the particular spin configuration of state i. $\beta = 1/k_B T$ is simply a measure of the inverse system temperature, (times the Boltzmann constant k_B). In actuality, it turns out that our system also follows the Boltzmann distribution [1]. Since these are probabilities, we know that they must necessarily obey the normalization condition

$$1 = \frac{1}{z} \sum_i e^{-\beta E_i}, \tag{4}$$

where we sum over all possible states, which in the 2×2 gives us $2^4 = 16$ different possibilities. Fortunately, (4) tells us that we can quite easily determine the partition function of a system, if we know the energy E_i associated with a given state. Inserting from (1), we get

$$z = \sum_{i=1}^{16} e^{2\beta J(s_1+s_3)(s_2+s_4)},$$

where we have rewritten the energy expression in a somewhat more suggestive form. To simplify matters, we can use a bit of combinatorics, and the fact that the number of different energies is limited. If only there is only one spin up, or one down, for example, the exponent goes to zero, something which can be accomplished in $\binom{4}{1} + \binom{4}{3} = 8$ different ways. We can also have all spins down or up, which can only be done one way each, accounting for two more possibilities, both with energy $-8J$. Finally, we can have two spins up, and and two down, which gives an energy of either $E = 0$, or $E = 8J$. The final option can occur in $\binom{4}{2} = 6$ ways, which completes our set of 16 possibilities. Putting this together, we end up with

$$z = 2e^{8\beta J} + 8e^0 + 2e^{-8\beta J} + 4e^0,$$

where we have used the fact that we can only obtain $(s_1 + s_3)(s_2 + s_4) = -8$ in two ways (s_1 and s_3 must point up, and the rest down, or vice versa). Tidying up, we find

$$z = 4\cosh(8\beta J) + 12,$$

in the 2×2 case.

Another interesting quantity we can determine quite easily, is the average absolute magnetization, $\langle |M| \rangle$. For a certain state i, the magnetization is just $M_i = \sum_j s_j$ for the 2×2 lattice, with $j = 1, 2, 3, 4$. Since the magnetization of the system is precisely determined by its spin configuration, the probability of getting a certain magnetization is given by (3), and the average value is

$$\langle |M| \rangle = \frac{1}{z} \sum_i^{16} |M_i| e^{-\beta E_i}, \tag{5}$$

where we once again sum over all possible configurations of the four spins. We can also use the fact that the magnetization of a given state M_i, is uniquely determined by the number of spins pointing up (or down), as we know the total number of spins. As such, we know that the absolute magnetization can be only 4, 2, or 0. The first case is simple, and achieved by either arranging all spins up, or all spins down. The second occurs when all but one particle have spin up or down, and the last when all spins cancel. We can however use this to find a neat expression for (5). As there are four particles, the sum over all states must contain 16 terms. However, as we noted, there are only three possible (absolute) values of the magnetization, one of which is zero, and therefore does not contribute to the sum. For the remaining states, there are only two ways of obtaining the maximum magnetization of 4, with corresponding energy $-8J$. The final possibilities are those with one spin up, or one spin down, which can occur in $\binom{4}{1} = \binom{4}{3} = 4$ ways each. If we once again write the energies in the more suggestive fashion $E_i = -2J(s_1 + s_3)(s_2 + s_4)$, we can see that both these possibilities carry $E = 0$. Putting all of this together, we find that

$$\langle |M| \rangle = \frac{1}{z}\left(4\left(e^{2\beta J\cdot 4} + e^{2\beta J\cdot 4}\right) + \binom{4}{1}2e^0 + \binom{4}{3}2e^0\right),$$

or that

$$\langle |M| \rangle = \frac{8}{z}\left(e^{8\beta J} + 2\right). \tag{6}$$

As for the squared magnetization, the probabilities (and possibilites) remain the same as for the absolute value case, we only need to square the actual value of the magnetization. Therefore, we can adapt our earlier expression, and obtain

$$\langle M^2 \rangle = \frac{32}{z}\left(e^{8\beta J} + 1\right) \tag{7}$$

We are also going to need the expected value of the actual magnetization, which is fortunately quite simple in this case. Due to symmetry, we can, for each possible value of the magnetization, simply flip all spins, and obtain the same absolute spin, with an opposite sign. Therefore, we must have that the sum over all states cancels, and

$$\langle M \rangle = 0. \tag{8}$$

We can also determine the expected value for the energy of the system, in the usual manner:

$$\langle E \rangle = \frac{1}{z}\sum_{i=1}^{16} E_i e^{-\beta E_i},$$

where we would have to sum over all states once again. But, the experienced reader might have noted another possibility, by observing that

$$\frac{\partial z}{\partial \beta} = \sum_{i=1}^{16} -E_i e^{-\beta E_i},$$

which should not be problematic, as z only consists of well-behaved exponentials. Therefore,

$$\langle E \rangle = -\frac{1}{z}\frac{\partial z}{\partial \beta} = -\frac{32J}{z}\sinh(8\beta J). \tag{9}$$

We can also find the expected squared energy, $\langle E^2 \rangle$ using the same approach, and differentiating z twice, which gives

$$\langle E^2 \rangle = \frac{256J}{z}\cosh(8\beta J). \tag{10}$$

Now that we have some essential building blocks, we can formulate a few more useful quantities, namely the heat capacity at constant volume, C_V, and the magnetic susceptibility, χ. The heat capacity tells us how much energy is required to heat a specific amount of substance by one degree [3]. For our purposes, it can be defined as

$$C_V = \frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right). \tag{11}$$

[1] Note that we can use (11) only as long as we keep the volume, or size of our system, which is the case for a fixed-sized lattice of spins, which we will focus on. Inserting for the expected squared energy, and squared expected energy, we get

$$C_V = \frac{256}{k_B T^2 z^2} \left(z \cosh(8\beta J) - 4 \sinh^2(8\beta J) \right).$$

The magnetic susceptibility is a measure of the degree to which a material is *susceptible* to being magnetized, and can be defined as

$$\chi = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right), \tag{12}$$

[1]and for our 2×2 lattice, we find

$$\chi = \frac{32\beta}{z} \left(e^{8\beta J} + 1 \right)$$

As a last, tantalising aspect of the Ising model, we will consider how it acts close to the critical temperature T_C, at which a phase transition occurs. For a two-dimensional model, this transition takes the form of a sudden discontinuity of the magnetic susceptibility and the heat capacity. As the temperature of the system approaches the critical point, the so-called correlation length of the system, tends toward infinity. The correlation length is, roughly speaking, a measure of the distance that can separate spins on the lattice, and still have them affect each other[1]. However, if we are to investigate the behaviour of the Ising model near the critical temperature, we first need to know what it might be. One possible way of doing so is by simply simulating different sized lattices, and extracting the temperature at which a discontinuity appears in the value of the magnetic susceptibility, for instance. However, it turns out that the critical temperature of the Ising model scales with the lattice size l as

$$\hat{T}_c(l) = aL + \hat{T}_c(\infty), \tag{13}$$

[4]where $\hat{T}_c(\infty)$ is the critical temperature of an infinite lattice of spins, and a some constant. Therefore, if we can determine the critical temperature for different lattice sizes, we can also approximate the critical temperature for the infinite case, by performing a linear regression for different values of $\hat{T}_c(l)$. The exact value of $\hat{T}_c(\infty) = 2/\ln(1+\sqrt{2})$ is actually known, and is due to Norwegian mathematician Lars Onsager [1].

2.2 The Metropolis Algorithm

As we can see from the 2×2 lattice, finding analytical solutions describing the Ising model can be difficult, even in the very simplest case. Motivated by this, we will attempt to use a Monte Carlo method to analyze a system of $l \times l$ spins. Specifically, we will attempt to outline and apply the Metropolis algorithm, a Monte Carlo algorithm tailored to the Ising model.

The general strategy of the Metropolis algorithm is to first "position ourselves" randomly at some spin site on the $l \times l$ lattice. We then try to see what happens to the energy of the system if we flip the selected spin, and if the change in energy is negative, we automatically accept the new configuration. If the change in energy is non-negative, however, we need some selection rule to determine if the flip should be approved or not.

While it is tempting to simply reject any positive change in energy, as physical systems tend to move toward lower energy states, this approach can bias our model, and we may never, for example, find all interesting energy states. As a general example, we can imagine a situation where we end up in a local energy minimum. To escape such a minima, we may need to make moves which increase the energy locally. Therefore, we require that our system is ergodic, or in other words that every possible state is accessible to the system, given enough time.

As we have already seen, the spins that make up the lattice follow the Boltzmann distribution, with probability density of being in a certain energy state given by (3). While we do not know the probability of transitioning from one state to another, we can model the probability of moving from a state with energy E_i to one with energy E_j as

$$p_{i \to j} = P(E_i) T_{i \to j} A_{i \to j},$$

where $A_{i\to j}$ is the probability of accepting a transition, while $T_{i\to j}$ is the probability of said transition occuring. Simply put, our model is then that for a transition to occur, we need for the system to be in a state with energy E_i, *and* have that a transition from state i to j occurs, *and* that we accept the transition. We are also going to require that we have so-called detailed balance, which means that $p_{i\to j} = p_{j\to i}$ [5]. In this text, we will also simply assume that the transition probabilities are equal, and therefore that

$$\frac{A_{i\to j}}{A_{j\to i}} = e^{-\beta(E_j - E_i)},$$

where we have equated $p_{i\to j}$ and $p_{j\to j}$, and inserted the respective probabilities from the Boltzmann distribution. While we do not know the acceptance probability, we have already mentioned that we automatically accept changes which lead to lower energies. In other words, if we consider two states i and j, and the j-state carries a greater energy, we must set $A_{j\to i} = 1$, as such a move would lower the energy. The acceptance probability of performing the oppsite transition must then be

$$A_{i\to j} = e^{-\beta(E_j - E_i)}, \tag{14}$$

and in the opposite case, where $E_i > E_j$, the acceptance probability is simply 1. Now that we have a selection rule for our Monte Carlo simulation, we can, for each proposed spin flip, find the resulting change in energy, and calculate the acceptance probability according to (14). In order to accept or reject a move, we can simply draw a random uniform number between 0 and 1, and compare this to the acceptance probability, which we can call w. If the drawn number is smaller than w, we accept the move, if not, we reject it. The reason it should be smaller, is simply due to the fact that we wish that large increases in energy should be accepted more rarely than small ones.

3 Methods

The Ising model was implemented in c++ using Monte Carlo simulation, according to the Metropolis algorithm. For all simulations, a scaled, dimensionless temperature $\hat{T} = k_B T/J$ was used. The spins were in all cases required to be on a $l \times l$ square grid, and the system was initialized using either an ordered, all spin up- or down state, or a random configuration. For the random initialization, the spin value at a given site was determined by drawing a pseudorandom uniform number between 0 and 1, using the c++ standard library function rand(). If the drawn number was less than 0.5, the spin was set to -1, and 1 otherwise.

A Monte Carlo cycle (MC cycle) was taken to be $l \times l$ suggested steps using the Metropolis algorithm, such that all spin sites were likely to be visited, for a sufficient number of MC cycles. As the total number of steps might be quite large, the coordinates of a suggested spin site were drawn (pseudo)randomly from a uniform integer distribution, generated using the c++ mt19937 Mersenne Twister random number generator (RNG). For each step, the energy associated with a selected spin s_i was found according to (1). To save computations, only the resulting change in energy due to flipping s_i to $-s_i$ was found, as

$$\Delta E = 2s_i \sum_{k=1}^{4} s_k,$$

where s_k is the value of a neighbouring spin. In accordance with the discussion on the acceptance probability of (14), negative changes in energy were automatically accepted. If an increase in energy was found, a pseudorandom, uniform random number between 0 and 1 was generated using the Mersenne Twister RNG, and compared to the acceptance probability of (14). If the drawn number was smaller than the acceptance probability, the spin flip was accepted, otherwise it was rejected. Note that the possible acceptance probabilites were precalculated at initialization to save computations. For each accepted spin flip, the change in energy was logged, and the magnetization was updated according to

$$M_2 = M_1 + 2s_2,$$

where the subscripts 1 and 2 denote the values of magnetization before and after the spin flip, respectively. The above simply entails that flipping a spin must necessarily change the magnetization by 2, as the spin

is not removed, but reversed. For all simulations, natural units were used, by setting $J = 1$, and $k_B = 1$. By doing so, the computed expectation values were actually scaled according to $\langle E \rangle / J$, $\hat{C}_V = C_V / k_B$, and $\hat{\chi} = J \cdot \chi$, which are all dimensionless. Note that the magnetization was already dimensionless before scaling.

In order to verify the Ising model implementation, a simulation of a 2×2 lattice of spins at dimensionless temperature $\hat{T} = 1.0$ was run for $n = 10^5$ MC cycles. The average energy, absolute magnetization, magnetic susceptibility, and heat capacity per spin was then computed, and compared with the analytical results of (9), (6), (2.1) and (11), respectively. The comparison was performed by determining the logarithmic absolute relative error. In addition, unit tests were implemented, which compared results from the implemented model with the 2×2 lattice analytical results. These unit tests verified, for a 2×2 model, that initial energies were calculated correctly, to a tolerance of 10^{-16}, and that the magnetization tended towards zero after 10^6 MC cycles, to a tolerance of 0.01.

To investigate the equilibration time of the Ising model at different temperatures, a 20×20 spin lattice was simulated for $n = 10^6$ MC cycles, and the average absolute magnetization, as well as the scaled mean energy was logged. Simulations were performed for $\hat{T} = 1.0$, and $T = \hat{} 2.4$, and in both cases both an ordered, as well as a random initial spin configuration was used. For the ordered configuration, all spins were taken to be up. For all these cases, the average values were inspected visually, and the equilibration time was approximated as the MC cycle at which the average value appeared to have stopped changing. For these simulations, the number of accepted spin flips was also logged at the end of each MC cycle.

For the 20×20 lattice simulations, the current energy of the system was logged at the end of each MC cycle. Using these energies, the discrete probability distribution of the system energy per spin was approximated. This was done simply by counting the number of times a given energy appeared during simulation, and normalizing with respect to the number of MC cycles and spins. Note that for $\hat{T} = 1.00$, the results using an ordered spin configuration was used, and the first 1000 MC cycles were not included, to ensure that equilibrium had been reached. For $\hat{T} = 2.40$, the results for a random initialization was used, and the first 2000 MC cycles were not included.

In order to uncover the behaviour of the Ising model near the critical temperature $\hat{T}_c$, the model implementation was parallelized using the external Message Passing Interface (MPI) library. This was done in order to run multiple instances of the Ising model simultaneously, at different temperatures. As a verification of parallelism, timing was performed on some trial runs, with and without vectorization compiler flags. Using the parallelized Ising model, simulations were performed for 40×40, 60×60, 80×80, and 100×100 lattices, at temperatures ranging from $T = \hat{} 2.0$ to $\hat{T} = 2.6$, with a temperature step of 0.025. For each of these simulations, a random initialization was used, and all simulations were performed using $n = 10^6$ MC cycles.

Using results from the parallel computations, the critical temperature for an infinite sized lattice was approximated by performing a linear regression of critical temperature versus lattice size, in accordance with (13). Note that the critical temperature was taken as the temperature at which the scaled heat capacity and magnetic susceptibility had their maximum values.

4 Results

Fig. 2 shows the absolute relative error ($\log_{10}$) of the scaled thermodynamic quantities, i.e. the average energy, absolute magnetization, as well as magnetic susceptibility and heat capacity at constant volume, per spin for a 2×2 lattice of spins, using periodic boundary conditions at scaled temperature $\hat{T} = 1.0$. It appears that the scaled average energy, absolute magnetization and heat capacity reach their equilibrium value after around 10^4 MC cycles, after which point they appear to oscillate around the exact value, which was found to be approximately 1, -2, 4, and 0.03 for the average absolute magnetization, scaled energy, magnetic susceptibility, and heat capacity, respectively. For the magnetic susceptibility, no oscillation is observed, and and apparent equilibrium is reached only after approximately $2 \cdot 10^4$ MC cycles. It is worth noting that the average energy and absolute magnetization appear to be, neglecting oscillations, correct to around the third digit, while the magnetic susceptibility and heat capacity only appear to be correct to around the first and second digit.

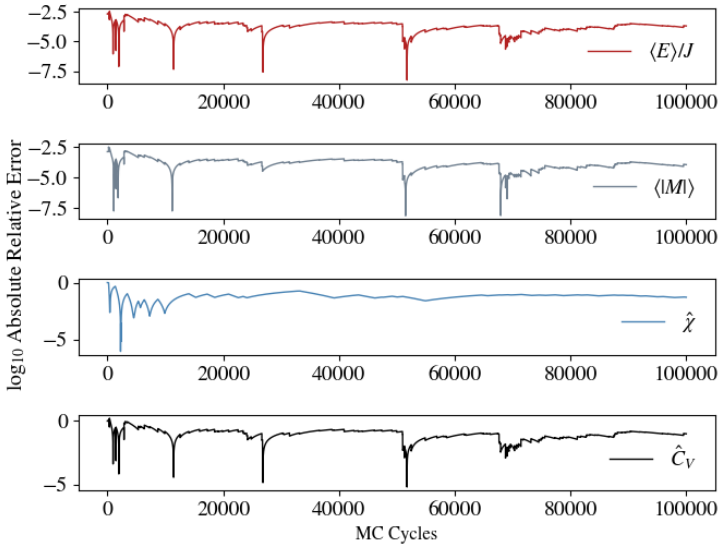

Figure 2: $\log_{10}$ absolute relative error of the scaled average energy, average absolute magnetization, magnetic susceptibility, and heat capacity at constant volume, for an Ising model of lattice size 2×2, simulated using $n = 10^5$ Monte Carlo cycles at scaled temperature $\hat{T} = 1.0$, using the Metropolis algorithm

Fig. 3 shows the scaled average energy and absolute magnetization per spin, as a function of simulation length in terms of the number of MC cycles, for an Ising model of lattice size 20×20. Results are indicated for both ordered, as well as random spin initializations, for scaled temperatures $\hat{T} = 1.0$ and $\hat{T} = 2.4$. For the $\hat{T} = 1.0$ case, we can see that both the average absolute magnetization, and the scaled average energy appear to stabilize after approximately 1000- 2000 MC cycles for an ordered initialization. For the random initialization, the results appear to converge more slowly, and the absolute magnetization only appears to begin to settle after approximately 10^4 MC cycles, towards a value just below unity, the same value as for the ordered case. The scaled average energy appears converge to more quickly, requiring approximately 4000 MC cycles to get close to the equilibrium value of around -1.997, as found for the ordered case. For the $\hat{T} = 2.4$ case, we can see that it takes roughly 1000 MC cycles for the scaled energy to converge to a value of approximately -1.23, both for the ordered and random cases. For the magnetization, however, the ordered simulation appears to take approximately 5000 MC cycles to settle to a value of approximately 0.45, while the random initialization appears to do so after approximately 2500 cycles.

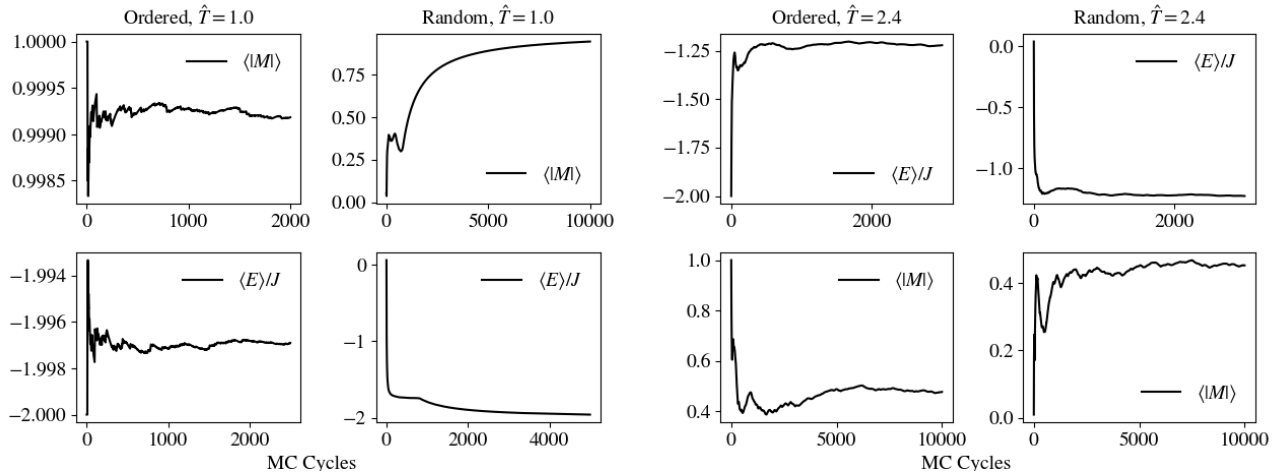

Figure 3: Average values of absolute magnetization $\langle|M|\rangle$, and scaled energy, $\langle E\rangle/J$, for an Ising model of lattice size 20×20 spins. Shown are simulations for scaled temperatures of both $\hat{T} = 1.0$ and $\hat{T} = 2.4$, for different numbers of Monte Carlo cycles. For each temperature, both random and ordered (all spin up), initial spin configurations were used, as indicated.

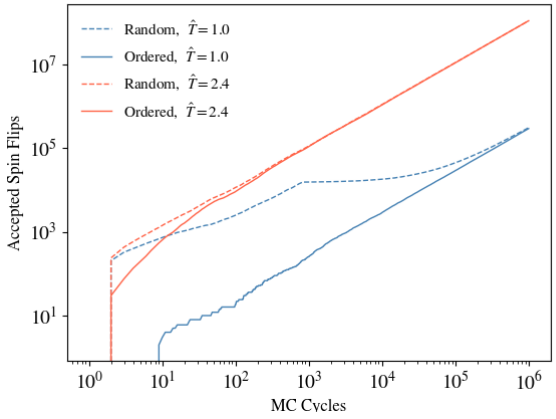

Figure 4: log-log plot of the total number of accepted spin flips, versus the total number of Monte Carlo cycles. Inset are the number of accepted moves using both random and ordered (all spin up), initial spin configurations, simulated using scaled temperatures $\hat{T} = 1.0$ and $\hat{T} = 2.4$.

Fig. 4 shows a log log-plot of the total number of accepted spin flips, as a function of the number of MC cycles for the same simulation as in Fig. 3. We can see that the number of accepted moves in all cases increases steadily with the number of MC cycles, but that is generally lower for a lower temperature. For the $\hat{T} = 1.0$, ordered case, we see that the number of accepted flips stabilizes at around 1000 MC cycles, indicating that equilibrium is reached, which is also in agreement with the finding from Fig. 3. We also see that the random initialization takes much longer to stabilize, as the number of accepted flips only approaches that of the ordered initialization after approximately 10^5 MC cycles. For $\hat{T} = 2.4$, we observe that the number of accepted flips is much greater for a given MC cycle, but that the random configuration appears to stabilize more quickly (and equilibrium may have been reached), which is also in agreement with what is observed in Fig. 3. We can also note that after equilibrium is reached, the number of accepted moves increases linearly with the number of MC cycles, as the slope of loglog curve is approximately 1.

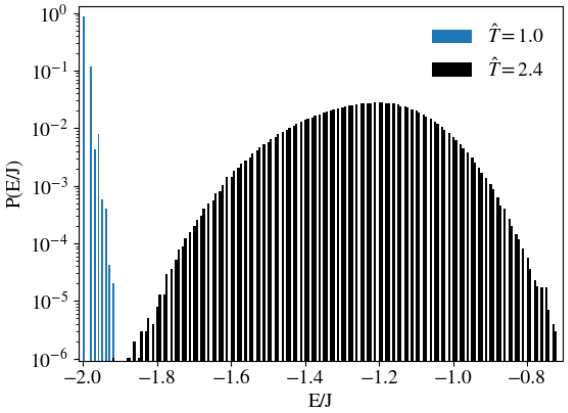

Figure 5: Relative frequency of the scaled energy states per spin, for an Ising model of lattice size 20×20. Shown are the relative number of appearances of a given scaled energy per spin, after system equilibration. Shown are the approximate probability distributions for a scaled temperature of $\hat{T} = 1.0$, and $T = \hat{} 2.4$. Note that the total simulation time was 10^6 Monte Carlo cycles, but the first 1000, and 2000 cycles were discarded for the $\hat{T} = 1.0$, and $\hat{T} = 2.4$ case, respectively, to ensure that equilibrium had been (approximately) reached.

Fig. 5 shows the relative frequency, or approximate probability distribution, of the total energy per spin of the 20×20 lattice Ising model, simulated for a duration of 10^6 MC cycles. The relative frequencies are indicated for scaled temperatures of $\hat{T} = 1.0$ and $\hat{T} = 2.4$. For the $\hat{T} = 1.0$ case, an ordered initial spin state was used (all spin up), and in accordance with previous findings, the first 1000 MC cycles were not included, so as to ensure that the equilibrium had been reached. For $\hat{T} = 2.4$, the spins were initialized randomly, and the first 2000 MC cycles discarded on the same grounds.

For $\hat{T} = 1.0$, it is evident that only a select few energy states are occupied by the system at equilibrium, from approximately $E/J = -2.0$ to $E/J = -1.92$ per spin. The most likely state carried $E/J = -2.0$, with a relative frequency of approximately 0.86. The variance of the energy, σ_E^2, was determined from (11) as $\hat{T}^2\hat{C}_V$ and found to be 0.03 for $\hat{T} = 1.0$.

When the temperature is increased, at $\hat{T} = 2.4$, we can see that the energy distribution is much wider, and that the system visits, or occupies states with energies ranging from approximately $E/J = -1.9$ to $E/J = -0.7$. The most probable state carried $E/J \approx 1.2$, and a relative frequency of 0.03. The energy variance was found to be $\sigma_E^2 = 8.09$. Interestingly, we have in both cases that only certain energies are possible, which is evident as gaps in the distributions.

Table 1 shows the execution time for selected runs of the Ising model, both for single process- and parallel processes, as well as runs with added compiler flags. Compared to the baseline, non-vectorized, non-parallel run, the parallel process provided a speedup of approximately 2.7 when running 10^4 cycles of the Ising model, using a temperature step of $\Delta\hat{T} = 0.05$ in the range $[2.0, 2.6]$. For the same simulations, the vectorized (compiler flag -O2), parallel run provided an average speedup of approximately 7.9. Note that for all runs, the last for temperature steps were shared by only four processes, as the temperature step divided the simulation into 12 steps, distributed on 8 parallel processes, and the values in Table 1 might therefore not reflect the maximum achievable speedup.

Table 1: Execution time for Ising Model, for various lattice sizes, $l \times l$, for $n = 10^4$ Monte Carlo cycles, in the temperature range $T \in [2.0, 2.6]$, with temperature step $\Delta T = 0.05$. Values are tabulated for the baseline run, with no added compiler flags, and only one process, as well as parallel runs, with 8 attempted parallel processes. Also shown is the same parallel processes, compiled with the -02 compiler flag. Lastly, the speedup of the -02 run compared with the baseline is shown.

Execution time $[s]$				
L	Baseline	Parallell	Parallel -02	Speedup $[s/s]$
40	73.4	27.2	9.5	7.73
60	167.7	61.5	21.6	7.76
80	305.3	106.9	37.4	8.16
100	474.1	170.0	59.9	7.91

Fig. 6 shows the scaled energy and absolute magnetization, per spin, as a function of scaled temperature for different lattice sizes. We can observe that both the scaled energy, as well as absolute magnetization appear to have an inflection point near $\hat{T} = 2.3$. We can also note that for the scaled energies, the response of the system appears to be similar for all lattice sizes, as opposed to the absolute magnetization, which drops off more slowly at higher temperatures for smaller lattice sizes. Also noteworthy is the fact that the absolute magnetization appears to go to zero at large temperatures, indicating that all spins are oppositely aligned, while for lower temperatures, the absolute magnetization per spin tends towards 1, indicating spins align. A similar behaviour is also observed for the scaled energy per spin, only opposite in nature, as a low temperature (and spin alignment) appears to decrease the system energy per spin.

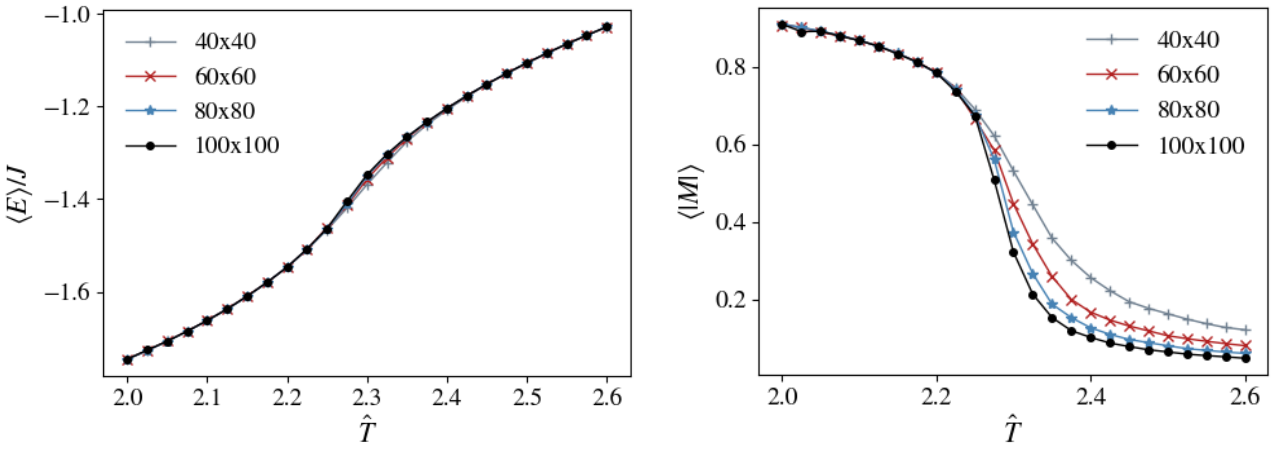

Figure 6: Scaled average energy per spin (left hand side), and average absolute magnetization per spin, for Ising models of lattice sizes 40×40, 60×60, 80×80, and 100×100, as a function of scaled temperature $\hat{T}$. Each data point represents the final average value of the quantity in question, extracted after the simulation was run for 10^6 Monte Carlo cycles.

Finally, Fig. 7 shows the temperature response of the scaled magnetic susceptibility $\hat{\chi}$ and heat capacity at constant volume $\hat{C}_V$ per spin, for Ising models of various lattice sizes. For both quantities, we notice a distinct peak near $\hat{T} = 2.3$, close to the critical temperature, but for the magnetic susceptibility per spin, models with smaller lattice sizes appear to peak at slightly lower temperatures, with the peak of the 60×60 case occuring closer to $\hat{T} = 2.2$, for instance. For the heat capacity per spin, the response profile appears more symmetric, and the peaking is more localized across lattice sizes. For the 60×60, 80×80, and 100×100 lattice size models, the maximum recorded value occurred at $\hat{T} = 2.2750$, while the 40×40 model peaked at $\hat{T} = 3.0$. In terms of magnitude, we can tell that the magnetic susceptibility has more of a pronounced peaking effect, at least for greater lattice sizes.

By extracting the point at which the response profiles of Fig. 7 peaked, the critical temperature of the

two-dimensional Ising model was estimated to be 2.31 ± 0.016 using only values from the scaled heat capacity at constant volume, and 2.25 ± 0.016 using only values obtained from the scaled magnetic susceptibility. If the average of the peak temperatures of the two quantities were used, the critical temperature was estimated as 2.245 ± 0.016. Note that for all these estimates, the uncertainty was taken to be the statistical uncertainty in the linear regression performed for (13).

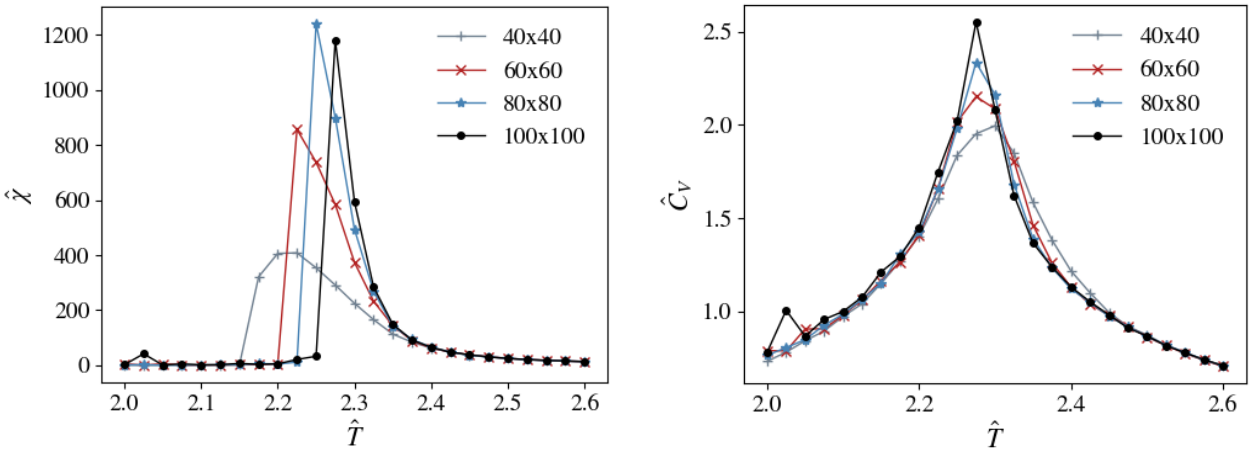

Figure 7: Scaled magnetic susceptibility per spin (left hand side), and scaled heat capacity per spin, for Ising models of lattice sizes 40×40, 60×60, 80×80, and 100×100, as a function of scaled temperature $\hat{T}$. Each data point represents the final average value of the quantity in question, extracted after the simulation was run for 10^6 Monte Carlo cycles.

5 Discussion

While the results of Fig. 2 indicate that the implemented Ising model does not converge exactly towards the analytical expected values, for a 2×2 lattice, it seems to show that the expected values which are found, tend to oscillate around the true value, given enough Monte Carlo cycles. In fact, this is to be expected, as Monte Carlo methods are inherently random, and the ergodicity of our system implies that we should always be able to escape equilibrium states. As for the scaled magnetic susceptibility, the most likely reason why it does not oscillate, or achieve the same level of precision as the other quantities, might be due to the fact that it depends directly on the magnetization of the system, not only the absolute magnetization. The magnetization of the system, while not adressed directly in this text, appears to converge more slowly than the absolute magnetization, which might help to explain the lower degree of precision. In actuality, the 2×2 case is somewhat unphysical, at least when compared to a real magnetic solid, which may consist of millions or billions of particles arranged on a lattice. As such the 2×2 case should mostly be valued for its ability to test our implementation of the Ising model, which seems to be able to find the scaled average values of all of the thermodynamic quantities of interest, down to one or two digits precision, taking approximately 10^4 MC cycles for most average values per spin to approach their true value.

For the 20×20 lattice, we can also see that there are differences in convergence time for the average scaled energy per spin, and the absolute magnetization per spin. However, these differences are rather small compared to the effect of changing the spin initializations. For the $\hat{T} = 1.0$ case, for instance, we can observe that the convergence time increases by almost an order of magnitude when going from an ordered, to a random spin initialization. A similar result is seen for the high-temperature case, with randomly initialized system appearing to converge somewhat faster. This does, however, make some intuitive sense: at lower temperatures, one would expect the system to be more ordered, as there is less thermal energy available, and an ordered initialization would seem reasonable. Likewise for the $\hat{T} = 2.4$, one would expect that a higher thermal energy level would bring about a more disordered state, and that a disordered initialization would be closer to the equilibrium state of the system.

For all simulations, it would have been beneficial to use a more rigorous method for determining whether equilibrium had been reached. The current method of simply saying that a steady state has been reached when the simulated value visually appeared to settle down, is fraught with error, and quite ad hoc. It would therefore be an interesting future development, to introduce some equilibration criterion, such as demanding a persistent, maximum variance over several samples. Perhaps even better would be to perform time-autocorrelation of the computed quantities, and demand that calculated averages remain self-similar over many samples, as we would expect at equilibrium.

Judging from Fig. 4, we can also tell that a higher temperature brings about a higher number of accepted spin flips, throughout the simulation. This might also be expected, as a system at higher temperature should experience more thermal fluctuations. Interestingly, Fig. 4 also shows that the low-temperature, randomly initialized system behaves somewhat similarly to the high-temperature case, before it settles into an equilibrium shared by the system initialized using an ordered spin configuration. It is likely that the randomly initialized system begins in a state of low magnetization, but that for low temperatures, it is energetically favourable to be aligned, which allows for many flips, until equilibrium is reached and most spins are aligned, after what is approximately $10^5 - 10^6$ spin flips.

We can also see evidence of this in the estimated probability distribution of Fig. 5, as the probability of being in anything but the lowest lying energy states is zero or vanishingly small, in the $\hat{T} = 1.0$ case. For the $\hat{T} = 2.4$ case, however, we observe a much larger spread in the energy per spin, and the probabilities are also more evenly distributed, in the sense that many different energy states are quite likely. This is also reflected by the variance in energy for the two temperatures, of 0.03 and 8.09 for $\hat{T} = 1.0$ and $\hat{T} = 2.4$, respectively. While especially the latter seems high, it should be noted that this is the variance in energy per spin for the very last calculated value of the heat capacity, after 10^6 MC cycles, not of the estimated probability distribution itself. A more suitable measure of the error might be $\sigma_E/\sqrt{n}$, with $n = 10^6$ being the number of MC cycles. However, this is not the main takeaway, as the point of this comparison is mainly to show that the width of the estimated probability distribution is related to σ_E^2, which we can see by the fact that the $\hat{T} = 1.0$ case carries a lower value of σ_E^2 *and* a narrower estimated probability distribution, compared to the $\hat{T} = 2.4$ case.

It is useful to note that the low-temperature initialization was chosen to be ordered, as this lead to a faster equilibration time, and allowed for more of the 10^6 MC cycles to be included in the probability distribution estimation. For the high-temperature case, a random initialization was used for the same reason, and although slightly fewer samples were used (2000 initial values omitted, versus 1000 for the low-$\hat{T}$, ordered case), this should not significantly impact the statistics shown in Fig. 5, as there are very nearly still $\approx 10^6$ samples used in both cases. It could, however, have been interesting to run the simulation for even longer, to see if this would have any effect, but Fig. 4 seems to indicate that equilibrium has been reached for all cases after 10^6 samples.

For the timing results shown in Table 1, it is interesting to see that the parallel process, without vectorization, only achieves a speedup of around 2.7, running 8 parallel processes. However, there is one caveat to this, as the temperature step used for the timing analysis necessitated 12 simulations, but of course only 8 of these could be performed in parallel, and so we would estimate the maximum theoretical speedup, by extrapolating the time used by the baseline, to run 16 simulations, which should take the same time as 12 for 8 parallel processes. Doing so, we get an maximum theoretical speedup of around 3.6 for the parallel, and approximately 10 for the parallel -O2 runs. The reason why the parallel-only speedup is not close to 8, is suspected to be that the simulation computer just has 4 *cores* available, not 8, as was initially believed. Ideally then, the timing should be re-examined.

For Fig. 6 and 7, there are at least two obvious problems, namely the use of a rather coarse step in scaled temperature of $\Delta\hat{T} = 0.025$, as well as the small number of different lattice sizes used. Due to our choice of using linear regression to determine $\hat{T}_C(\infty)$, more samples, evaluated over a smaller temperature interval, for instance, could substantially improve our estimate. One possible way of doing so, would be to limit the temperature interval to $\hat{T} \in [2.2, 2.4]$, based on initial findings, for example. Unfortunately, as can be judged from the timing found in Tab 1, simulating large lattice size models is time-consuming, with 10^6 MC cycles taking close to 3 hours to complete for a lattice size of 100×100, $\Delta\hat{T} = 0.05$ and the temperature interval of (6) and (7). An additional complication, is that single-flip Monte Carlo methods, such as the Metropolis algorithm, can fail miserably near the system's critical temperature. The reason for this is that the correlation length near $\hat{T}_C$ tends towards infinity, and when a spin is flipped, *all* the other spins tend to

react, as they are corrolated, and the system can take an infinite amount of time to equilibrate[6]. Another possible source of error, is that the average magnetization was used to find the magnetic susceptibility, (not the average absolute magnetization), which seems to converge quite slowly, based on previous results, which might further compound this problem. Therefore, other simulation methods should actually be used near T_C, which could be an interesting future development. It might also be worthwhile to calculate the scaled magnetic susceptibility using the absolute magnetization, not the magnetization itself, as it tends to converge more quickly. On the other hand, the scaled heat capacity produced similar estimates for $\hat{T}_C(\infty)$, but it does not depend on the average magnetization. Therefore, it is likely that the problem is not only with convergence of the average magnetization, but rather convergence using the Metropolis algorithm in general.

As for our estimate of the scaled critical temperature $\hat{T}_C(\infty) \approx 2.245 \pm 0.016$, it seems reasonable to use the average temperatures, obtained from both the scaled magnetic susceptibility and the heat capacity at constant volume, as there is no strong grounds to select one over the other. From the exact value, $\hat{T}_C(\infty) \approx 2.269$, we see that the average value almost contains the exact value within its uncertainty, but not quite. This strongly suggests that there is room for improvement in our approach, for example using the methods proposed above.

6 Conclusion

In this text we have explored the two-dimensional Ising model with periodic boundary conditions, describing particles interacting magnetically on a square lattice, with no applied magnetic field. Analytical results were found for a 2×2 lattice, and expressions were found for the expected values of magnetization, scaled energy, heat capacity at constant volume, as well as magnetic susceptibility. These analytical expressions were then used to test a c++ implementation of the two-dimensional Ising model, utilizing the Metropolis algorithm, showing agreement to the third digit or better for the simulated absolute magnetization and scaled energy at equilibrium, after 10^5 Monte Carlo cycles. The scaled magnetic susceptibility and heat capacity at constant volume were found to be correct to the first and second digit at equilibrium.

As the implementation successfully simulated a 2×2 lattice, a 20×20 lattice was simulated for 10^6 MC cycles, and its equilibration time and energy distribution studied. It was found that at low temperature, $\hat{T} = 1.0$, the equilibration time of the scaled average energy for an ordered spin initialization was approximately 1000 MC cycles, and 4000 for a random initialization, while at a higher temperature $\hat{T} = 2.4$, the absolute magnetization of the randomly initialized spin lattice reached equilibrium more quickly, after approximately 2500 MC cycles, versus around 5000 for an ordered initialization. This finding was mostly supported by examining the number of accepted spin flips, which also showed that the number of spin flips was consistently higher at greater temperatures. The accepted spin flips did however suggest that the low-temperature, random initialization took longer to fully equilibrate than was first assumed. This suggests that the method for determining equilibrium should be reconsidered, as it was done by visual inspection in this work. It would for example be an interesting future development to implement an equilibrium criterion by using time-autocorrelation.

By looking at the relative frequencies of the scaled energy states per spin of the 20×20 lattice size Ising model, it was found that the spread in energy was much lower for the $\hat{T} = 1.0$ case, than for $\hat{T} = 2.4$. This was also confirmed by computing the end-of-simulation variance in energy, which was $\sigma_E^2 = 0.03$ for $\hat{T} = 1.0$, and $\sigma_E^2 = 8.09$ for $\hat{T} = 2.4$. It was also found that only certain energies states were occupied by system, indicating that certain energies are impossible.

Finally, the critical temperature of the Ising model was investigated, by simulating its temperature response and computing average values for absolute magnetization, scaled energy, magnetic susceptibility, and heat capacity at constant volume using lattice sizes of 40×40, 60×60, 80×80, and 100×100. Using the scaled heat capacity and magnetic susceptibility, the approximate critical temperatures were extracted as the temperature at which these quantities took on their maximum value. Using the average of these temperatures for each lattice size, the scaled critical temperature of an infinite lattice of spins was estimated to be 2.245 ± 0.016, which almost contains the exact value of $\hat{T}_C(\infty) = 2.269$. This discrepancy was found to likely be due to the single spin-flip dynamic of the Metropolis algorithm, which may cause very slow convergence rates. It might therefore be interesting to consider using other Monte Carlo methods near the critical temperature as a development.

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