Final Report: Multi-Dimensional Computer Simulation of the Ising Model

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Abstract

This project aims to simulate the Ising model in two, three, and four dimensions, and to determine the Curie Temperature in all cases. These simulations were written in Python and run many times. Each simulation produced Magnetization vs. Temperature plots, which were fitted to sigmoid curves. For each of these plots, the point of inflection was found and determined to be the Curie Temperature. After running the 2D simulation 500 times, the average curie temperature was 2.340 with a standard deviation of 0.230. The average Curie Temperature for 200 runs of the 3D simulation was 4.083 with a standard deviation of 0.412, and the average across 50 runs of the 4D model was 4.502 with a standard deviation of 0.805. There is an exact solution for the 2D Ising Model only. When compared to Onsager's exact solution, the 2D Ising model had an average percent error of 3.12%. Ultimately, the Ising Model was successfully simulated in two, three, and four dimensions. Future improvements on the simulation could invlove increasing simulation efficiency so that larger lattices may be simulated.

1 Introduction

The Ising Model is a statistical model of phase transitions, specifically the transition from paramagnetic to ferromagnetic as a material cools. This project simulates the Ising Model in two, three, and four dimensions using Python in order to find the Curie Temperature.

This research builds on a 2D Ising Model simulation program previously created by Dr. David Heddle. It also extends the capstone project completed by Richard Munroe in 2012, entitled "Simulation of the two-dimensional square lattice Lenz-Ising model in Python."

2 Theory

2.1 Theory of Operation

The Ising Model is a mathematical model of ferromagnetism. As ferrous materials cool, their atoms settle into spin up or spin down states which results in the magnetization of the material. The Ising model consists of a lattice of atoms, each of which can be in either a spin up or spin down state. The partition function is used to determine the probability that the lattice will enter a particular state. Using the resulting lattice at each temperature, the magnetization is calculated, and a magnetization vs. temperature plot is produced. The goal of this simulation is to find the Curie Temperature at which the magnetization of the material sharply changes.

2.2 Mathematical Theory

The materials modeled in this project consist of 2D, 3D, and 4D lattices composed of molecules which will be referred to as "sites." Each site $i = 1, ..., N$ is assigned a value σ_i which can be either +1 or -1 representing spin up and spin down. The Hamiltonian for the system is found by summing the energies associated with each site's nearest-neighbor interactions. The Hamiltonian is given by

$$H(\sigma) = -\sum_{i,j} E\sigma_i\sigma_j - \sum_i J\sigma_i \tag{1}$$

The second sum represents the sum over all lattice sites, and the first is the sum over all nearest-neighbor pairs. E and J are parameters; E represents the material's magnetization and J corresponds to an external magnetic field.

The partition function is given by

$$Z(\beta, E, J, N) = \sum_{\pm 1} e^{-\beta H(\sigma)} \tag{2}$$

The probability of the lattice entering a particular configuration is given by

$$\text{Prob}(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z} \tag{3}$$

Because of the minus sign in the exponent, lower energy states are associated with a higher probability of occurrence. β, which is given is the reciprocal of the fundamental temperature, is higher when temperature is lower and lower

when temperature is higher. Therefore, a lower temperature and a higher β tends to accentuate the higher probabilities of lower energy states, while a higher temperature and a lower β tends to make all configurations closer to equally likely.

In this simulation, a random configuration is generated. Then, a trial configuration is generated, and its hamiltonian is calculated. If the energy of this next configuration is lower than that of the previous configuration, this new configuration is accepted. If the energy of this new state is higher than the last, the probability function is used to determine the probability that this new configuration will occur, which is then used in the program to decide if the new configuration will or will not be accepted. This process is repeated at different temperature steps until this material is cooled to equilibrium and the final configuration is accepted.

The magnetization of the material is calculated at each temperature step, resulting in a magnetization versus temperature plot. The temperature at which the magnetization spikes as the material cools is the Curie Temperature. The method for finding the Curie Temperature from data plots is not agreed upon. In order to find the Curie Temperature for this project, the magnetization versus temperature plots were each fitted to a sigmoid curve. Then, the point of inflection was found and determined to be the Curie Temperature.

2.3 Data and Error Analysis

The Ising Model has an exact solution only in 2D, so in 2D the simulated results were directly compared to the theoretical solution. For the higher dimension simulations, the program was run multiple times and the standard deviations of spin and energy were analyzed.

3 Methods

The code for the 2D, 3D, and 4D simulations went through several stages of development. First, a 2D simulation of the Ising Model by Mr. P Solver on YouTube was adapted for this project's 2D simulation. Then, this code was altered to work in three and four dimensions. Figure 1 shows the flowchart for the simulation code. After adapting the code into three and four dimensions, visualization functions were added to both the 2D and 3D simulations, and functions outputting magnetization versus temperature plots were added to each simulation.

At this stage, the magnetization versus temperature plots were not behaving as expected. Rather than a sigmoid shape, these plots were an exponential shape. Additionally, instead of the magnetization spiking at a consistent temperature, it would spike towards the bottom end of the temperature range, no matter what the lowest temperature was set to. To troubleshoot this issue, the 2D simulation was compared to several existing simulations, and the issue was determined to be the method for calculating the energy of

the configuration. This was adjusted in the original 2D, 3D, and 4D simulations and the magnetization versus temperature plots began to behave as expected.

Finally, a function for determining the Curie Temperature was added to each simulation. This function entailed fitting the plot to a sigmoid curve, finding the point of inflection (the Curie Temperature), and finding the two points of greatest curvature, which were used as the positive and negative boundaries of error.

For analysis, the 2D Ising Model simulation was run many times and the average Curie Temperature was compared to Osanger's (1944) exact solution of the two-dimensional Ising Model. There is no exact solution for the three- and four- dimensional models, so the standard deviations of the Curie Temperatures were analyzed.

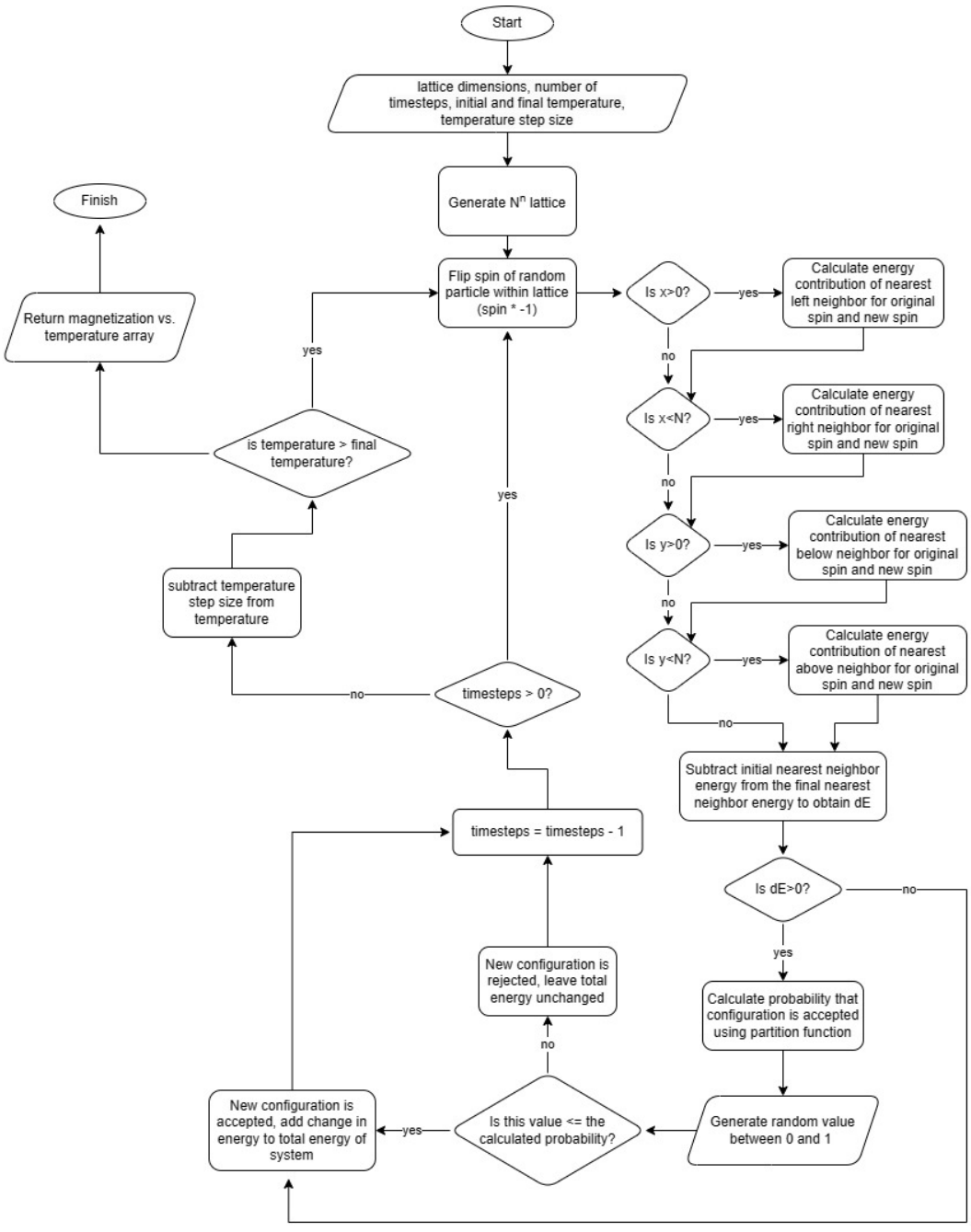
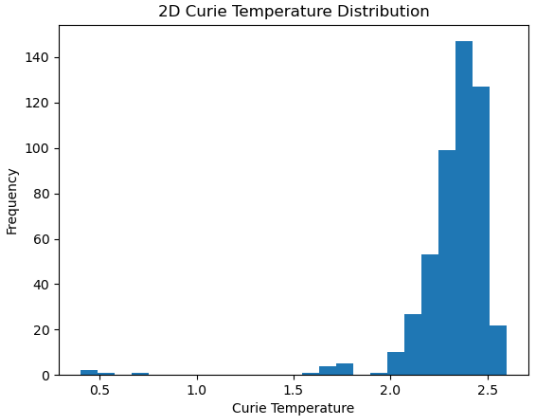


Figure 1: 2D Ising Model simulation flowchart

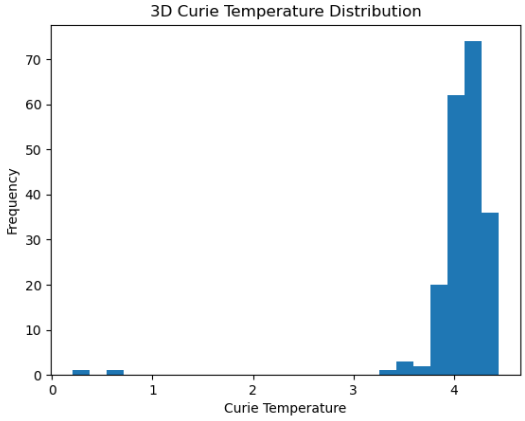
4 Results

4.1 Data

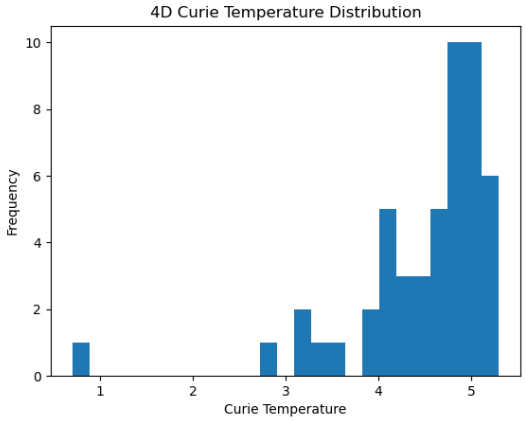
The expected Curie Temperature value for the 2D simulation was 2.269. When the 2D simulation was run 500 times, the average value was 2.340 with a standard deviation of 0.230. The average Curie Temperature for 200 runs of the 3D simulation was 4.083 with a standard deviation of 0.412, and the average across 50 runs of the 4D model was 4.502 with a standard deviation of 0.805. The histograms of these results are below.



2D results for 500 trials



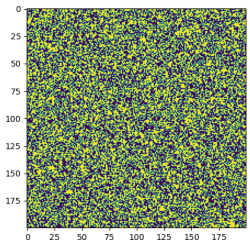
3D results for 200 trials



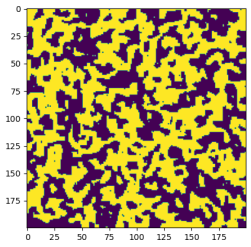
4D results for 50 trials

4.2 Visualization

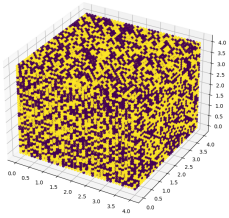
In addition to magnetization versus temperature plots, the code also outputs visuals of simulated annealing for the 2D and 3D simulations. Below are examples of these visuals. Each shows the randomly generated lattice before and midway through annealing, before all of the spins aligned and the magnetization reached 1.0.



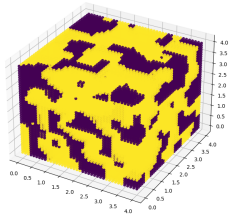
[2D Before]



[2D After]



[3D Before]



[3D After]

4.3 Discussion

The goal of this project was to simulate the Ising Model in two, three, and four dimensions, and to identify the Curie Temperature for each run. Because there is an exact solution for the Curie Temperature of the two-dimensional

Ising Model, the accuracy of the two-dimensional simulation is known. After 500 trials, the 2D simulation had an average percent error of only 3.12%. The 3D and 4D Ising Model do not have exact solutions to compare to; however, as can be seen in the narrow histogram in the "results" section, the results of the 3D simulation were very consistent with a standard deviation of 0.412. The 4D simulation was less so, with a standard deviation of 0.805. This simulation could possibly be made more consistent by slowing the cooling rate. Because the 4D lattices are so large, to do many runs within a reasonable timespan requires a faster cooling rate than is necessary to achieve the cleanest annealing possible.

Another goal of this project was to create visualizations of the annealing process in two and three dimensions. These visualizations can be viewed in the "results" section. Both simulations behaved as expected, beginning with randomly generated lattices, then forming regions of spin up and spin down, and finally settling into entirely spin up or spin down after reaching the Curie Temperature.

If I were to improve this project, I would alter it to handle larger lattices. The 2D simulation can handle up to 3-digit by 3-digit lattices, but the 3D and 4D simulations are much more limited.

References

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[3] Lee, T. D., & Yang, C. N. (1952). Statistical theory of equations of state and phase transitions. II. Lattice gas and Ising model. Physical Review, 87(3), 410.

[4] Onsager, L. (1944). Crystal statistics. I. A two-dimensional model with an order-disorder transition. Phys. Rev., Series II, 65 (3–4): 117–149, doi:10.1103