Project: Monte Carlo simulations of the 2D Ising model

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Square-lattice 2D Ising model

Consider a square lattice Λ of linear size L.

Your task is to write a computer code based on the Metropolis Monte Carlo method to simulate the dynamics of the nearest-neighbor ferromagnetic Ising model with hamiltonian:

$$H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \; i,j \in \Lambda, \; J > 0$$

where $\sigma = \{\sigma_i, i \in \Lambda\}$ denotes a configuration of spins on Λ, with $\sigma_i = \pm 1$, and the sum is over pairs of adjacent spins (every pair is counted once).

In the thermodynamic limit the 2D Ising model undergoes a phase transition at the inverse critical temperature:

$$\beta_c = \frac{ln(1+\sqrt{2})}{2J}$$

For $\beta > \beta_c$, the 2D Ising model exhibits a spontaneous magnetization

$$m_\beta = \left[1 - \frac{1}{sinh^4(2\beta J)}\right]^{\frac{1}{8}}$$

In your simulations set $k_B = J = 1$ (in this case $T_c = \beta_c^{-1} \approx 2.269$) and L = 100.

Time is measured in number of sweeps $N = L^2$.

Use <u>periodic boundary conditions</u> and consider the following <u>initial configurations</u> $\{\sigma_i\}$: (i) $\sigma_i = +1$ (“i.c. P”), (ii) $\sigma_i = -1$ (“i.c. N”) and (iii) $\sigma_i = \pm 1$ with probability $1/2$ (“random i.c.”).

Compute the following observables:

- the magnetization (per spin) $m(\sigma) = 1/N \sum_{i \in \Lambda} \sigma_i$ as a function of time (for $T = 2 < T_c$ and $T = 2.5 > T_c$, and using the i.c. above);
- the energy $e(\sigma) = H(\sigma)/N$ as a function of time (for $T = 2 < T_c$ and $T = 2.5 > T_c$, and using the i.c. above);
- the mean magnetization $\langle m \rangle$ as a function of the temperature T;
- the mean energy $\langle e \rangle$ as a function of the temperature T;
- the magnetic susceptibility $Xi = \beta N(\langle m^2 \rangle - \langle m \rangle^2)$ as a function of T;
- the specific heat $c = \beta^2 N(\langle e^2 \rangle - \langle e \rangle^2)$ as a function of T;
- the microscopic configurations $\{\sigma_i\}$ sampled at different times: $t_k = 2 \times 10^3 k$, with $k = 1, ..., 9$, for $T = 2 < T_c$ and $T = 2.5 > T_c$.

1. Numerical results

We used $k_B = J = 1$.

1.1 Thermalization time

In our numerical simulations we considered a square lattice with $L = 100$, interaction energy $J = 1$, Boltzmann constant $k_B = 1$. Time is measured in units of $N_{sw} = L^2$, where N_{sw} denotes the number of sweeps.

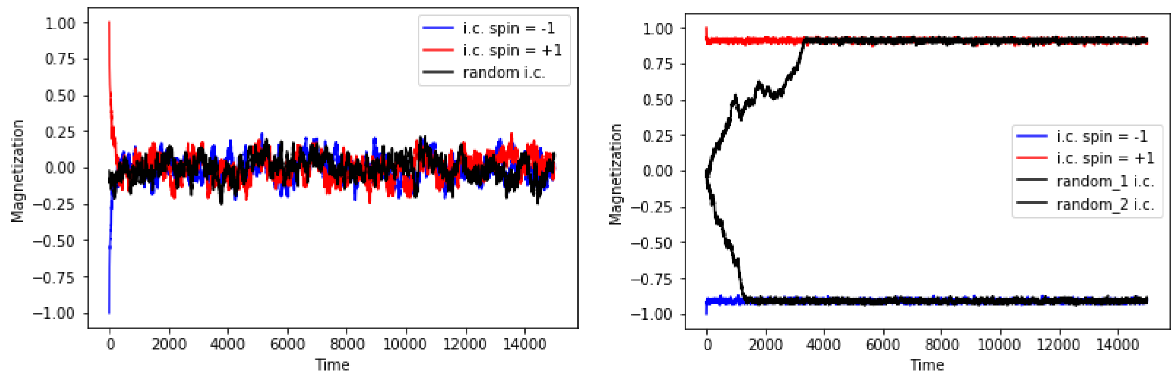

Figure 1: (Magnetization per site vs time). Shown are the results for $\beta = 0.4$ (left panel) and $\beta = 0.5$ (right panel). The different colours of the curves refer to different initial data.

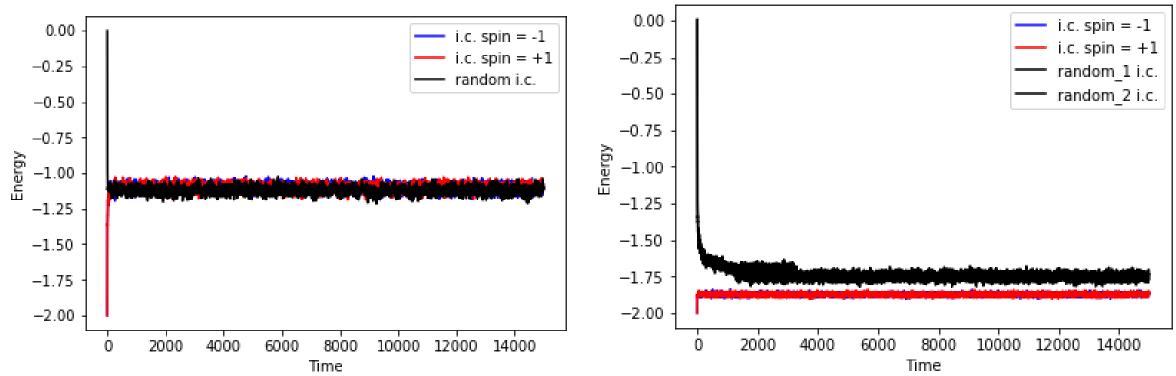

Figure 2: Energy per site of a two-dimensional Ising model on a square lattice with $L = 100$ for $\beta = 0.4$ (left panel) and $\beta = 0.5$ (right panel). The different colours of the curves refer to different initial data.

1.2 Phase transition

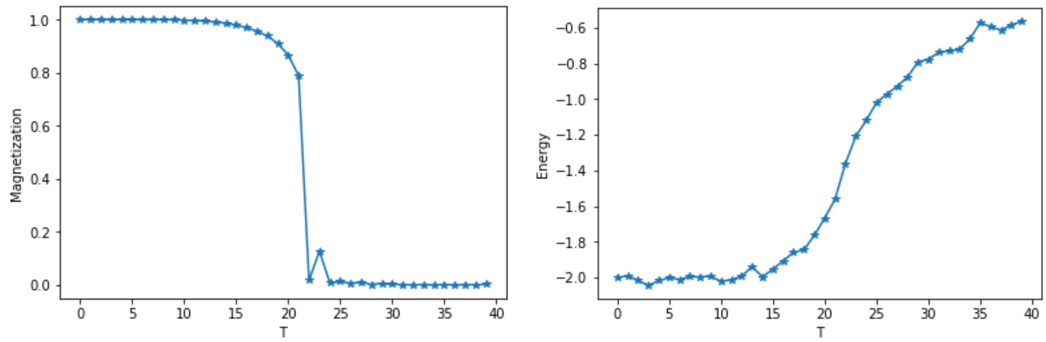

Figure 3: Left panel: Magnetization per site vs temperature T . The blue stars denote the results of the MC simulations with the Metropolis algorithm. Right panel: Energy per site as a function of T .

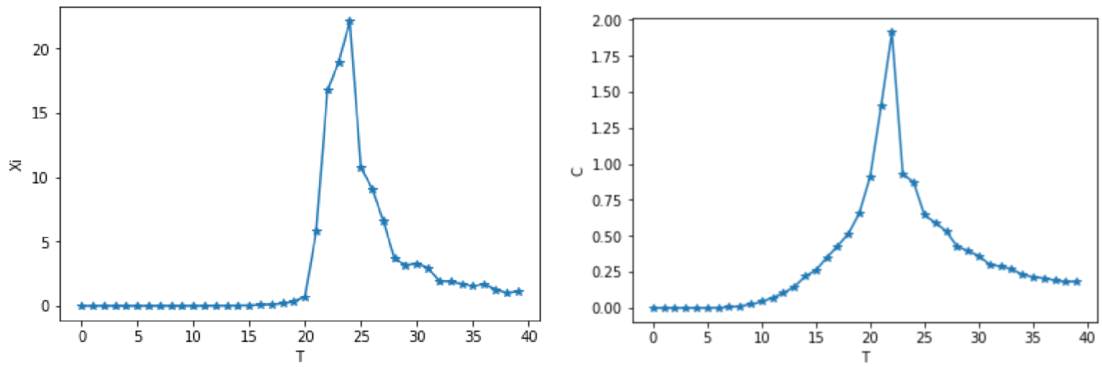

Figure 4: Left panel: Magnetic susceptibility (left panel) and specific heat (right panel) as functions of T .

1.3 Microscopic configurations

We will consider the dynamics of the 2D Ising model starting from a fully disordered initial configuration.

1.3.1 Case with $\beta < \beta_c$:

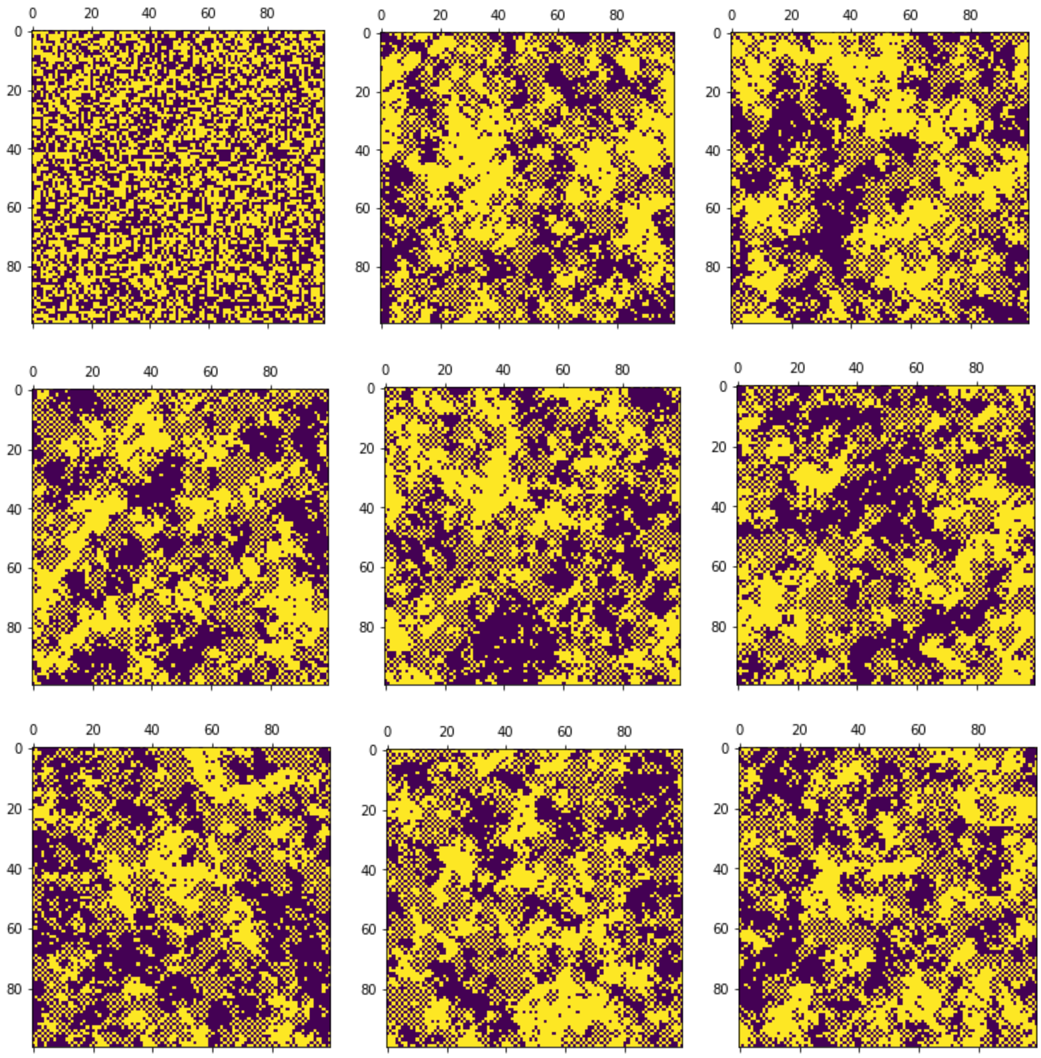

Figure 5: Microscopic configurations corresponding to $\beta = 0.4 < \beta_c$ at times (left to right, top to bottom) 2×10^3 , 4×10^3 , 6×10^3 , 8×10^3 , 10^4 , 1.2×10^4 , 1.4×10^4 , 1.6×10^4 and 1.8×10^4 .

1.3.2 Case with $\beta > \beta_c$:

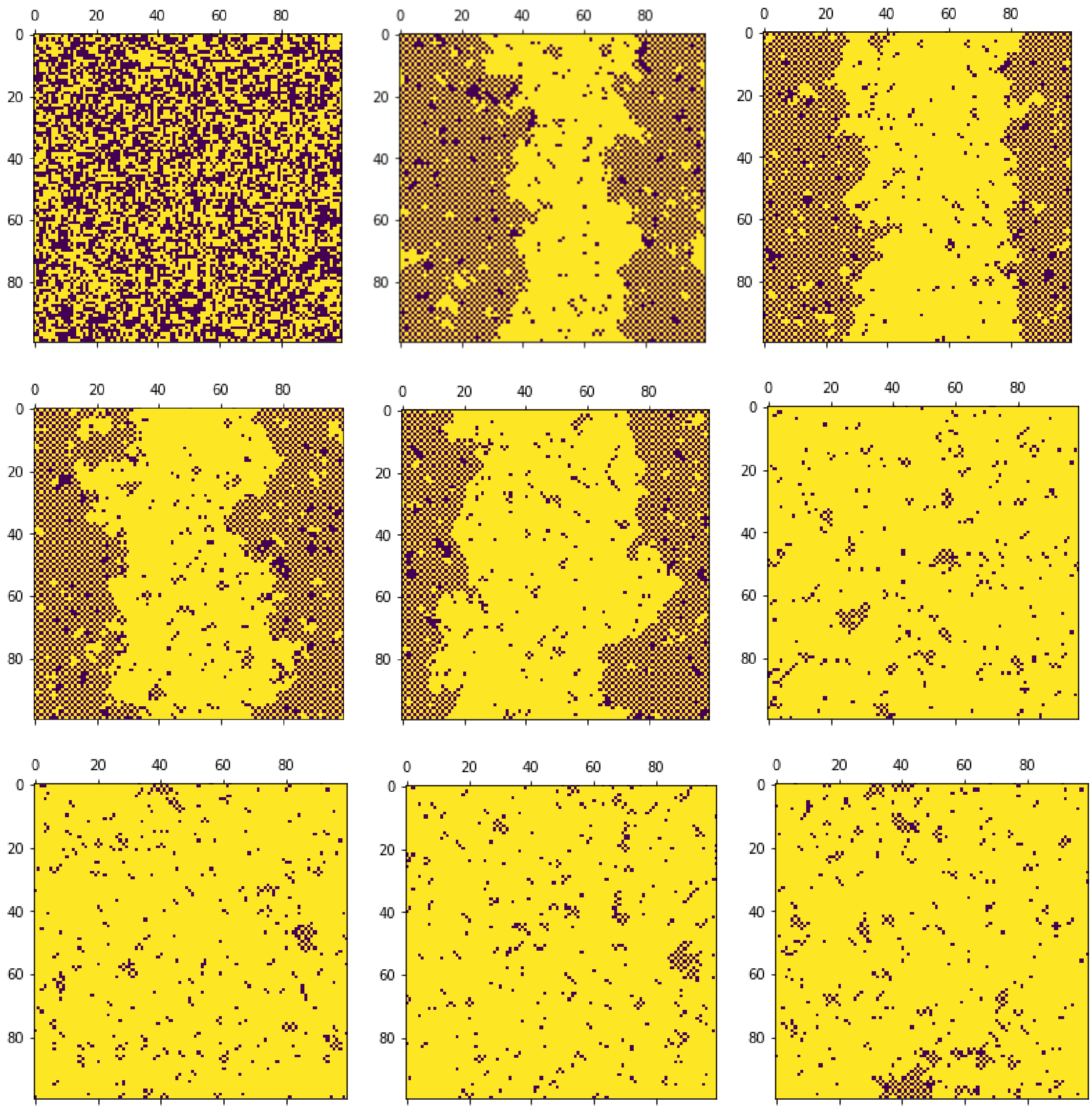

Figure 6: Microscopic configurations corresponding to $\beta = 0.5 > \beta_c$ at times (left to right, top to bottom) 2×10^3 , 4×10^3 , 6×10^3 , 8×10^3 , 10^4 , 1.2×10^4 , 1.4×10^4 , 1.6×10^4 and 1.8×10^4 .