Markov Chain Monte Carlo Simulation of the 2D Ising Model

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November 28, 2023

1 Introduction

The 2D Ising model consists of a lattice of spins, with each spin $s_{i,j}$ at lattice coordinates (i, j) capable of being either up (+1) or down (-1). The model is explored to investigate the critical temperature at which the system undergoes a phase transition from an ordered (magnetized) state to a disordered (non-magnetized) state.

The Hamiltonian of the system is expressed as

$$H(\{s_{i,j}\}) = -J \sum_{i,j} s_{i,j}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1}), \tag{1}$$

where J denotes the interaction energy between adjacent spins. This summation considers nearest neighbor interactions, assuming periodic boundary conditions. The state probability is given by the Boltzmann distribution:

$$W(\{s_{i,j}\}) = \frac{1}{Z(\beta)} \exp[-\beta H(\{s_{i,j}\})], \tag{2}$$

with $\beta = \frac{1}{k_B T}$, k_B being Boltzmann's constant, and T the temperature. The partition function $Z(\beta)$ is

$$Z(\beta) = \sum_{\{s_{i,j}\}} \exp[-\beta H(\{s_{i,j}\})]. \tag{3}$$

Theoretical analysis of the 2D Ising Model reveals that the critical temperature T_c for an infinite lattice can be calculated exactly, which is given by

$$k_B T_c = \frac{2J}{\ln(1 + \sqrt{2})}. \tag{4}$$

Our computational approach uses the Metropolis-Hastings algorithm to approximate this critical temperature by analyzing the system's behavior. The mean magnetization is calculated as

$$\langle M \rangle = \frac{1}{N} \sum_{\{s_{i,j}\}} M(\{s_{i,j}\}), \tag{5}$$

where N is the number of configurations.

2 Method

We started with initializing a lattice, where each spin at a lattice site can take a value of +1 or -1. The script allows the user to choose if the initial lattice is randomly generated (a mix of +1s and -1s), uniformly +1 states, or uniformly -1 states. The simulation works by trying out new configuration states and determining if these new states are accepted using an acceptance fraction. This will continue for a number of iterations.

There are several important components of the MCMC method that need to be defined using what we know about the 2D Ising Model. The Boltzmann distribution that we defined earlier in 2 is our "likelihood", because this function represents how likely a certain spin configuration is. We can ignore the denominator $Z(\beta)$ because it will cancel out in our acceptance fraction. Our "prior" in this case is represented by the fact that we have preselected certain temperature values that will be tested. Therefore, the likelihood function ends up being our posterior.

The posterior is used to calculate the acceptance fraction, which determines whether we accept a new lattice configuration. The acceptance fraction is defined as

$$\begin{aligned} \alpha &= \frac{p(\{s_i\})}{p(\{s_i^{'}\})} \\ &= \frac{exp(-\beta H(\{s_i\}))}{exp(-\beta H(\{s_i^{'}\}))} \\ &= exp(-\beta(\Delta E)) \end{aligned} \tag{6}$$

At each step of the simulation, a lattice site is randomly selected, and the change in energy (ΔE) resulting from a potential spin flip is computed. This change in energy is given by $\Delta E = 2J \cdot S_{i,j} \cdot \sum S_{\text{neighbors}}$, where J is the interaction strength between neighboring spins and $S_{\text{neighbors}}$ is the sum of the nearest neighbor spins.

The spin flip is accepted with a probability of $\exp(-\beta \Delta E)$ if ΔE is positive; otherwise, the flip is always accepted. This criterion ensures that the system explores lower energy states while still allowing for thermal fluctuations.

The total magnetization M is computed as the sum of all spins, and the total energy E is determined from the spin interactions. From these primary measurements, additional thermodynamic properties are calculated: the specific heat C is derived from the energy variance as $C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}$, and the magnetic susceptibility χ from the magnetization variance as $\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}$.

The lattice size was $N = 32$, total number of steps was set to 1,000,000 to make sure balance between computational feasibility, system equilibrium demand and sufficient resolution to capture collective phenomena. The interaction strength J was set to 1, no external field considered (h=0) and the Boltzmann constant Kb was also set to 1 for simplicity.

Quantitative measurement such as multiple chain analysis and Gelman-Rubin statistics was performed to assess the convergence of multiple chains. Each chain k in a total of m chains produces a series of observations. For a given property (energy and magnetization), we calculated the within-chain variance W and the between-chain variance B. Within-Chain Variance (W): This is the average of the variances within each chain. Mathematically, it is given by $W = \frac{1}{m} \sum_{k=1}^{m} s_k^2$ where s_k^2 is the variance of the k-th chain. Between-Chain Variance (B): This measures the variance of the chain means. It is calculated as $B = \frac{n}{m-1} \sum_{k=1}^{m} (\bar{x}_k - \bar{x})^2$ where n is the number of observations per chain, $\bar{x}_k$ is the mean of the k-th chain, and $\bar{x}$ is the mean of the means of all chains. The Gelman-Rubin statistic ($\hat{R}$) is then computed using these variances. It is defined as $\hat{R} = \sqrt{\frac{\hat{Var}^+}{W}}$ where $\hat{Var}^+$ is the pooled variance estimate, a weighted combination of W and B: $\hat{Var}^+ = \frac{n-1}{n} W + \frac{1}{n} B$. A $\hat{R}$ value close to 1 indicates that the within-chain and between-chain variances are comparable, suggesting that the chains have likely converged to the target distribution. Values significantly greater than 1 suggest non-convergence and necessitate further investigation or additional simulation steps.

3 Testing/Validation

Visual examination of the spin configurations at various temperatures can provide qualitative insights into the phase transition process. We expect to see a clear change from ordered to disordered states as the temperature crosses the critical threshold.

In order to validate the results of our handwritten MCMC, we ran a variety of tests with different initial lattice states (random mix of +1s and -1s, uniformly +1s, or uniformly -1s) and temperature values. The script outputs various plots that give us a good idea of the physical characteristics of the system. Repeated testing of each situation yields similar results.

Figure 1 shows results from testing with a random initial lattice state. We can see a clear increase in energy, which is what we expect to see. We also see a large jump in the average magnetization at a temperature of 2.2 K, signifying a state change. This jump is also present in the specific heat and susceptibility plots, which further validates our results. From these plots, we can guess that the critical temperature is around 2.2 K. The magnetization over time plot also reflects this. We see that the magnetization starts around the same values for most of the temperatures, but eventually temperatures around 2.2 K and above separate and their magnetization ends up being much higher. This jump is present in the energy over time and average energy plots as well, although it is much less noticeable. These results overall seem consistent with what we expect and know of the 2D Ising Model.

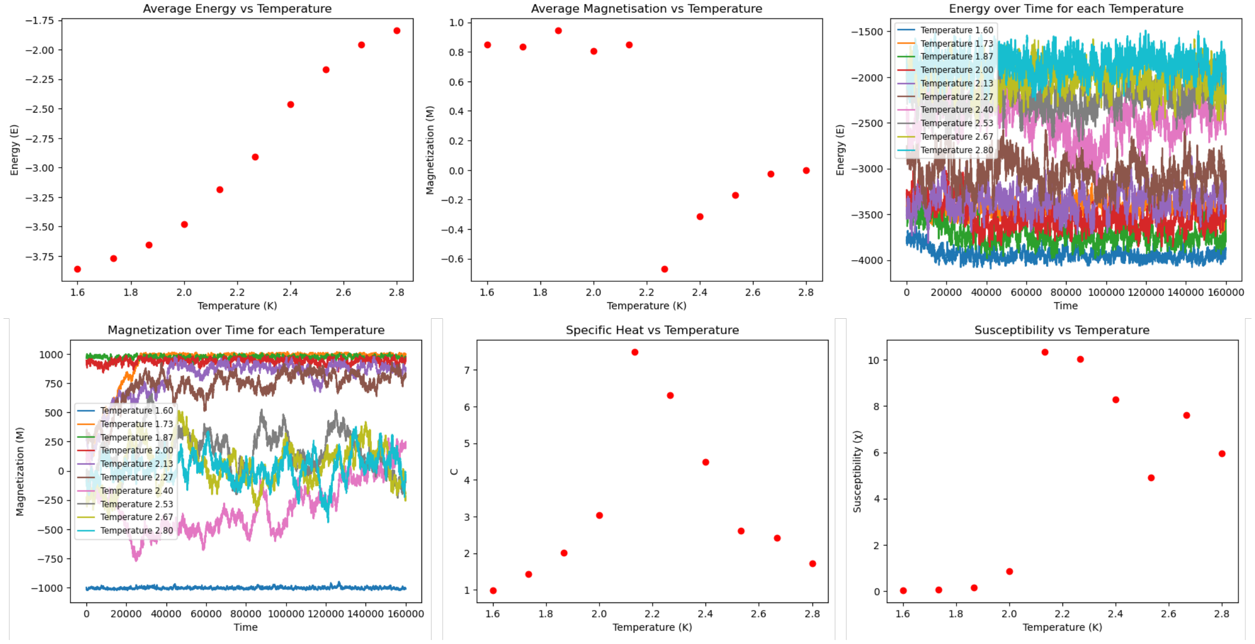


Figure 1: Results of the handwritten MCMC using a random initial lattice state

Figure 2 shows the results now for an initial lattice state that is uniformly +1 for each spin. We see similar results in terms of the jumps made around the critical temperature representing a state change. We also see the average magnetization decrease over time, which makes sense because the magnetization depends on the spins, which all start being +1 in this case.

Figure 3 shows the results now for an initial lattice state that is uniformly -1 for each spin. Again, we see the jumps made around the critical temperature representing the state change. This time, the average magnetization begins negative and increases due to the spins all being -1 initially.

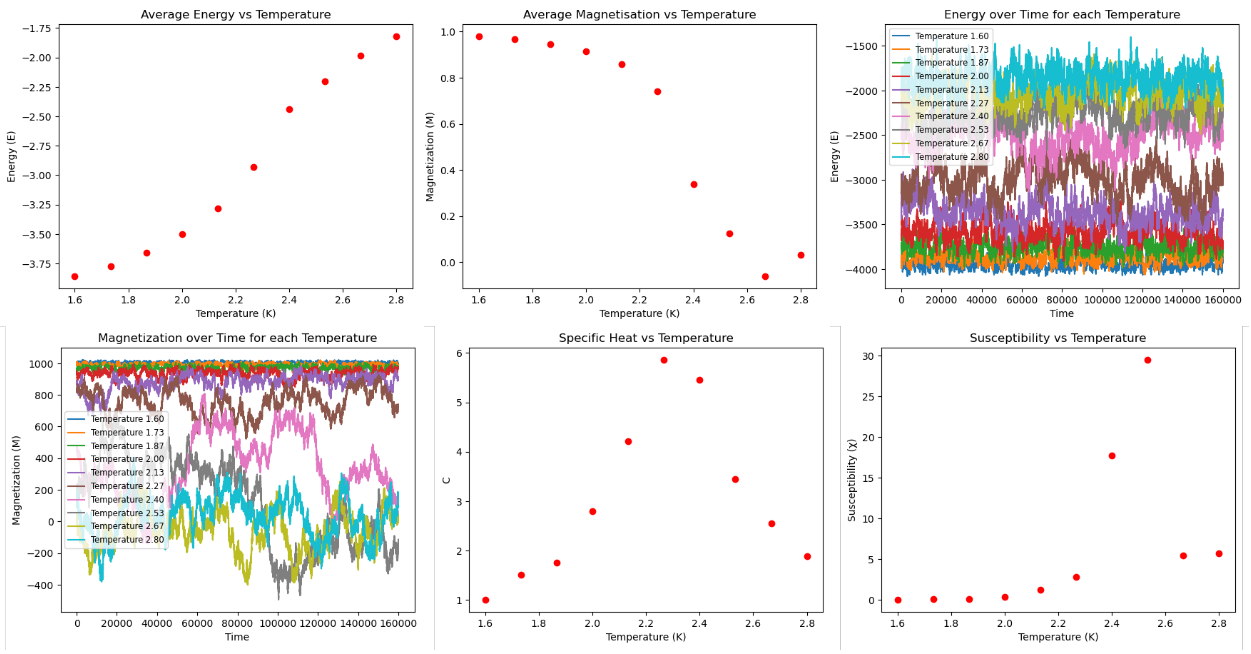


Figure 2: Results of the handwritten MCMC using a uniform +1 initial lattice state

We also utilized the pymc3 package, which is a premade python package that can run an MCMC simulation. Our package outputs the final lattice state for each temperature value for both our handwritten method and the pymc3 method. Here, we will compare the results from the two.

Figure 4 shows the final lattice states for both our handwritten method and the pymc3 method when the initial lattice is randomly generated. Immediately, you can see that the pymc3 method tends to result in spin states grouping together, which is what we expect from the 2D Ising Model. Our handwritten code tends to have spin states positioned more randomly across the lattice. It gets better at higher temperatures, where you can start to see some clumps and shapes. I believe this is due to the fact that our handwritten code does not take into consideration the effect that one atom flipping its spin will have on the other atoms around it. Each run randomly selects which atom to test, without considering the previously tested/flipped atom. This is an area in which our code falls short and could be improved on in the future.

Figure 5 shows the final lattice states for both our handwritten method and the pymc3 method when the initial lattice is uniformly +1. Similar to the results from the random initial lattice, we see that our handwritten code has a more random distribution of spin states as compared to the pymc3 model. And again, it does better at higher temperatures. It appears that once we exceed the critical temperature at which a state change occurs, our script is able to group spin states better. This also makes sense considering our acceptance

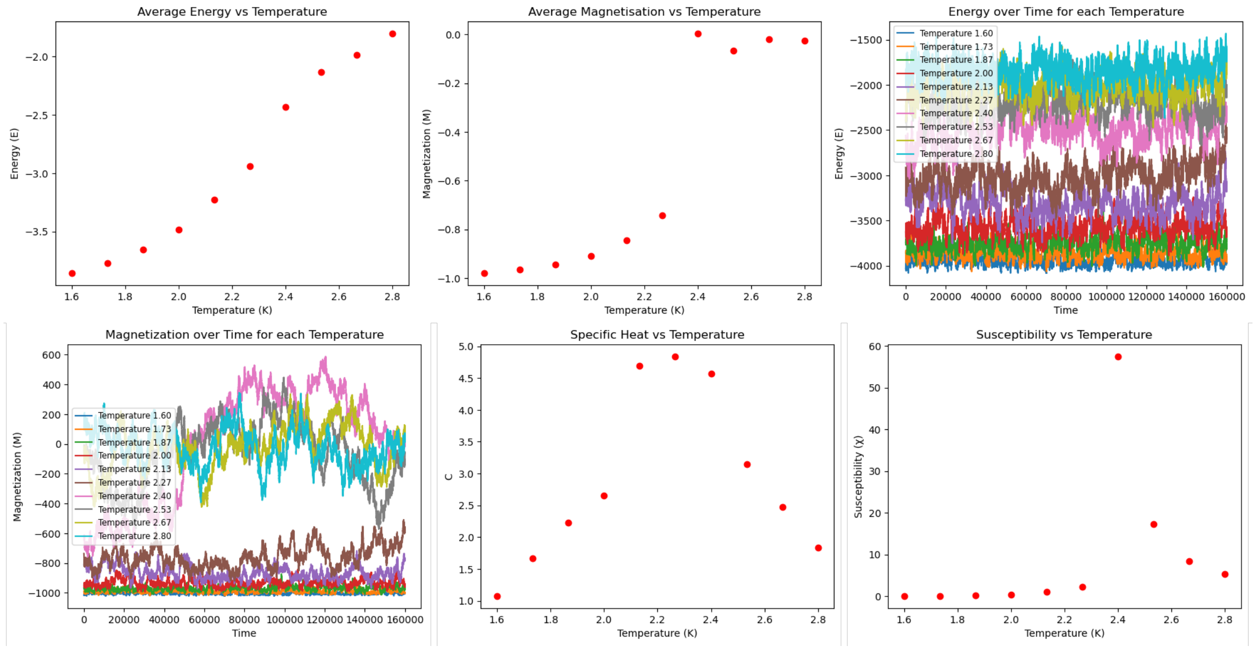


Figure 3: Results of the handwritten MCMC using a uniform -1 initial lattice state

function's temperature dependence. With a uniform initial state, it struggles quite a bit. It is likely that it is unfavorable for the spin states to flip when they are all already uniform, and since our script does not consider the effects of one atom flipping on the next atom we test, it struggles to do more than flipping a few random spins.

Figure 5 shows the final lattice states for both our handwritten method and the pymc3 method when the initial lattice is uniformly -1. This one struggles similarly to how the uniformly +1 initial lattice test struggled, and adds more evidence to my suspicions about what is causing these struggles.

All three initial state tests show that the handwritten script struggles more at lower temperatures compared to the pymc3 model. Our script trends towards uniform spin states below the critical temperature. Above the critical temp, our script does better about forming groups of matching spin states, similar to what the pymc3 model does. I believe our struggles with this come from the fact that we randomly select which atom to test each time instead of considering the previously tested/flipped atom.

3.1 Convergence Test

In order to test the convergence, multiple-chain analysis and Gelman-Rubin statistics test were explored. The autocorrelation function (ACF) was also explored to visualize and validate the correlation between the present and past state of a particular spin configu-

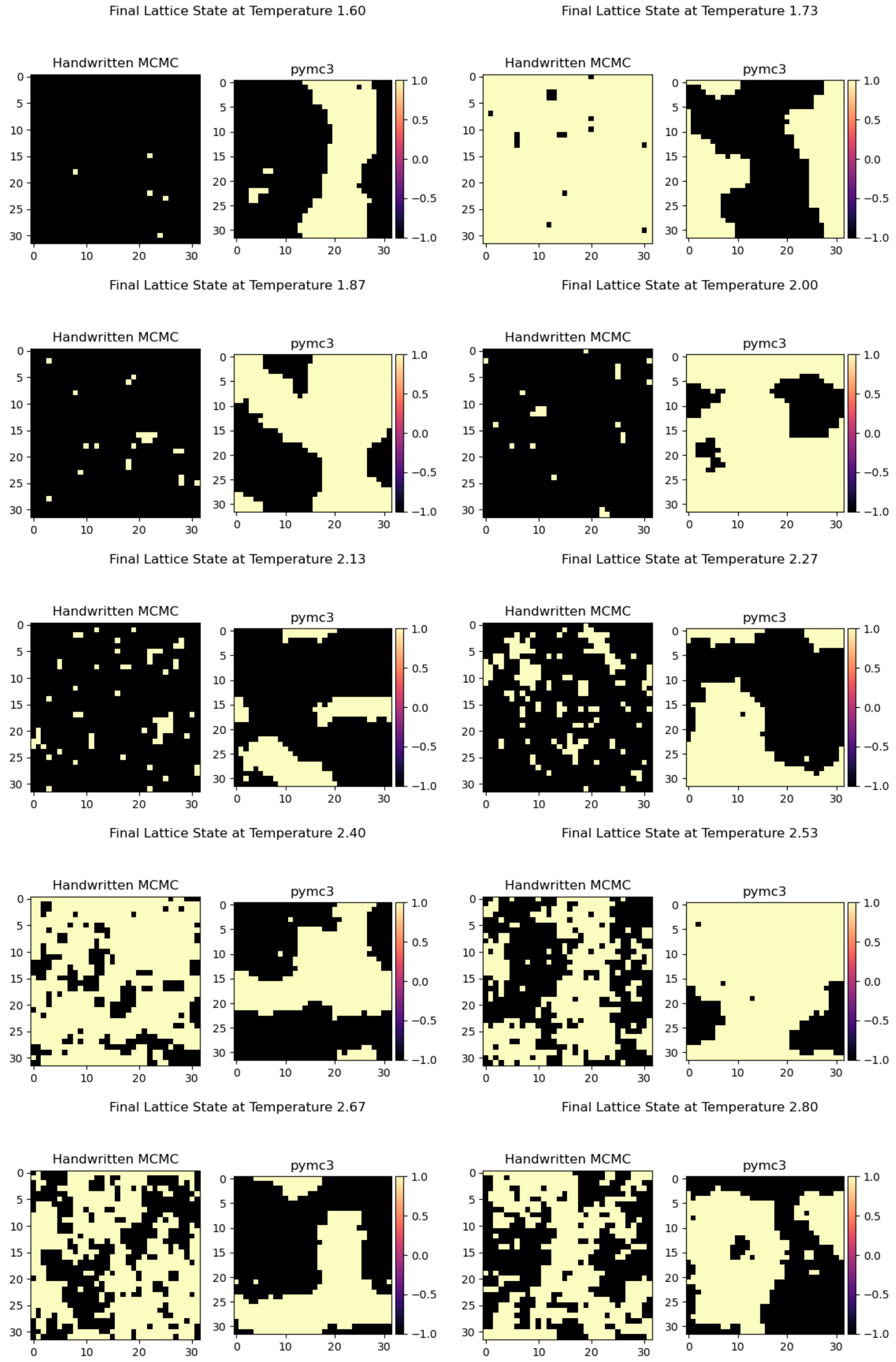


Figure 4: Final lattice states at a variety of temperatures, with a random initial lattice state, comparing the handwritten MCMC to pyMC3

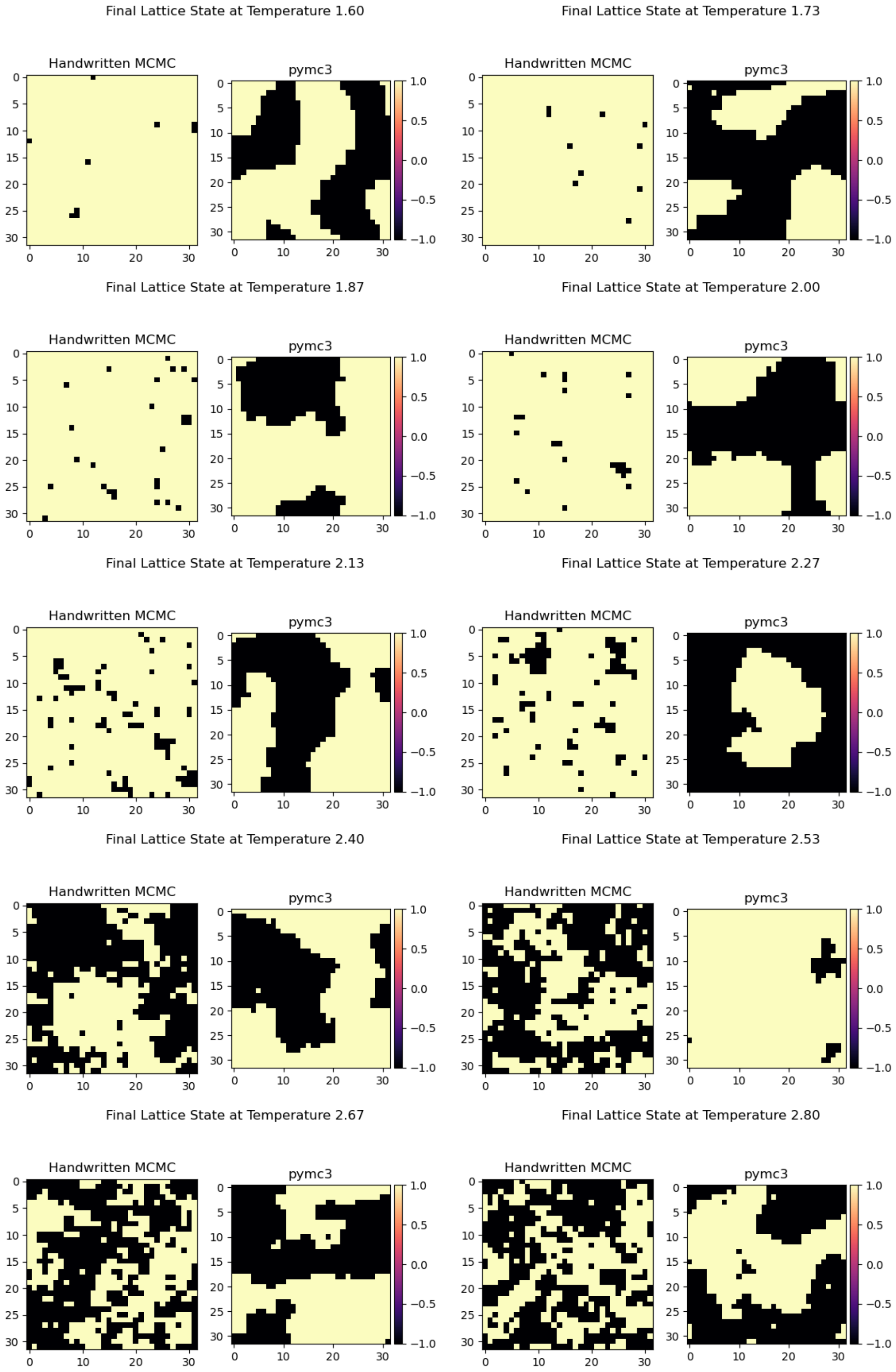
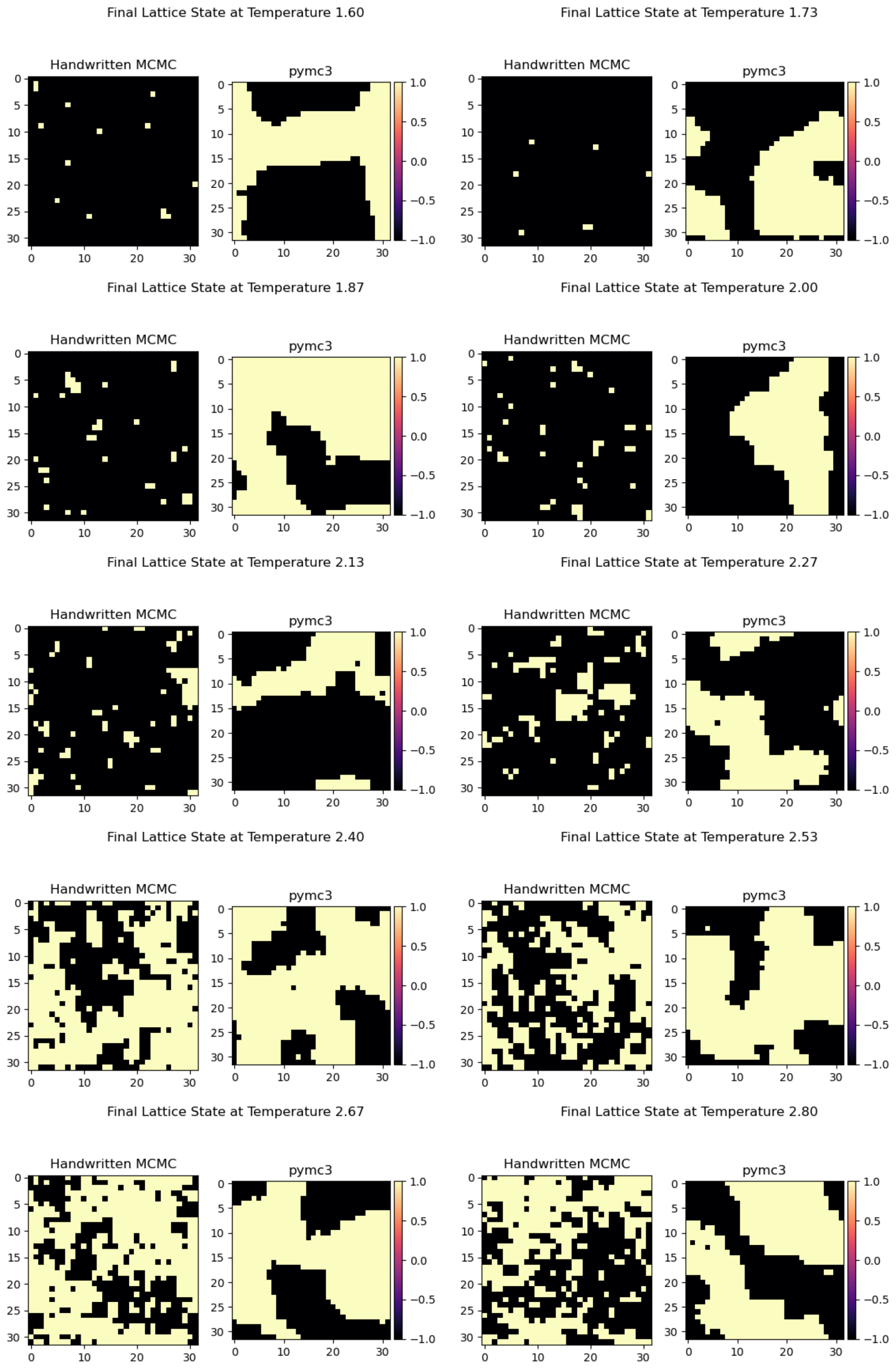


Figure 5: Final lattice states at a variety of temperatures, with a uniformly +1 initial lattice state, comparing the handwritten MCMC to pyMC3



Final Lattice State at Temperature 1.60

Final Lattice State at Temperature 1.73

Final Lattice State at Temperature 1.87

Final Lattice State at Temperature 2.00

Final Lattice State at Temperature 2.13

Final Lattice State at Temperature 2.27

Final Lattice State at Temperature 2.40

Final Lattice State at Temperature 2.53

Final Lattice State at Temperature 2.67

Final Lattice State at Temperature 2.80

Figure 6: Final lattice states at a variety of temperatures, with a uniformly -1 initial lattice state, comparing the handwritten MCMC to pyMC3

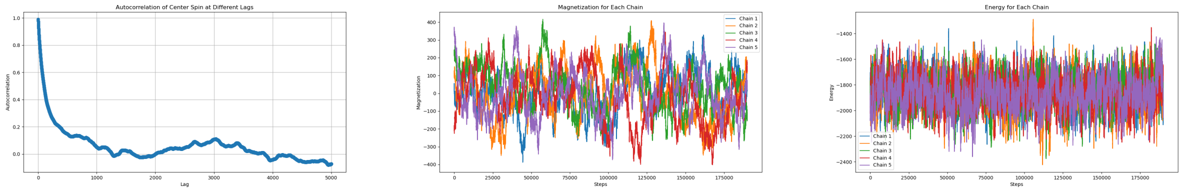


Figure 7: Plots showing autocorrelation and convergence test results, multiple chain analysis and Gelman-Rubin statistical test was performed

ration. The first graph displayed in Fig.7 indicates how the state of the center spin (at position $(16, 16)$ in a 32×32 lattice) is related to its past states (the 'lag' represents the time difference between comparisons). The autocorrelation graph showed a rapid decline as it progresses. There are several factors that played important roles in generating and assessing the correlation and convergence, such as the `equilibration_steps` which was defined at 20%, however, it was also tested for 10% or 5% (0.05) as well as a burn-in period was also implemented at the later part of the code. For the final convergence test, the equilibration steps, was set at 5% of the total steps, serve as a pre-burn-in phase to allow the system to reach a 'steady state' before collecting data as a well-chosen equilibration period helps in achieving a state that is independent of the initial conditions. When testing these parameters, we closely monitored values of Gelman-Rubin as well as graphical results from multiple chain analysis, no significant difference was found within the range between $5 - 20\%$ burn-in period. The steepness of the decay in autocorrelation values with increasing lag provides a measure of how quickly past information is lost, with different lag values from 50 to 5000 tested. The `measurement_gap` or thinning samples was also explored and kept at a value for consistency. The values obtained from the Gelman-Rubin diagnostic assess the convergence of multiple chains. A value close to 1 suggests that inter-chain variance is comparable to intra-chain variance, a sign that the chains are converging to the target distribution. The reported values near 1 (1.0208270273770934 for magnetization and 1.0022680666778951 for energy) indicate good convergence. The plots from multiple chain analysis (other two plots in Fig.7) demonstrated variability over time for each independent chain. Ideally, after an adequate burn-in period, the chains displayed overlapping behaviors, indicating that they are sampling from the same distribution which we observed, however, a lot more fluctuation was observed for magnetization and this was always reflected in the Gelman-Rubin statistics test.

4 Conclusion

Compared to pymc3, our handwritten code appears to struggle with recognizing the effect atoms would have on their neighbors, which results in more random results. I believe that this would be fixed if we changed the way we decide which spin to test so that it's dependent on the location of the previously testing atom (example: More likely to choose atoms close to the current one for the next test). This could have been done with a proposal function that is some sort of 2D Gaussian probability, but it can only select integers which tell us how far away and in which direction the next spin state to test is.

Our model does much better at higher temperatures, which makes sense given the dependence of our likelihood function on temperature. Our model also does quite well at identifying state changes at a critical temperature. There is a clear jump in the magnetization, specific heat, and susceptibility plots when the state change occurs. The Gelman-Rubin test also reveals that our model converges well after a relatively small burn-in period.

Our model is quite computationally and time expensive, as it produces and saves a significant amount of data over many iterations in order to produce the results we want. It takes about 5-10 minutes to run on average, but overall produces decent results that match with our expectations for the 2D Ising Model.