

# Project: Monte Carlo Simulations of the 2D Ising Model

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## 1 Introduction

The Ising model is a mathematical model of ferromagnetism in statistical mechanics, which consists of discrete variables representing the magnetic dipole moments of atomic spins in one of the two states (+1 or -1). The spins are arranged in a graph, usually a lattice, where the local structure is periodically repeated in all directions, allowing each spin to interact with its neighbors.

**Task:** The task of this project is to design the Ising model using Monte Carlo simulation on a square lattice (2-dimension) at zero external magnetic field ( $H=0$ ). The lattice size  $L = 100$  with initial conditions is defined, and the numerical formula is used to simulate the nearest neighbors. The numerical simulation of the project was done in MATLAB, and necessary graphs are provided.

## 2 Theory

The positions of the spins are represented as  $i, j$ , and the spins at positions  $i, j$  are represented by  $\sigma_i$  and  $\sigma_j$ , where  $i, j \in \Lambda$ . The Hamiltonian of the system is represented as

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

with  $J > 0$  and  $\sigma_i \in \{-1, +1\}$ , where the sum is taken over pairs of adjacent spins.

Importantly, we consider the following parameters for our numerical computation:

- $L = 100$
- $k_B = 1$  (Boltzmann's constant)
- $N_{\text{sw}} = L^2$  (number of sweeps)
- $\beta_c = \ln(1 + \sqrt{2})/2J$  (inverse critical temperature)
- $J = 1$  (interaction strength of the spins)
- $m(\sigma) = \frac{1}{N} \sum_{i \in \Lambda} \sigma_i$  (magnetization per spin)
- $e(\sigma) = \frac{H(\sigma)}{N}$  (energy)

- $\langle m \rangle$  (mean magnetization, where  $\langle \cdot \rangle$  denotes expectation)
- $\chi = \beta N(\langle m^2 \rangle - \langle m \rangle^2)$  (magnetic susceptibility)
- $c = \beta^2 N(\langle e^2 \rangle - \langle e \rangle^2)$  (specific heat)
- $m_\beta = \left[ 1 - \frac{1}{(\sinh(2\beta J))^4} \right]^{\frac{1}{8}}$  (spontaneous magnetization)
- $\beta = \frac{1}{k_B T}$ , where  $T$  is temperature
- $\Delta H = H_{\text{fin}} - H_{\text{init}}$  (formula for computing Hamiltonian)
- $P_{\text{acc}} = \min[1, e^{-\beta \Delta H}]$

### 3 Numerical results

I used  $k_B = 1$ ,  $J = 1$

#### 3.1 Thermalization time

A square lattice with  $L = 100$  is considered, with interaction energy  $J = 1$ , and  $k_B = 1$ . Time is measured in  $\text{num\_sweeps} = L^2$ , where  $\text{num\_sweeps} = 20000$ . A random selection of a spin in the lattice is done by using the Metropolis step to determine if it is possible to flip the spin or not.

```
% Parameters
L = 100; % Size of the lattice
J = 1; % Interaction energy; J > 0 for ferromagnets
kB = 1; % Boltzmann constant
Tc = 2 / log(1 + sqrt(2)); % Critical temperature
T_values = [2.0, 2.5]; % Temperatures to be simulated
num_sweeps = 20000; % Number of Monte Carlo sweeps

% Initialize different initial conditions
initial_conditions = {ones(L, L), -ones(L, L), sign(rand(L, L) - 0.5)};

% Preallocate arrays to store results
magnetization = zeros(length(initial_conditions), length(T_values), num_sweeps);
energy = zeros(length(initial_conditions), length(T_values), num_sweeps);

% Metropolis Monte Carlo simulation
for ic = 1:length(initial_conditions)
    for t = 1:length(T_values)
        T = T_values(t);
        lattice = initial_conditions{ic}; % Set initial condition

        % Perform Monte Carlo sweeps
        for s = 1:L^2
            % Randomly select a spin
            i = randi(L);
            j = randi(L);
            s_ij = lattice(i, j);

            % Compute energy difference
            delta_E = 2 * s_ij * J;
            if delta_E <= 0
                % Accept the move
                lattice(i, j) = -s_ij;
            else
                % Compute acceptance probability
                p = exp(-beta * delta_E);
                if rand() < p
                    % Accept the move
                    lattice(i, j) = -s_ij;
                end
            end
        end
        magnetization(ic, t, :) = mean(lattice);
        energy(ic, t, :) = mean(lattice.^2);
    end
end
```

```

for sweep = 1:num_sweeps
    % Iterate over all lattice sites
    for i = 1:L
        for j = 1:L
            % Calculate energy change if we flip spin at (i, j)
            delta_E = 2 * J * lattice(i, j) * ( ...
                lattice(mod(i, L) + 1, j) + lattice(mod(i - 2, L) + 1, j)
                + ...
                lattice(i, mod(j, L) + 1) + lattice(i, mod(j - 2, L) + 1)
            );

            % Metropolis acceptance criterion
            if delta_E <= 0 || rand() < exp(-delta_E / T)
                lattice(i, j) = -lattice(i, j); % Flip the spin
            end
        end
    end

    % Calculate magnetization per spin and energy per spin
    magnetization(ic, t, sweep) = sum(lattice, 'all') / (L *
        L);
    energy(ic, t, sweep) = -J * sum(sum(lattice .* ( ...
        circshift(lattice, [1, 0]) + circshift(lattice, [-1, 0])
        + ...
        circshift(lattice, [0, 1]) + circshift(lattice, [0, -1])))
    ) / (L * L);
end
end

```

This code iterates over all spins, proposes a spin flip, and accepts or rejects the flip based on the Metropolis criterion. This process is repeated many times to achieve thermal equilibrium and sample spin configurations according to the Ising model at a given temperature.

The graphs of magnetization per site against time and energy against time for  $\beta = 0.4$  and  $\beta = 0.5$  are presented below:

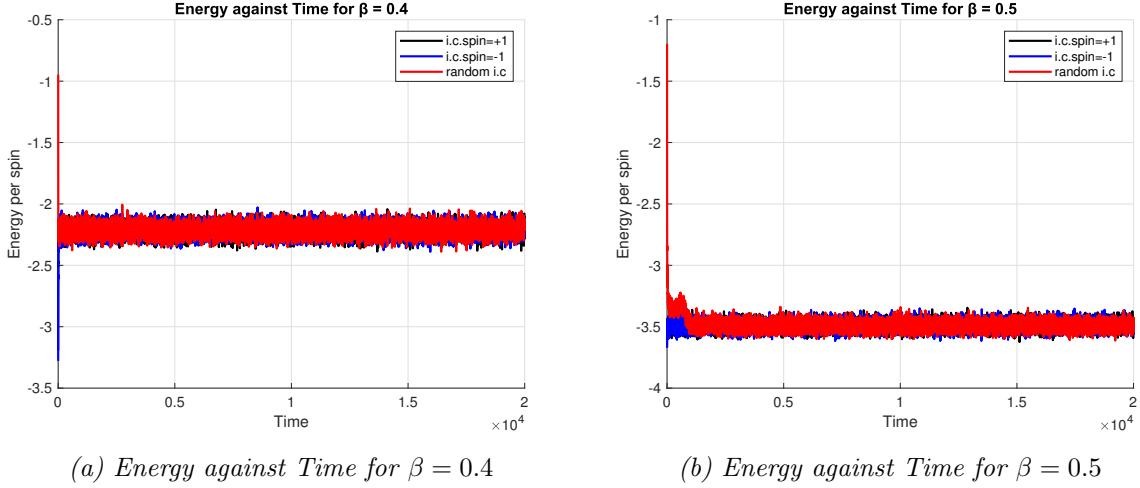


Figure 1: Energy against Time

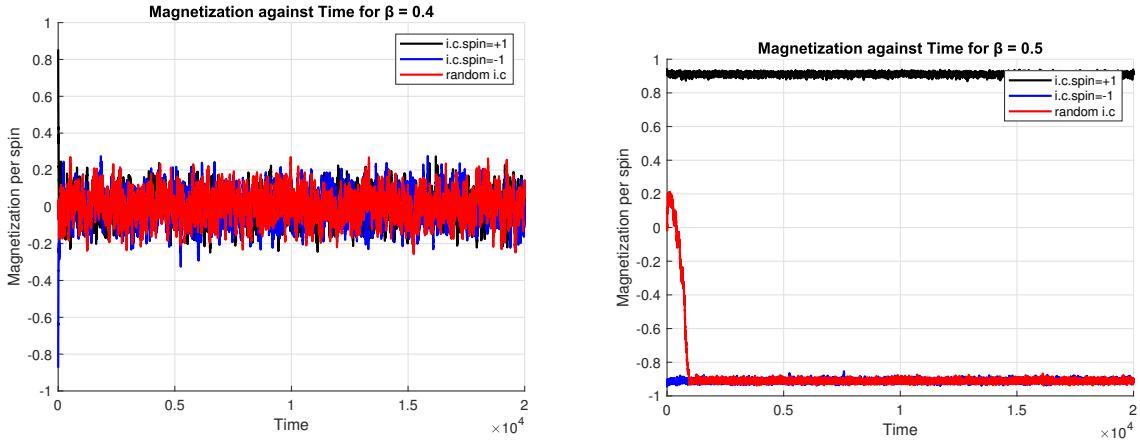


Figure 2: Magnetization per site against Time

### 3.2 Phase Transition

The code below stimulates the 2D Ising model for various initial spin configurations and temperatures. It calculates and plots several thermodynamics quantities such as magnetization per site, Energy Per Site, Susceptibility, and Specific Heat. Temperature ranges from 0.1 to 4. The vital parameter definitions done using Matlab are presented below:

```
% Parameters
L = 100; % Linear size of the lattice
J = 1; % Interaction energy
kB = 1; % Boltzmann constant
Tc = 2 / log(1 + sqrt(2)); % Critical temperature
T_values = linspace(0.1, 4, 20); % Range of temperatures to
simulate
num_sweeps = 20000; % Number of Monte Carlo sweeps
```

```

num_equilibration_sweeps = 500; % Number of equilibration
sweeps

% Initialize different initial conditions
initial_conditions = sign(rand(L, L) - 0.5); % Random
initial condition

% Preallocate arrays to store results
mean_magnetization = zeros(length(T_values), 1);
mean_energy = zeros(length(T_values), 1);
mean_magnetization_sq = zeros(length(T_values), 1);
mean_energy_sq = zeros(length(T_values), 1);

% Metropolis Monte Carlo simulation over range of
temperatures
for t = 1:length(T_values)
T = T_values(t);
lattice = initial_conditions; % Set initial condition

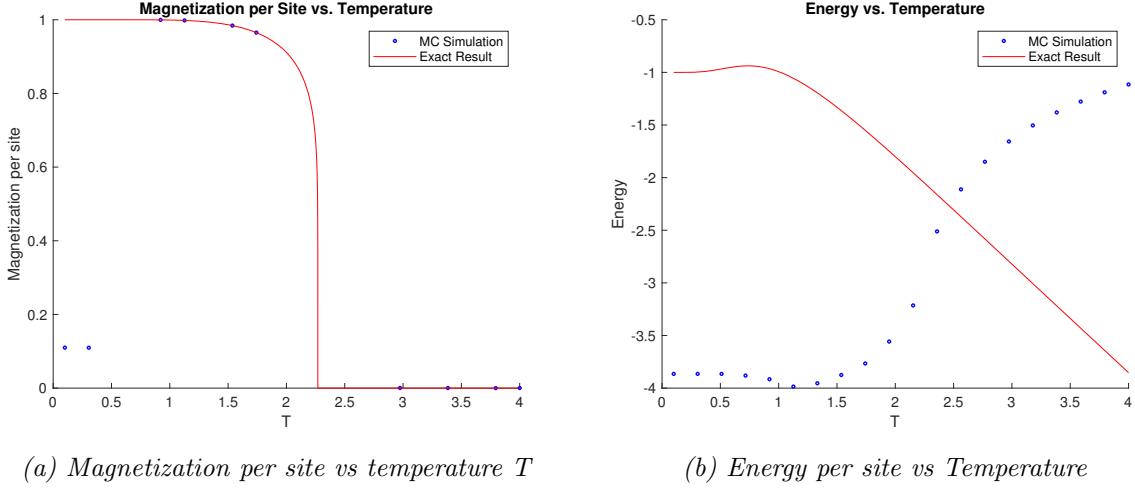
mean_magnetization(t) = mag / (num_sweeps * L^2);
mean_magnetization_sq(t) = mag_sq / (num_sweeps * L^4);
mean_energy(t) = eng / (num_sweeps * L^2);
mean_energy_sq(t) = eng_sq / (num_sweeps * L^4);

% Calculate susceptibility and specific heat
susceptibility = L^2 * (mean_magnetization_sq -
mean_magnetization.^2) ./ T_values;
specific_heat = L^2 * (mean_energy_sq - mean_energy.^2) ./ (
T_values.^2);

% Exact results for magnetization and energy (for comparison)
exact_magnetization = @(T) (1 - sinh(2./T).^(-4)).^(1/8) .* (T
< Tc);
exact_energy = @(T) -J * (1 + (2./sinh(2 * J ./ T)).^2) .* *
tanh(J ./ T);

```

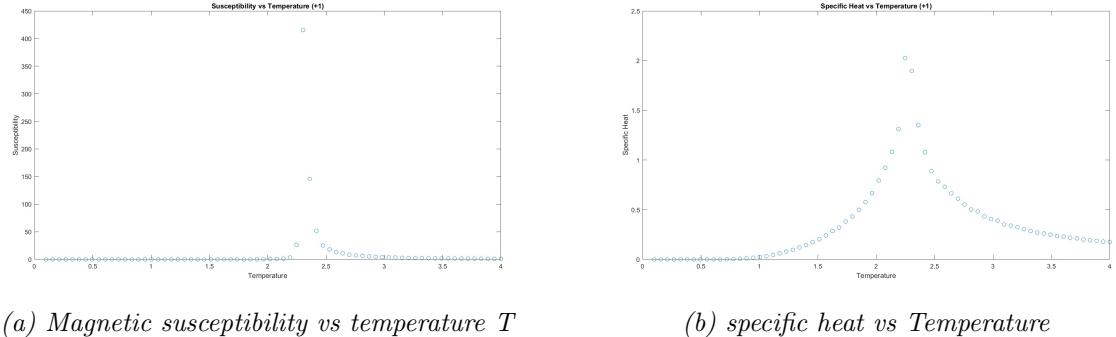
The graph of Magnetization per site, results for energy, result for susceptibility, result for specific heat are presented below:



(a) Magnetization per site vs temperature  $T$

(b) Energy per site vs Temperature

Figure 3: Left panel: Magnetization per site vs temperature The blue circles denote the results of the MC simulations with the Metropolis algorithm: The solid line is the exact result obtained. Right panel: Energy per site as a function of  $T$ .



(a) Magnetic susceptibility vs temperature  $T$

(b) specific heat vs Temperature

Figure 4: Left panel: Magnetic susceptibility (left panel) and specific heat (right panel) as functions of  $T$

### 3.3 Microscopic Configuration

Here I considered the dynamics of the 2D Ising model starting from disordered initial configuration. The graph differs a bit from the one in the numerical project guide given in class because they are randomized variables.

There are two cases considered:

1.  $\beta = 0.4 < \beta_c$
2.  $\beta = 0.5 > \beta_c$ , where time changes in both cases from  $t = 2000$  to  $t = 18000$ .

#### 3.3.1 Case with $\beta < \beta_c$

The graph of  $\beta = 0.4 < 0.44$  is presented below:

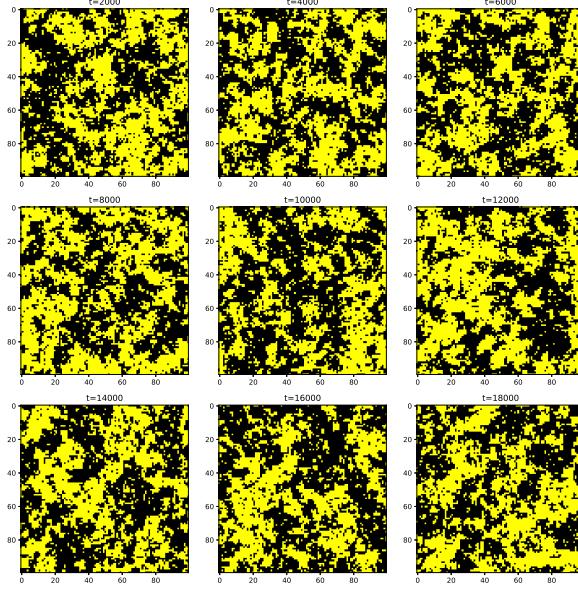


Figure 5: microscopic configurations corresponding to  $\beta = 0.4 < \beta_c$  at times (left to right, top to bottom  $2 \times 10^3 k$ , for  $k = 1, 2, \dots 9$ )

### 3.3.2 Case with $\beta > \beta_c$

The graph of  $\beta = 0.5 > 0.44$  is presented below:

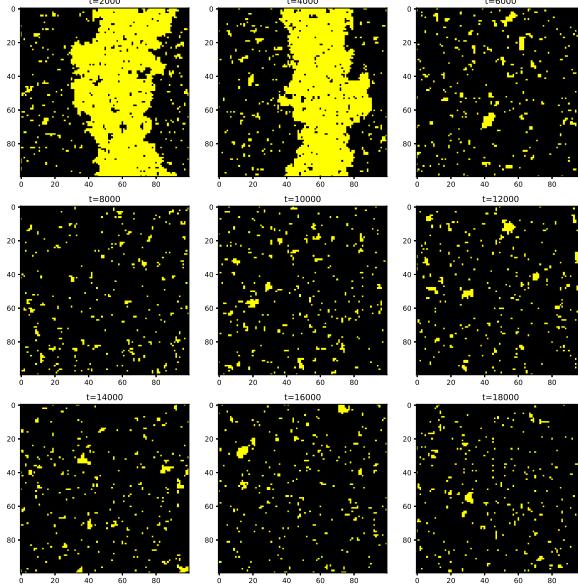


Figure 6: Microscopic configurations corresponding to  $\beta = 0.5 > \beta_c$  at times (left to right, top to bottom  $2 \times 10^3 k$ , for  $k = 1, 2, \dots 9$ )

## 4 Conclusion

The 2D Ising model done in this project was carried out using MATLAB and the methodology adopted was the Metropolis algorithm. The thermalization times, phase transition,

and microscopic configurations were numerically computed, and their graphs were presented.