# Statistical Properties of the 2D Ising Model

Report by: Mea Railo

## Introduction

The report explores the statistical properties of the 2D Ising model using Markov Chain Monte Carlo (MCMC) simulations. The Ising model is a system of a square lattice of N-by-N binary spins, where each spin takes on a value of -1 or +1. The report uses periodic boundary conditions to minimize energy effects.

The Hamiltonian energy function is used to calculate the cost of a particular configuration, by examining a spin's interactions with its neighbors. For this assignment, the coupling constant $J_{ij}$ is set to 1. The Hamiltonian energy function, which calculates the cost of a system, is defined as

$$H(s) = -\frac{1}{2}\sum_i \sum_{j\in N(i)} J_{ij} s_i s_j.$$

To simulate thermal equilibrium, configurations are sampled from the Boltzmann distribution

$$P(s) \propto e^{-\beta H(s)},$$

and this is done using the Metropolis algorithm, where single spin flips are accepted based on the probability

$$P_{acc} = min\{1, \, exp(-\beta\Delta H)\}.$$

This report aims to explore the phase transitions between the ordered and disordered phases. Moreover, the report estimates critical temperature using magnetization and susceptibility. The code for all tasks can be run from Ising_main.py, though the logic for Task 3 is found in Ising_properties.py.
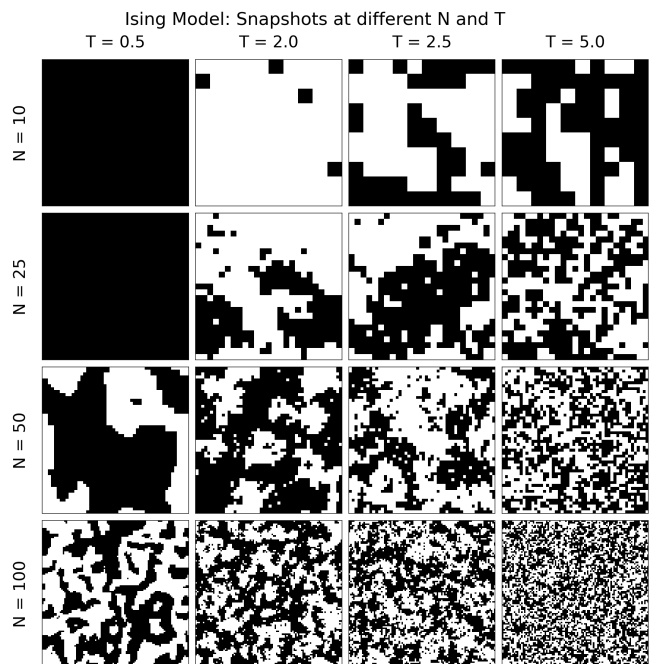
## Task 1: Implementation of Ising class

The Ising class was successfully completed to handle the core mechanics of the simulation. The cost() method computes the total Hamiltonian energy of the system by summing the bottom and right neighbors of each pair and it enforces periodic boundary conditions. The delta_cost() method was implemented to reduce computational cost, as the method computes only the energy difference caused by a single spin flip rather than the energy of the entire system. Then, find_clusters() was implemented following the Breadth-First Search that was outlined in the pseudocode. It uses a mask array and a todo to go over the lattice and identify domains of spins (spins that have the same sign).

## Task 2: Exploring MCMC parameters

### Task 2.1: Visualization of spin configurations

**Methodology** The 2D Ising model was simulated using MCMC for various system sizes ($N \in \{10, 25, 50, 100\}$) and temperatures ($T \in \{0.5, 2.0, 2.5, 5.0\}$). A burn-in period of 100,000 to eliminate bias from initial values was used. The display() method shows snapshots of the final spin configurations.

**Findings** With high temperatures (T=5.0), as seen in the figure on the right, the system is in disorder. There are no sizable clusters, and the spin configurations resemble random noise. At temperatures well above the phase transition, thermal fluctuations are more



Ising Model: Snapshots at different N and T

important than magnetic coupling, preventing order from forming.

At intermediate temperature (2. 5), more ordered systems can be seen. With smaller systems (N=10, 25), the system seems to be mostly magnetized. With larger systems (N=50, 100), there are large clusters of spins. The system is in between order and disorder. This behavior suggests that the system is close to phase transition, where spins influence each other over large distances, thus forming clusters.
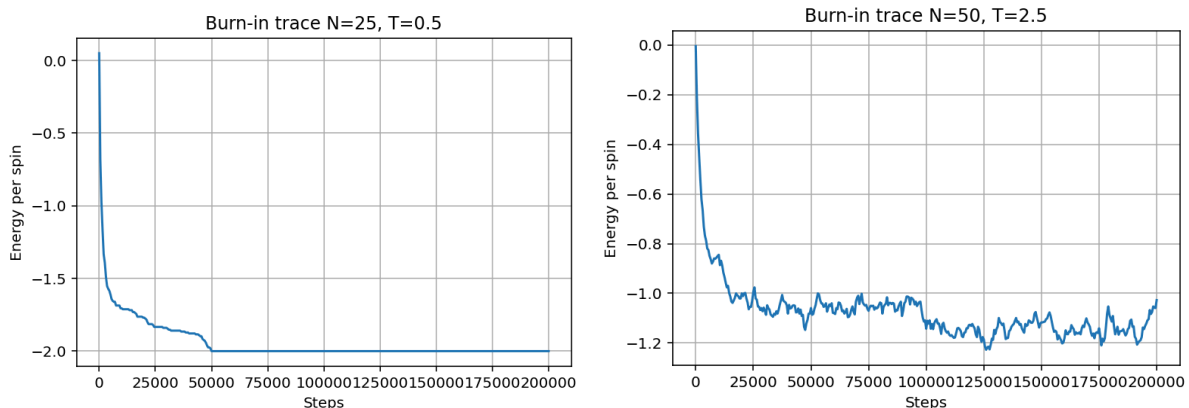
Just below this transition (T=2.0), the system attempts to order, but some small islands of unaligned spins are seen. This represents thermal noise.

At low temperature (T=0.5), large systems (N=50, 100) show large domains. These are metastable states where the system did not align because of stable domain walls. More iterations, so a larger burn-in, would be needed to fully align to a single color.


**Task 2.2: Suitable burn-in, acceptance rate, costs**

**Finding optimal burn-in**

To determine the optimal trade-off between a sufficiently high burn-in while keeping computational cost low, different burn-in times with different lattice sizes and temperatures were plotted along total energy (cost). Visually, helped determine where the total energy reaches a stable point (i.e., where it is no longer consistently increasing or decreasing). The visualization was done for lattice sizes 10, 25, 50, and 100 along temperatures 0.5, 2.0, 2.5, and 5.0. The stable point (optimal burn-in) was determined visually for each; these results can be found in the burn-in table in Ising_main.py. Two examples are shown below.



N = 25, T = 0.5 → burn-in = 60,000 (Left figure)

The energy drops rapidly into the ordered phase and reaches the ground-state value early. By around 50,000 steps, the curve is completely flat. So, to be conservative, a value of 60,000 was chosen as the smallest burn-in that guarantees fully equilibrated samples.

N = 50, T = 2.5 → burn-in = 120,000 (Right figure)

Near the critical temperature, the energy relaxes much more slowly: even after the initial drop, there is gradual downward drift for tens of thousands of steps. Only around 100,000 steps does the curve settle into a stable fluctuation band. A burn-in of 120,000 was chosen as the optimal burn-in.
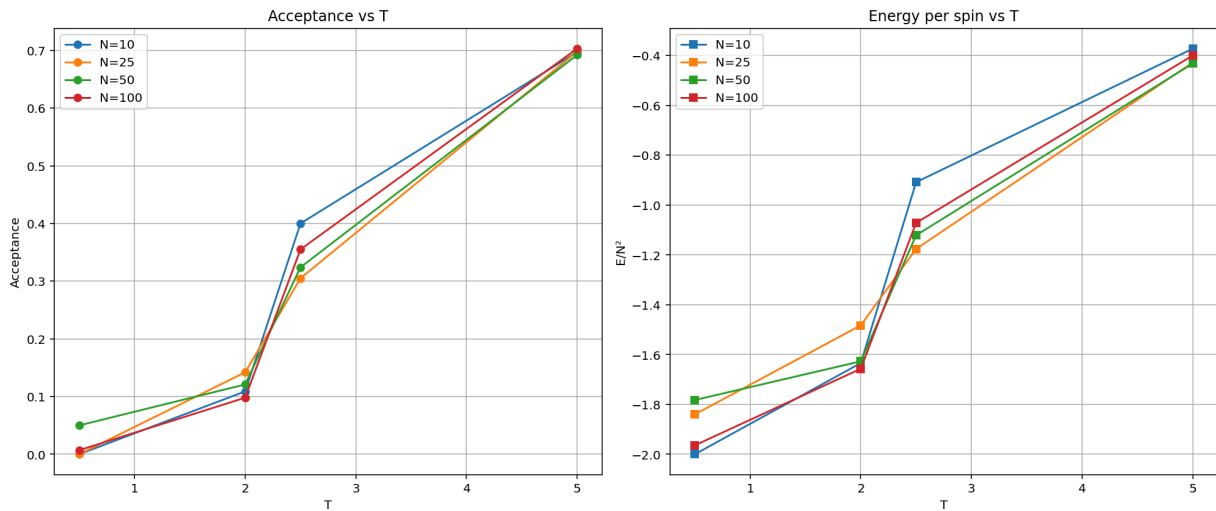
From these visualizations, some conclusions about the effect of N and T on burn-in can be drawn.
- System size (N): Larger systems require longer burn-in times. The larger systems in general did not reach the ground state energy while the smaller systems did, meaning that the burn-in value must scale with system size.
- Critical region (where T is around the critical temperature): Close to the critical temperature  around 2.26), the system experiences critical slowing down. Large clusters means that the system moves slowly. Thus, the burn-in period required to reach the final ordered state is maximal near the critical temperature, which means it needs more steps than in the high-temperature phase.

**Acceptance rate and cost**

***Methodology*** To investigate the Metropolis algorithm's efficiency, the cost (total energy $H$) of the system was tracked. To allow for comparison along the different system sizes ($N \in \{10, 25, 50, 100\}$), the value was normalized by the total number of spins ($N\text{\textasciicircum}2$) to calculate the average energy per spin. This was measured alongside the acceptance rate, which is the fraction of proposed flips that were accepted, for temperatures $T \in \{0.5, 2.0, 2.5, 5.0\}$.

***Output & Findings***



As shown in the figure on the left, the acceptance rate increases with temperature across all lattice sizes, nearly reaching 70% at T=5.0. At low temperature (T=0.5), the system is strongly ordered due to the fact that almost all proposed flips increase energy, resulting in a very low acceptance rate (most ΔH > 0 flips are rejected). At intermediate temperatures and around the critical temperature, the ΔH penalties become less important, so the acceptance rate is slightly higher. At high temperatures, when the system is disordered, the energy cost becomes close to irrelevant. In this phase, spins flip freely and the acceptance stays around 70% for lattices of all sizes.

The average energy per spin, or cost, of each system is shown in the figure on the right. At low T, all lattices have an energy per spin that is close to the ground-state value of E/(N^2) = -2 (specifically, at T=0.5, we observe that N=10 reaches this ground state). As the temperature increases, the thermal fluctuations result in domain walls, so energy begins to rise closer to 0. The sharpest rise in temperature is around the critical region (between 2.0 and 2.5), which is consistent with the system moving from a phase of order to disorder.
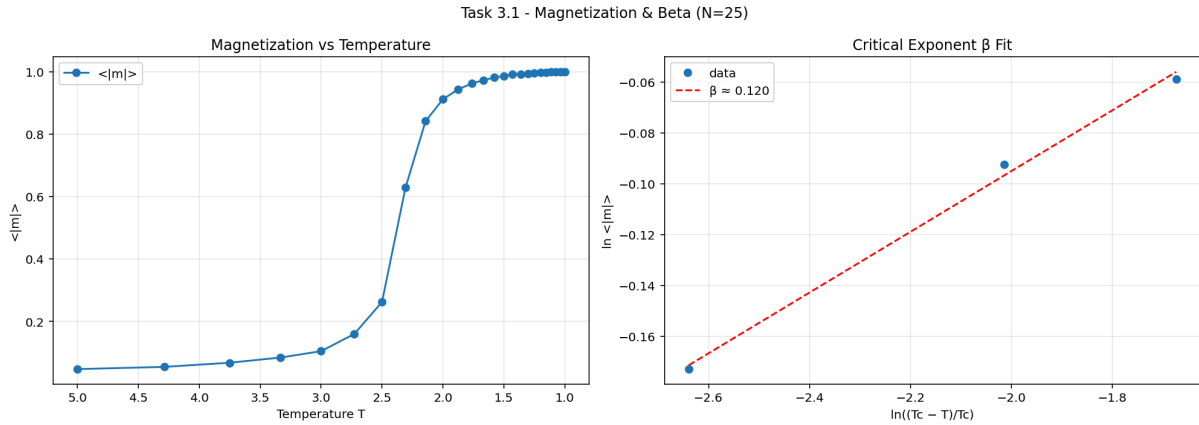
## Task 3: Statistical properties and estimating critical temperature

### Task 3.1: Estimating critical temperature via magnetization

***Methodology*** To estimate the critical temperature, the behavior of average absolute magnetization < |m| > as a function of temperature was measured. The MCMC simulations were performed on a lattice of size $N = 25$. This was chosen as a trade-off between accuracy and computational cost. The program uses a long burn-in period with a long waiting time to reduce autocorrelation. Additionally, performing a linear regression on the log-transformed data (near the critical temperature) allows to estimate the critical exponent β. This tests the theoretical power law prediction:

$$m(T) \sim \left(\frac{T_c - T}{T_c}\right)^{\beta}, \text{ with } \beta = \frac{1}{8}.$$

## Output & Findings

The resulting magnetization curve, shown on the figure on the left, follows the theoretical behavior of the 2D Ising model. At high temperatures, the system is disordered with a magnetization of approximately 0, while at low temperatures the system becomes ordered, approaching a magnetization of 1.0. The transition between this ordered and disordered phase is sharp, shown in the graph by the steep curve from about 2.5 to 2.2. The critical temperature can be visually identified where the system sees the highest increase in absolute magnetization. The value for the critical temperature can therefore be identified at around 2.3 and 2.4. This is close to the theoretical critical temperature of T=2.269, though slightly higher, resulting from the finite size of the system (N=25).
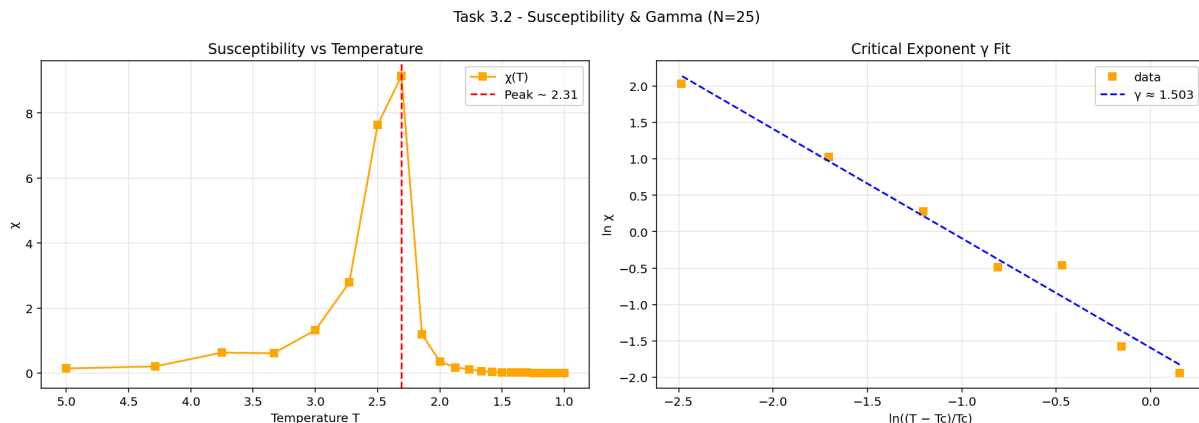
To calculate the critical exponent, three values around the critical temperature were used, giving a beta value of 0.120. This is similar to the theoretical prediction of 0.125, thus confirming the expected critical behavior, though the value could be made more accurate with a larger amount of samples close to the critical temperature.

## Task 3.2: Estimating critical temperature via susceptibility

*Methodology* Another method of measuring critical temperature is by calculating the susceptibility, which measures the magnitude of magnetization fluctuations at temperature T. For each temperature, with the range used in task 3.1, the same MCMC simulation was run as in Task 3.1 (N=25, long burn-in and waiting time). The susceptibility curve $\chi(T)$ was plotted against temperature, and the location of the peak was used as another estimator of critical temperature. To determine the critical exponent $\gamma$, only the temperatures above the critical point were used, and the logarithm of the power law was taken:

$$\chi(T) \sim \left(\frac{T-T_c}{T_c}\right)^{-\gamma}.$$

## Output & Findings

As shown in the figure on the left, the susceptibility shows a pronounced peak at T=2.31. This peak gives the temperature at which the magnetization fluctuations are maximized, which indicates the start of the system becoming ordered. At high T, χ is small because the spins behave independently, while at low T, χ is also small because the system is almost fully ordered, meaning that there are close to no fluctuations.

The log fit for the critical temperature gives a value of about $\gamma = 1.5$. The theoretical value for the Ising model is 1.75, so the value from the simulation is slightly lower, though still close.
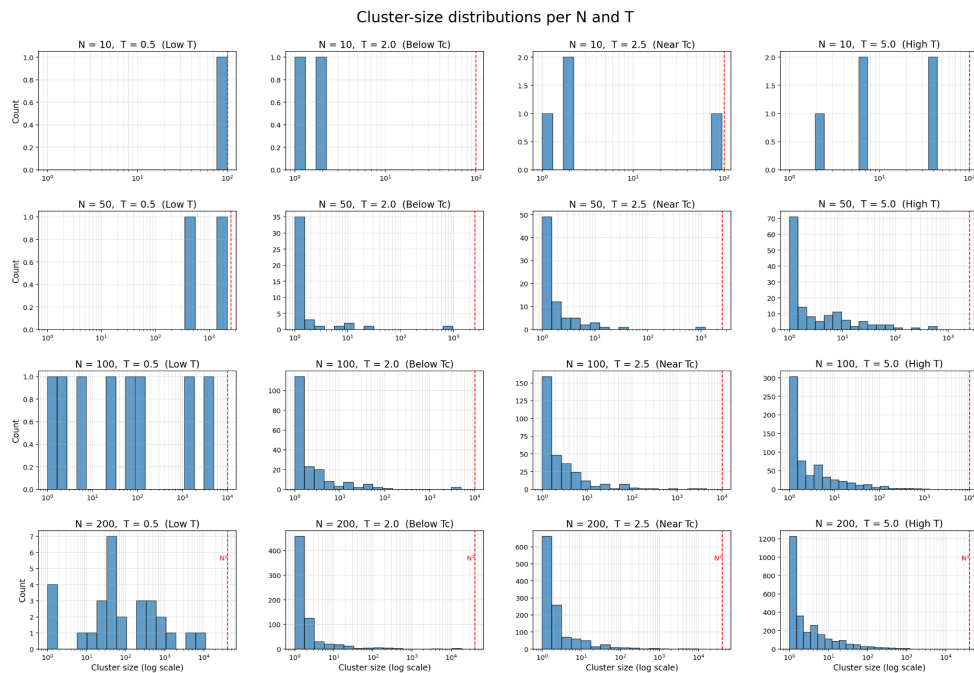
### *Connection between magnetization and susceptibility*

In the Ising model, susceptibility is essentially the derivative of magnetization with respect to an external field. Therefore, large susceptibility corresponds to rapid changes in magnetization. This is why both observables give the same critical temperature (around 2.3). Visually, it is easier to understand the critical temperature with susceptibility, as it is simply the peak.

### Task 3.3: Investigating cluster size

*Methodology* The simulation was run for lattice sizes 10, 50, 100, and 200 with temperatures 0.5, 2.0, 2.5, and 5.0. For each temperature, a long burn-in period was used to reach equilibrium. A single sample was calculated and plotted. The find_clusters() method was completed and used to count the size of every connected component of spins. The results were then plotted in histograms with a logarithmic scale for the cluster sizes on the x-axis, and the count of the number of clusters of this size on the y-axis. The red line shows the maximum possible size of a cluster (so the area of the whole lattice N^2).

### *Output & Findings*



Cluster-size distributions per N and T

The above figure plots the cluster size distribution for the different sized lattices with different temperatures. As can be seen in the rightmost column, in the highest temperature (T=5.0), the systems are in a disordered state. Large clusters are non-existent, and the configuration resembles random noise. Near the critical temperature (T=2.5, 2.0), we observe an increase in the size of clusters. For example, for N=100 at 2.5 and 2.0, there exist clusters of over 1000. When the system reaches T=0.5, the system is in an ordered state. For the lattice of size 10, there exists one cluster of size 100, so the system is ordered. For N=50, there are two clusters, indicating a domain wall. For N=100 and N=200, there exist large clusters and some smaller clusters. The large lattices fail to reach the ground state fully, which demonstrates critical slowing down. This is when the domain walls move extremely slowly, and an extremely large burn-in is required to resolve the domains into one cluster