Simulating the 2D Ising Model via the Metropolis-Hastings Algorithm

A Study in Statistical Mechanics, Phase Transitions, and Monte Carlo Methods

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Contents

1 Abstract

This project investigates the thermodynamic behavior and phase transition of a two-dimensional ferromagnetic Ising Model through a numerical simulation driven by the Metropolis-Hastings Monte Carlo algorithm. The Ising Model serves as a paradigmatic system in statistical mechanics for demonstrating spontaneous symmetry breaking and continuous phase transitions.

In this computational study, we model a 10×10 lattice of discrete magnetic dipole moments (spins). The primary objective is to observe how localized nearest-neighbor interactions compete with global thermal fluctuations to determine the macroscopic state of the system. We explore the limitations of computing the canonical partition function analytically and circumvent this $O(2^N)$ computational bottleneck by employing Monte Carlo importance sampling.

Furthermore, the model addresses finite-size edge effects by mapping the finite rectangular grid onto a topological torus using periodic boundary conditions. The simulation is stress-tested across three distinct thermal regimes: well below the critical temperature ($T \ll T_c$) to observe magnetic ordering, exactly at the critical temperature ($T \approx 2.269$) to observe scale-invariant fractal clustering, and well above the critical temperature ($T \gg T_c$) to observe a high-entropy paramagnetic state. The results validate the efficacy of the Metropolis criterion in steering high-dimensional systems toward thermodynamic equilibrium.

2 Introduction & Motivation

The phenomenon of ferromagnetism—where certain materials exhibit a spontaneous macroscopic magnetization in the absence of an external magnetic field—was a profound mystery in classical physics. According to the Bohr-Van Leeuwen theorem, classical mechanics cannot explain diamagnetism or ferromagnetism; these phenomena are fundamentally rooted in quantum mechanics and the Pauli exclusion principle, which give rise to the exchange interaction between electron spins.

In 1920, Wilhelm Lenz proposed a highly simplified mathematical model of this behavior, which was subsequently analyzed by his student Ernst Ising in 1924. The resulting "Ising Model" strips away the complex quantum mechanical details, reducing the material to a regular lattice of discrete variables called spins, s_i, which can only take two values: $+1$ (spin up) or -1 (spin down).

While Ising famously proved that the 1D model does not undergo a phase transition at any temperature greater than absolute zero ($T > 0$), Lars Onsager published an exact analytical solution for the 2D model in 1944. Onsager proved that the 2D Ising Model does indeed exhibit a continuous phase transition at a finite critical temperature, T_c.

2.1 The Computational Imperative

The motivation for treating this system computationally rather than analytically lies in the scaling of macroscopic systems. For a lattice of N spins, the number of possible microstates is 2^N. For a modest 10×10 grid, this yields $2^{100} \approx 1.26 \times 10^{30}$ configurations. Calculating the exact thermodynamic observables by summing over all these states—evaluating the exact partition function—is computationally intractable.

This project bridges theoretical statistical mechanics and modern computational physics by implementing the Metropolis-Hastings algorithm. Instead of analyzing every possible state, we use a stochastic process to generate a sequence of states drawn directly from the equilibrium Boltzmann distribution. This "importance sampling" allows us to accurately estimate macroscopic observables (like total energy and magnetization) using only a minute fraction of the total phase space, demonstrating the immense power of Monte Carlo methods in modern physics.

3 Theoretical Basis

3.1 The Ising Hamiltonian

The total internal energy of a specific microstate (configuration of spins) in the absence of an external magnetic field is given by the Ising Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

Where:

- $s_i, s_j \in \{+1, -1\}$ are the discrete spin states at lattice sites i and j.
- J is the exchange interaction constant. For $J > 0$, the system is ferromagnetic (favoring aligned spins). For $J < 0$, it is antiferromagnetic. In this simulation, we set $J = 1$.
- $\langle i, j \rangle$ indicates that the sum is performed strictly over pairs of nearest neighbors. In our square lattice, the coordination number is $z = 4$.

3.2 Statistical Mechanics and the Partition Function

In the canonical ensemble, the probability $P(\mu)$ of finding the system in a specific microstate μ with energy E_μ at temperature T is given by the Boltzmann distribution:

$$P(\mu) = \frac{1}{Z} e^{-\beta E_\mu} \tag{2}$$

Where $\beta = \frac{1}{k_B T}$ and Z is the partition function:

$$Z = \sum_{\nu} e^{-\beta E_\nu} \tag{3}$$

Because computing Z directly is impossible for large N, we must rely on dynamic stochastic transitions that bypass Z entirely.

3.3 Detailed Balance and the Metropolis Algorithm

To sample from the Boltzmann distribution without knowing the partition function Z, the system's transition probability $W(\mu \to \nu)$ from state μ to state ν must satisfy the condition of **detailed balance**:

$$P(\mu) W(\mu \to \nu) = P(\nu) W(\nu \to \mu) \tag{4}$$

Substituting the Boltzmann probabilities yields:

$$\frac{W(\mu \to \nu)}{W(\nu \to \mu)} = \frac{P(\nu)}{P(\mu)} = e^{-\beta(E_\nu - E_\mu)} = e^{-\beta \Delta E} \tag{5}$$

Notice that the intractable partition function Z cancels out perfectly in the ratio.

The Metropolis-Hastings algorithm satisfies detailed balance by breaking the transition probability into a proposal probability (which is symmetric) and an acceptance probability. The acceptance criterion $A(\mu \to \nu)$ is defined as:

$$A(\mu \to \nu) = \begin{cases} 1 & \text{if } \Delta E \leq 0 \\ e^{-\beta \Delta E} & \text{if } \Delta E > 0 \end{cases} \tag{6}$$

Physically, this means:

1. A spin flip that lowers the system's energy (aligning with neighbors) is *always* accepted.

2. A spin flip that increases the system's energy (introducing disorder) is accepted with a finite probability dependent on the temperature. High temperatures allow frequent energy increases (entropy dominates), while low temperatures suppress them (internal energy minimizes).

4 Topological Framework: The Toroidal Array

One of the most significant challenges in computational solid-state physics is the "finite-size effect." In a small 10×10 rectangular grid, there are 100 spins. Of these, 36 lie on the boundary edges. This means 36% of the particles do not have a full set of 4 neighbors, heavily skewing the energy calculations and artificially suppressing the phase transition.

To correct this, we must eliminate the boundaries entirely without increasing the number of spins to infinity. We achieve this by altering the topology of the space, mapping the flat 2D grid onto a **torus** ($S^1 \times S^1$).

4.1 Mathematical Implementation of Periodic Boundaries

We implement Periodic Boundary Conditions (PBC) using the modulo operator. For a lattice of size $L \times L$, the indices run from 0 to $L - 1$. When calculating the neighbors of a spin at (i, j), we define them as:

- Right: $(i, (j + 1) \bmod L)$
- Left: $(i, (j - 1) \bmod L)$
- Down: $((i + 1) \bmod L, j)$
- Up: $((i - 1) \bmod L, j)$

4.2 Physical Implications of the Torus

If the algorithm queries the right neighbor of a spin on the far right edge ($j = 9$), the operation $(9 + 1) \bmod 10 = 0$ wraps the geometry around, pointing to the spin on the far left edge of the same row. Similarly, the bottom edge wraps to the top.

This mathematical "stitching" of edges means the lattice has no boundaries, no corners, and no "surface." Every single spin in the array now exists locally in an identical environment with exactly coordination number $z = 4$. By enforcing this translational invariance, our small 10×10 matrix simulates a localized patch within an infinite crystal lattice much more accurately than a hard-bounded grid.

5 Full Source Code

```
import numpy as np

choose = np.random.choice

IM_initial = np.zeros((10,10))
spins = [1,-1]
J = 1
k = 1.38
Temp = 2.269

def Probability(dE):
    p = np.exp(-1*dE/(k*Temp))
    return p

for r in range(10):
    for c in range(10):
       IM_initial[r,c] = choose(spins)

def neighbors(i, j, lattice):
    L = lattice.shape[0]
    n = [
        lattice[(i+1) % L, j],
        lattice[(i-1) % L, j],
        lattice[i, (j+1) % L],
        lattice[i, (j-1) % L]
    ]
    return n

def Hamiltonian(lattice):
    H = 0
    for r in range(lattice.shape[0]):
        for c in range(lattice.shape[0]):
            H += -1*J*(lattice[r,c])*(sum(neighbors(r,c,lattice)))
    return H/2

print(f'Initial Energy: {Hamiltonian(IM_initial)} Joules(e-23)')

def Metropolis(lattice):
    for i in range(10000):

        a = choose(range(lattice.shape[0]))
        b = choose(range(lattice.shape[0]))
        p = lattice[a,b]
        q = -1*p

        lattice1 = lattice.copy()
        lattice1[a,b] = q

        dE = Hamiltonian(lattice1)-Hamiltonian(lattice)

        if dE <= 0:
            lattice[a,b] = q
        else:
            prob = Probability(dE)
            if np.random.rand()<prob:
                lattice[a,b] = q
```

```
57
58      return lattice
59
60  def print_lattice(lattice):
61      for r in range(lattice.shape[0]):
62          row = ""
63          for c in range(lattice.shape[1]):
64              if lattice[r, c] == 1:
65                  row += "O "
66              else:
67                  row += "X "
68          print(row)
69
70  IM_final = Metropolis(IM_initial)
71  print_lattice(IM_final)
72  print(f'final Energy is {Hamiltonian(IM_final)} Joules(e-23)')
```

Listing 1: 2D Ising Model Simulation

6 Code Description: Block by Block

The numerical simulation is structured into distinct functional blocks, reflecting the underlying physics of the Ising Model.

6.1 Block 1: System Initialization

Lines 1-17: The simulation parameters are established. The physical constants are defined, notably setting the simulation exactly at the Onsager critical temperature $T_c \approx 2.269$. The 10×10 lattice `IM_initial` is populated with a totally random distribution of $+1$ and -1 spins. This represents the system starting at $T = \infty$, representing a state of maximum entropy.

6.2 Block 2: The Toroidal Neighbor Map

Lines 19-27: The `neighbors(i, j, lattice)` function applies the periodic boundary conditions discussed in Section 4. By returning the array of the four adjacent spins using the modulo `% L` operator, the function maps the 2D array onto a torus, ensuring translational invariance and eliminating boundary anomalies.

6.3 Block 3: Energy Calculation (Hamiltonian)

Lines 29-35: The `Hamiltonian(lattice)` function computes the macroscopic internal energy of the current microstate. It iterates through every spin, multiplying it by the sum of its four toroidal neighbors and scaling by $-J$. Crucially, the final return statement divides the total sum by 2 (`H/2`). This prevents double counting, as the nested loop counts the interaction between spin A and spin B twice (once when evaluating A, and once when evaluating B).

6.4 Block 4: The Metropolis-Hastings Engine

Lines 39-59: The `Metropolis(lattice)` function is the core thermodynamic engine. It runs for 10,000 "Monte Carlo steps."

- It selects a random spin at coordinates (a, b) and proposes a spin-flip ($q = -1 * p$).
- It evaluates the change in energy ΔE caused by this flip.
- If $\Delta E \leq 0$, the array is permanently updated.
- If $\Delta E > 0$, the flip is subjected to a stochastic test. It generates a uniform random number between 0 and 1. If this number is less than the Boltzmann probability $P = e^{-\Delta E / k_B T}$, the flip is accepted; otherwise, it is rejected.

6.5 Block 5: State Rendering

Lines 61-70: The `print_lattice` function translates the numerical array into a visual map. Spin-up states ($+1$) are represented by "O", and spin-down states (-1) are represented by "X". This provides an immediate visual confirmation of domain clustering and magnetic ordering.

7 Results and Analysis: Temperature Regimes

To validate the code, the simulation was executed at three distinct thermal regimes by adjusting the 'Temp' variable. The initial random configuration (maximum entropy) rapidly evolves toward a state dictated by the specific temperature. The initial energy for all runs began at approximately +4 to −12 Joules.

7.1 Regime 1: Low Temperature ($T = 0.5$)

At temperatures well below T_c, thermal fluctuations are highly suppressed. The Boltzmann probability for accepting a higher-energy state approaches zero. The system acts almost strictly as an energy-minimizer, resulting in spontaneous symmetry breaking. The lattice becomes highly ordered, collapsing into a single, massive ferromagnetic domain. The final energy approaches the absolute minimum (−200 Joules).

```
Low Temperature Output (T = 0.5)
O O O O O O O O O O
O O O O O O O O O O
O O O O O O O O O O
O O O O O O O O O O
O O O O O X O O O O
O O O O O O O O O O
O O O O O O O O O O
O O O O O O O O O O
O O O O O O O O O O
O O O O O O O O O O
Final Energy is -192.0 Joules(e-23)
```

7.2 Regime 2: Critical Temperature ($T = 2.269$)

At the exact critical temperature, the system undergoes a continuous phase transition. The competition between aligning forces (internal energy) and randomizing forces (entropy) is perfectly balanced. This results in the formation of fractal-like clusters of 'O' and 'X' of all scale lengths. The system exhibits large-scale fluctuations but retains significant localized order.

```
Critical Temperature Output (T = 2.269)
O O O X X X X O O O
O O O X X X X O O O
O O X X X X X X O O
O O X X X X X X X O
O X X X X X X X X X
O X X X X O O X X X
O O X X O O O O X X
O O O O O O O O O X
O O O O O O O O O O
O O O O O O O O O O
Final Energy is -116.0 Joules(e-23)
```

7.3 Regime 3: High Temperature ($T = 5.0$)

At temperatures significantly above T_c, the kinetic thermal energy completely overwhelms the nearest-neighbor exchange interaction J. The acceptance probability $e^{-\Delta E/k_B T}$ approaches 1 regardless of the energy penalty. The spins flip rapidly and randomly, resulting in a paramagnetic state characterized by maximum entropy and zero net macroscopic magnetization. The final energy remains close to zero.

```
High Temperature Output (T = 5.0)
X O X O O X O X X O
O X O X O O X X O X
X X X O O X O O X X
O O X O X X X O O X
X O O X X O X X O O
O X O O X X O O X O
X X X O X O X X X O
O O X X O O X O X X
X O O X X O O X O O
O X X O O X O X X O
Final Energy is -12.0 Joules(e-23)
```

8 Conclusion

This independent research project successfully implemented the Metropolis-Hastings Monte Carlo algorithm to simulate the 2D Ising Model. By projecting the 10×10 lattice onto a topological torus, we mitigated boundary edge anomalies and preserved the translational symmetry required to simulate bulk thermodynamic properties.

The integration of the physics engine produced highly accurate qualitative results across different temperature regimes. The transition from a totally disordered paramagnetic state at high temperatures, through scale-invariant clustering at the critical temperature T_c, to a highly ordered ferromagnetic domain at low temperatures strongly validates the model. The code proves that complex, macroscopic phase transitions can emerge entirely from the iterative application of localized, nearest-neighbor stochastic probabilities based on the fundamental principles of statistical mechanics.