Project: Monte Carlo simulations of the 2D Ising model

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1 Introduction. Ising Model

1.1 Square-lattice 2D Icing Model Problem

Consider a square lattice Λ of linear size L.

The 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:

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

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 computed 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

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

In the simulations consider k_β = 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 periodic boundary conditions and consider the following initial configurations σ_i: (i) σ_i = +1 ("i.c. P"), (ii) σ_i = -1 ("i.c. N") and (iii) σ_i = +1 with probability $\frac{1}{2}$ ("random i.c.").

Compute the following observables:

- the magnetization (per spin) $m(\sigma) = \frac{1}{N} \sum_{i \in \Lambda} \sigma_i$, as a function of time (for T = 2.0 < 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 = 2.0 < T_c and T = 2.5 > T_c and using the i.c. above);
- the mean magnetization $< m >$ as the function of the temperature T;
- the mean energy $< e >$ as the function of the temperature T;
- the magnetic susceptibility $\chi = N(< m^2 > - < m >^2)$ as a function of T;
- the specific heat $c = \beta^2 N(< e^2 > - < e >^2)$ as a function of T;
- the microscopic configurations σ_i sampled at different times: $t_k = 2{*}10^3 k$, with k = 1,...,9, for $T \ = \ 2 \ < \ T_c$ and $T \ = \ 2.5 \ > \ T_c$.

1.2 Metropolis Monte Carlo Algorithm

1. Initialization.

   A (L × L) square lattice is taken; positive, negative or random (with probability 0.5) spin configuration is taken as an initail lattice state assigning $\sigma_i = +1\ \forall i \in \Lambda$ ("P i.c."), $\sigma_i = -1\ \forall i \in \Lambda$ ("N i.c.") or $\sigma_i = +1$ with probability $\frac{1}{2}\ \forall i \in \Lambda$ ("R i.c.").

2. Updating.

   Given $X_t = \overrightarrow{\sigma}$:

   - Pick a coordinate $j \in V$ uniformly at random
   - Set the proposed new state $\overrightarrow{Y} = \sigma_1, ..., \sigma_{j-1}, -\sigma_j, \sigma_{j+1}, ..., \sigma_{|V|}$
   - Compute

     $$\alpha = \min\{1,\ \frac{\exp(-\beta H(Y))}{\exp(-\beta H(\sigma))}\}\ =\ min\{1,\ exp(-\beta \triangle H)\},$$

     where $\triangle H\ =\ H(Y)\ -\ H(\sigma)$

     Introducing $\triangle H$ into the simulation increases the productivity of the algorithm, since $\triangle H$ needs to be calculated only for the neighborhood of the chosen spin (for other spins it is equal to zero). Therefore, it is not necessary to compute H(Y) on the whole proposed set Y. Therefore, step of the algorithm can be modified:

     $$If\ \triangle H < 0\ set\ \alpha = 1.\ Else\ if\ \triangle H > 0\ =>\ \alpha = \exp\{-\beta \triangle H\}$$

   - Determine, wether to accept or decline the move. Generate $U \sim U[0, 1]$. If $U \leq \alpha$, then set $X_{t+1} = Y$, otherwise $X_t = \overrightarrow{\sigma}$
   - Reapeat all the steps at least L^2 times for each iteration of the algorithm.

3. Calculating the Energy and Magnetization of a Monte Carlo Iteration.

   The Magnetization and Energy as functions of time are calculated at each iteration of the algorithm. In order to obtain the total energy of the lattice, the energy of all nearest neighbor pairs must be considered. If the interaction energy of the right and down neighbors is considered of each spin on lattice, the total energy is calculated. Important condition that must be maintained while implementing the Metropolis algorithm is the periodic boundary condition. This condition is defined as follows: The Periodic boundary condition: For an $L \times L$ 2D lattice, grid points (0, j) and (L-1, j) are north-south neighbors and (i, 0) and (i, L-1) are west-east neighbors. Essentially, this defines a wrapped around lattice.

4. Repeat steps 2 and 3 over given period of time.

2 Simulation

2.1 Negative Initial Configuration

Initial lattice σ, where $\sigma_i = -1\ \forall i$. Microscopic configurations of the simulation, that are sampled at times $t_k = 2 * 10^3 k$, with k = 1,...,9, are shown on Figure 1. Where red color corresponds to the value -1 and yellow color corresponds to the value 1.

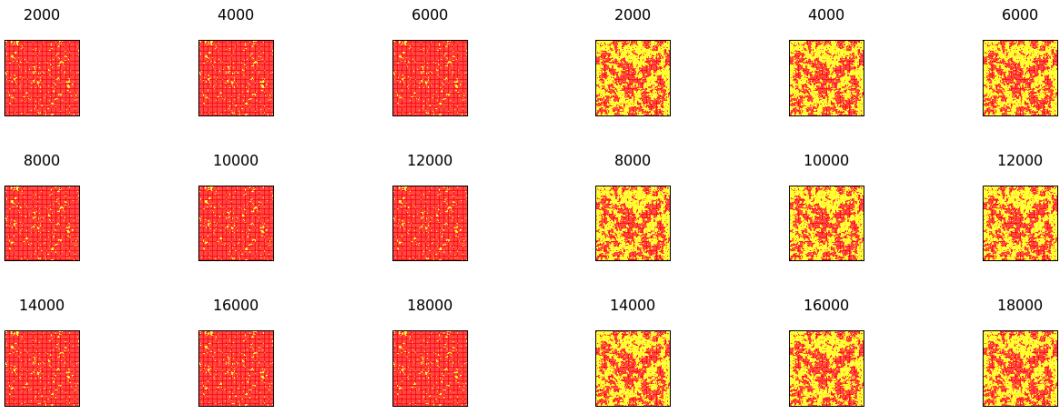
Figure 1a corresponds to the configurations sampled at temperature T = 2.0, most of its spins are red. The reason for this is the fact that small temperatures (large positive β) create tendency for spins to align. And the chance for spins to swap is small. Therefore, the lattice sticks to the initial condition. The material appeals to be ferromagnetic.

In the case where T = 2.5 (Figure 1b), different behavior is observed. Spins of the lattice do not seem to align. And the resulting configurations appear random, disordered. The reason for it is paramagnetic behavior. The high values of temperatures (small positive β) create tendency for spins to flip. Therefore, the material losses the magnetization.

An important observation is that the rate of oscillation is substantially bigger in case of the higher temperatures. This is due to the fact that in ferromagnetic regime spins in the lattice tend to align and change their values rarely. Therefore, the energy and magnetization per spin do not change much. This is not true in case of paramagnetic regime (high temperatures) as spins tend to change their values a lot, therefore, variables also tend to oscillate more.

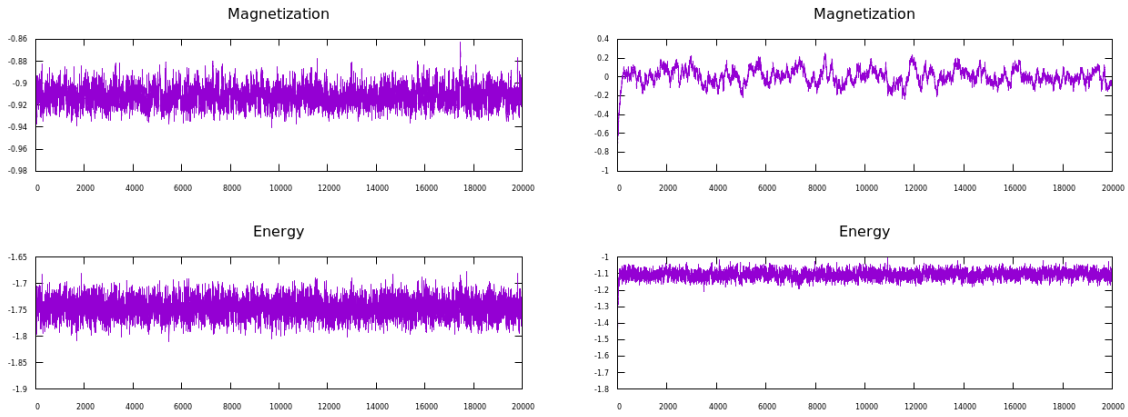
Figure 2a shows time dependence of the energy and magnetization per spin, where T = 2.0.

Figure 2b shows the dependency in case of T = 2.5.



(a) Configurations for T=2.0 (b) Configurations for T=2.5

Figure 1: Microscopic configurations sampled at different times (for N i.c.)



(a) T=2.0 (b) T=2.5

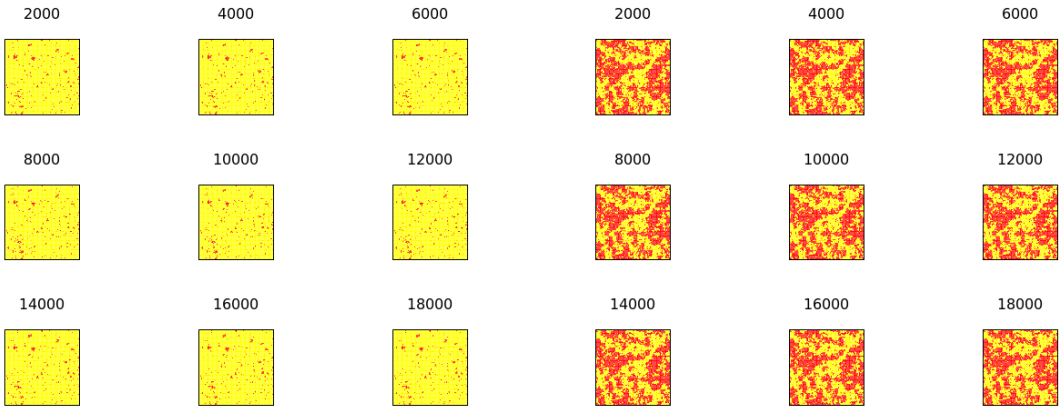
Figure 2: Energy and magnetization for N i.c.

2.2 Positive Initial Configuration

Statements for negative initial configurations are also valid in case of initial configuration where all spins are positive directed. Figures 3a and 3b show the microscopic configuration for T = 2.0 and T = 2.5 in the case of the positive initial configuration (P i.c.). Figures 4a and 4b show the time dependency of the energy and magnetization per spin.

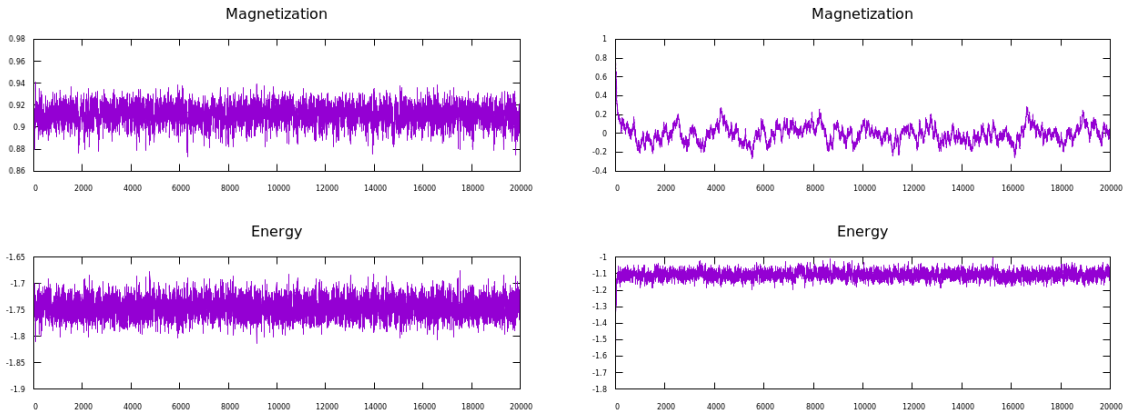
2.3 Random Initial Configuration

Random initial configuration is more time consuming, since the thermalization time may be very big. Therefore, it may take some time to compute simulations for random initial configurations.



(a) Configurations for T=2.0 (b) Configurations for T=2.5

Figure 3: Microscopic configurations sampled at different times (for P i.c.)



(a) T=2.0 (b) T=2.5

Figure 4: Energy and magnetization for P i.c.

Since in the low temperature regime the spins tend to align, after some time the lattice with dominating amount of either "-1" or "+1" is attained. The initial configuration is random, therefore, the case to which it will led is not known.

Figures 5a and 7a show the configurations for random initial conditions in case of T = 2.0. It is seen that in first case "+1" dominates in the configuration and in the other case "-1" dominates. The behavior for the case T = 2.5 (Figures 5b and 7b) is almost the same for different initial configurations.

Figures 6 and 8 show the behavior of the energy and magnetization per spin, depending on time. For T = 2.0 spins with value "+1" are in majority in the Figure 6a and spins with value "-1" are in majority in the Figure 8a.

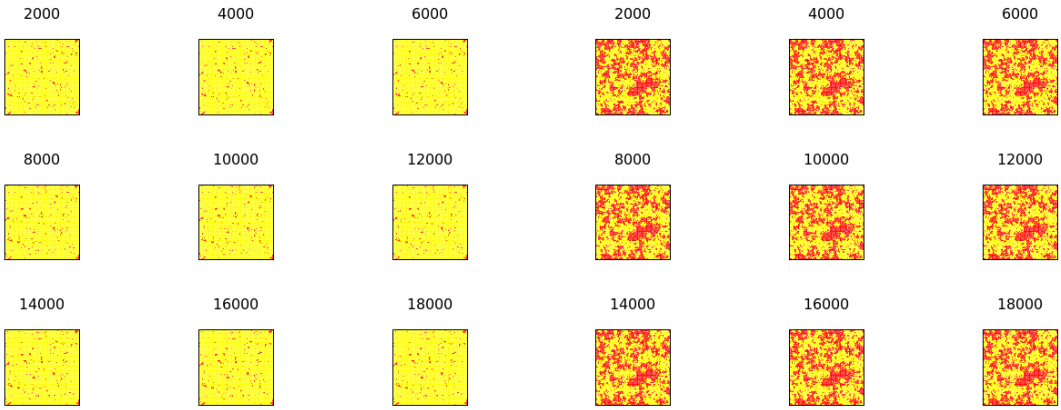
2.4 Observables That Depend on Temperature T

Define a set of temperatures $T_s = \{t_i\}$, i = 1,...,32.

$$T_s = \{1.0,\ 1.1,\ 1.2,\ 1.3,\ 1.4,\ 1.5,\ 1.6,\ 1.7,\ 1.8,\ 1.9,\ 2.0,\ 2.1,\ 2.2,\ 2.269,$$
$$2.3,\ 2.4,\ 2.5,\ 2.6,\ 2.7,\ 2.8,\ 2.9,\ 3.0,\ 3.1,\ 3.2,\ 3.3,\ 3.4,\ 3.5,\ 3.6,\ 3.7,\ 3.8,\ 3.9,\ 4.0\};$$

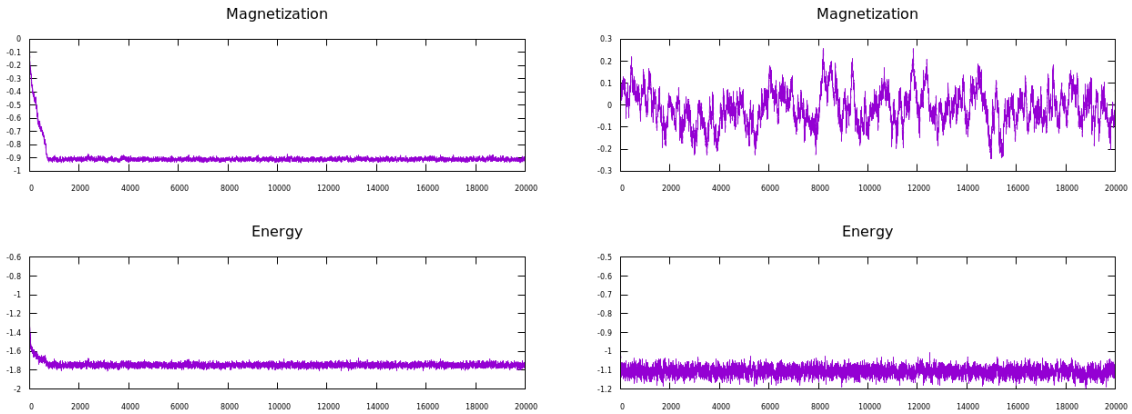
In order to compute mean energy and magnetization it is needed to first find a part of a timeline where the mean value computed on all previously obtained values do not change much. The value reaches its equilibrium.

Therefore, pression p is needed to be chosen and the time interval (the number of time steps that should satisfy the precision). The interval is used in order to avoid local equilibriums. On each time step difference between



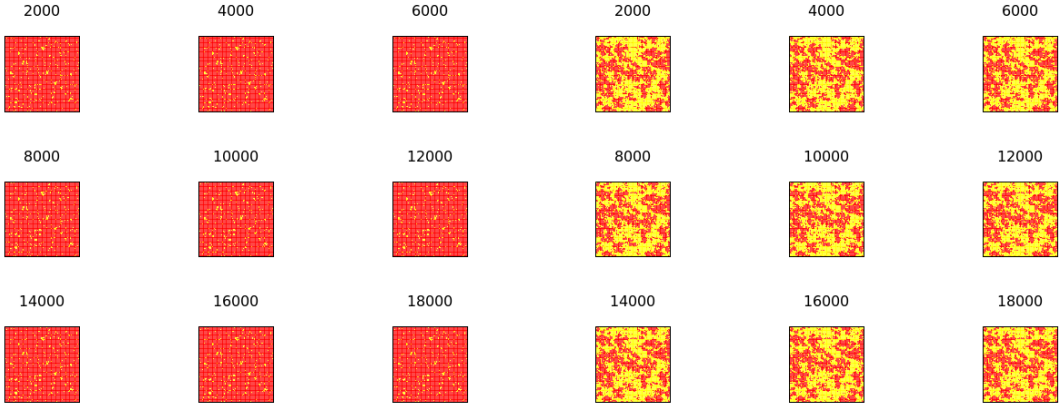
(a) Configurations for T=2.0 (b) Configurations for T=2.5

Figure 5: Microscopic configurations sampled at different times (for R i.c.)



(a) T=2.0 (b) T=2.5

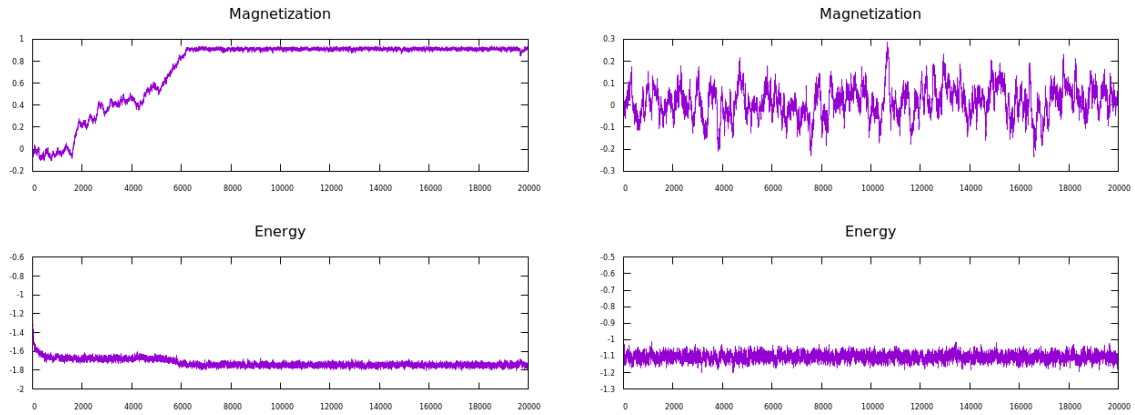
Figure 6: Energy and magnetization for R i.c.



(a) Configurations for T=2.0 (b) Configurations for T=2.5

Figure 7: Microscopic configurations sampled at different times (for another R i.c.)

variables (average energy and average magnetization) that were obtained in the current and in the previous step need to be compared with the precision. If the condition is satisfied for the whole interval, thermalization time is reached and mean variables are computed.



(a) T=2.0 (b) T=2.5

Figure 8: Energy and magnetization for another R i.c.

Thermalization time is the timeline on which average value (of energy and magnetization) converges. In this simulation were chosen such parameters:

- precision p = 10^{-5}
- interval on which difference of mean values should be less than precision = 5000

Figure 9 shows the mean energy, absolute value of mean magnetization, magnetic susceptibility and specific heat for R i.c. Minimal energy is obtained at minimal temperatures. The lattice losses the magnetization in the paramagnetic part (T ¿ T_c) in the case of positive i.c. and in the case of negative i.c. it losses the magnetization in the ferromagnetic part (T ¡ T_c). All of the plots have a break in the point T_c, where their values tend to infinity.

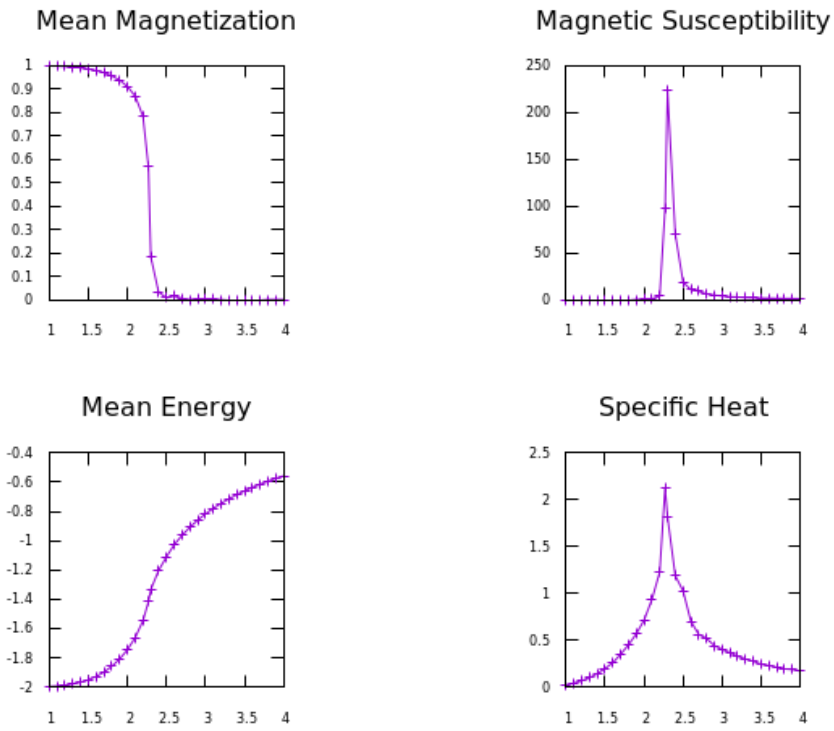


Figure 9: Observables that depend on temperature T for R i.c.