Exploring a 2D Ising model with Metropolis Algorithm to compute Mean Field Theory approximate solutions

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Abstract

Our project examines the thermodynamic quantities of a lattice of spins after the system has thermalized using MATLAB to simulate the Ising model.

1 Introduction

We investigate the phase transitions in simulated systems of particles through Monte Carlo simulations. We will fix the coupling exchange interaction to be $J = 1$ for simplicity, and also only investigate when $H = 0$ due to time constraints.

2 Part 1

3 Part 2

We use code from a GitHub repository as a starting base for our own. We had to make some modifications.

```
%%  Initial configuration
grid = sign(.5-randi([0 1],N,N)); % Random initial configuration
%%  Initialization
Elist=zeros(t,1); Mlist=zeros(t,1);

sumOfNeighbors = ...
      circshift(grid, [ 0  1]) ...
    + circshift(grid, [ 0 -1]) ...
    + circshift(grid, [ 1  0]) ...
    + circshift(grid, [-1  0]);

Em = -J*grid.*sumOfNeighbors;
Energy = .5 * sum(sum(Em));%initial Energy
Magnet=(sum(sum(grid))/N); %initial magnetization
```

Code for Initialization

First we create the matrix with a random state instead of cold configuration. This will take some time to compute but the machine running the code can handle it.

Next we take the equation

$$E = -J \sum_{i,j} \sigma_i \sigma_j$$

and deconstruct it a bit to make computation easier. We instead compute the sum of the neighbors for each location in the array using the function $circshift$. This function wraps around to ensure periodic boundary conditions are satisfied. We then do element wise multiplication to find the energy of the sum of each array location times its nearest neighbors. Initially the code we used summed up everything and divided it by two, but this was corrected when we ran our code.

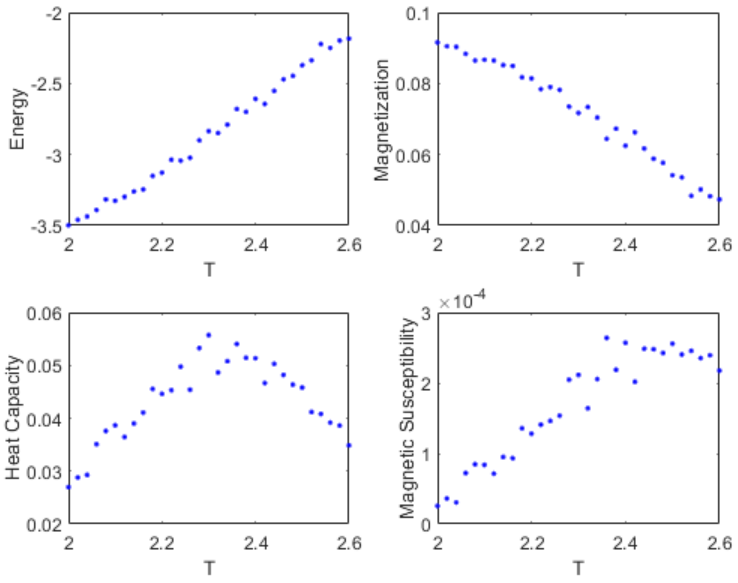
We then precomputed our Boltzmann factor for using use in importance sampling since the values ΔE_{2D} are finite in a 2D simulation. Since we only choose to use the Boltzmann factor when the change in spin would result in a gain in energy to the overall system and we are looking for a ground state we only consider when the change in energy added to the overall system. Since we know due to temperature that some microstates can have a higher energy, this importance sampling keeps that information.

To avoid making computations unnecessarily long, we do not use the Boltzmann constant in our computations. We will also use N=2500 and a 50x50 2D matrix to represent our Ising Model. We will run the metropolis algorithm 1,000,000 times to ensure there is less than 1% probability that a spin was not flipped at least 10 times. We can find the time to thermalization for each temperature by knowing with a high likelihood that the system has reached thermalization after the 500,000 iteration. We look for the first time step the energy of the system is within one standard deviation of the mean energy after equilibrium was reached.

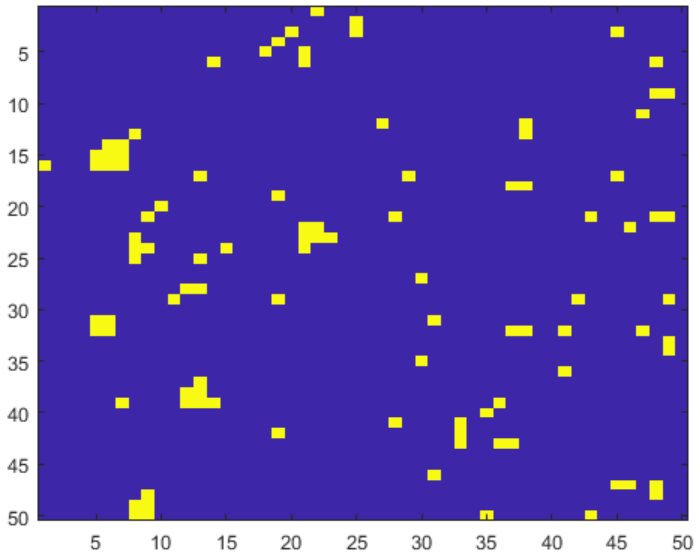
3.1 Investigating Critical Temp for N=10

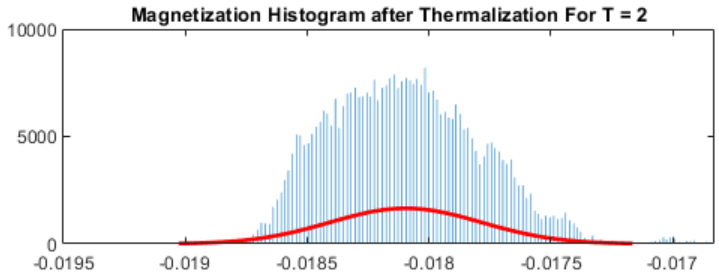
We were able to generate a plot of the magnetic susceptibility, which is how strongly magnetized an object will become if a magnetic field was applied, the heat capacity, and the energy and overall magnetization as a function of temperature.

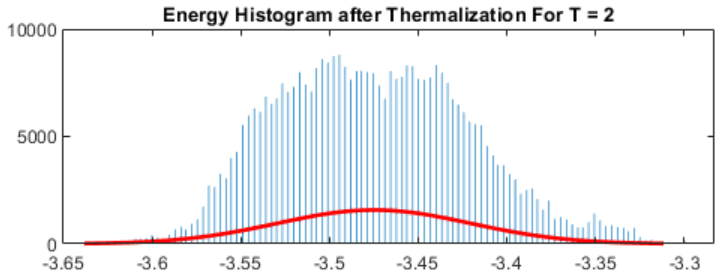
The magnetic susceptibility and heat capacity are the easiest graphs to use to identify where the critical temperature is located. These values peak around the critical temperature.



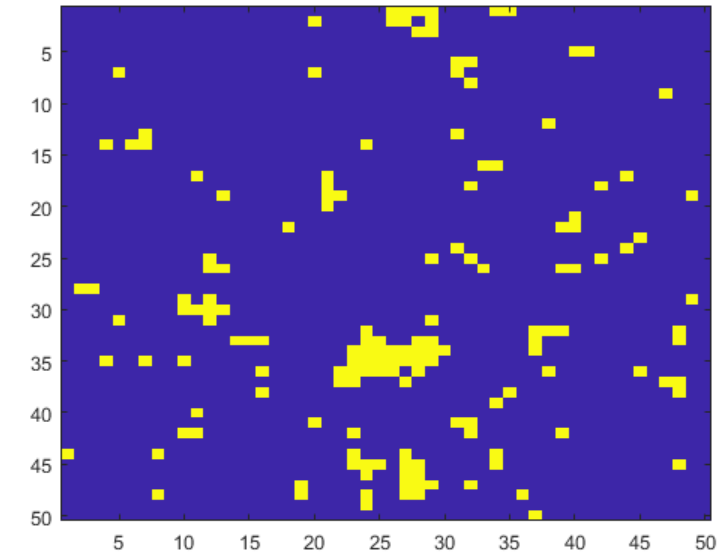
3.2 Inconclusive Results for N=50

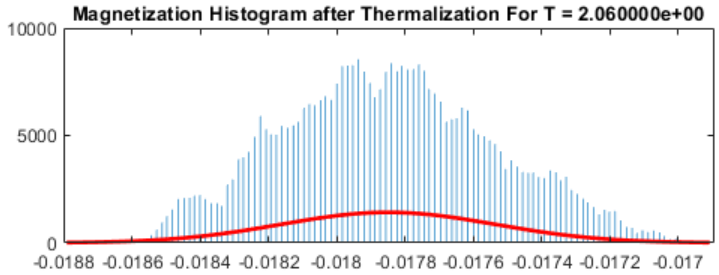


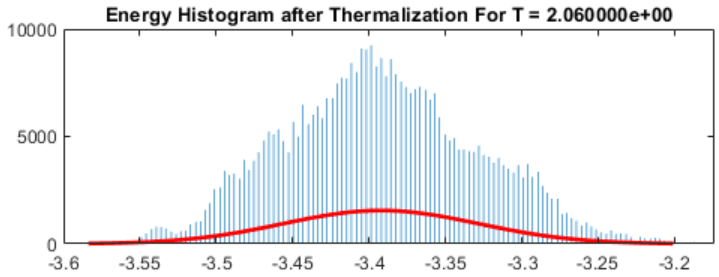




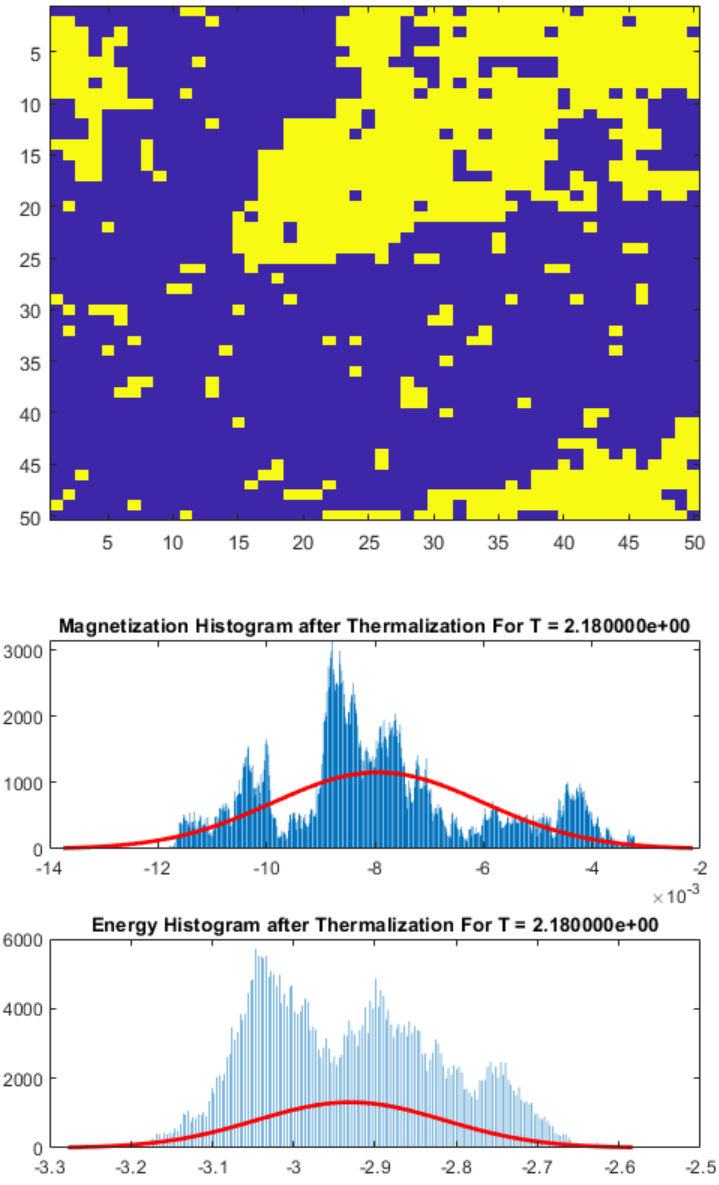
We can see that things seem to work but in actuality we found our code does not work properly. While trying to run the code for N=50 investigating the critical temp we got nonsense in return.



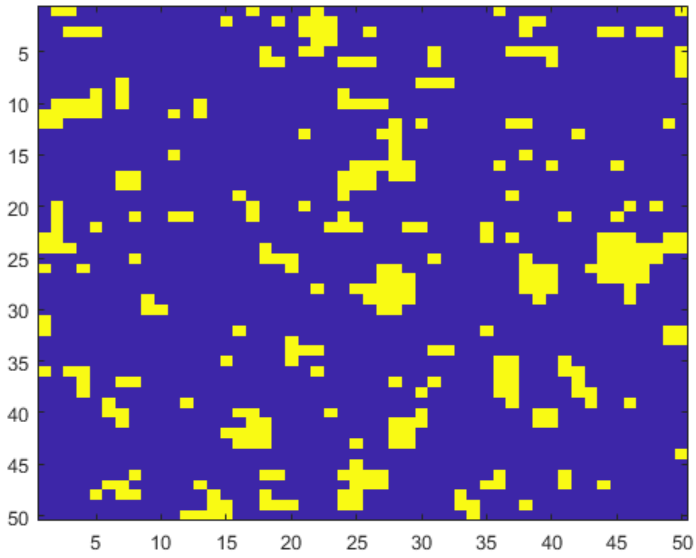


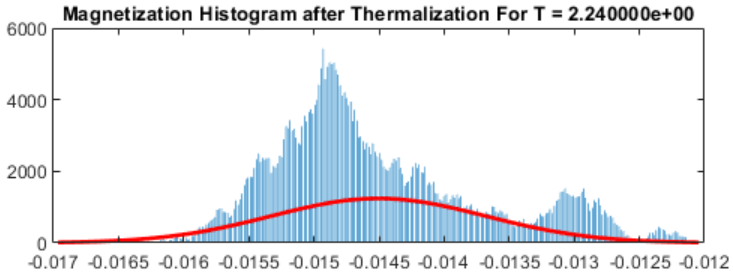


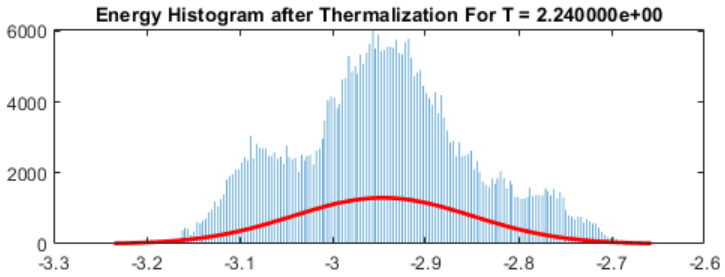
Things seem to work okay for temperatures nearer to $T = 2$. This is expected because the likelihood that a microstate has a higher energy is lower here.



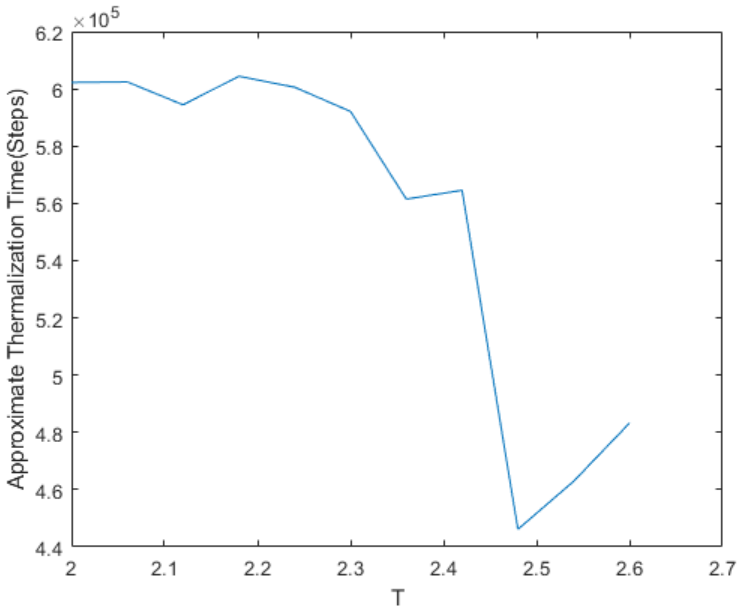
Here we see an instance where our code failed completely.







Even when it seems like our code may have reached an equilibrium, our histograms show that we are not strongly peaked around a central value and thus it cannot be yet at thermalization.



Even though our results were inconclusive, it is interesting to note that the time to thermalization decreases significantly as we approached what could be assumed to be the critical temp for N=10. More analysis is needed to verify this result. We do however expect that the time to thermalization should be smaller when we are already near the critical temp of the system for N=2500.