An Analytical and Numerical Analysis of the One Dimensional and Two Dimensional Ising Model

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Abstract:

The Ising model is one of the simplest mathematical models to describe a phase transition. Here, the Ising model in one and two dimensions has been discussed analytically, and analysed numerically using both the Metropolis and Wolff algorithms. It has been shown both qualitatively and numerically that the one dimensional model does not contain a phase transition, and that the two dimensional Ising model does contain a phase transition between the paramagnetically ordered and the ferromagnetically ordered phases at a finite temperature.

The Ising Model:

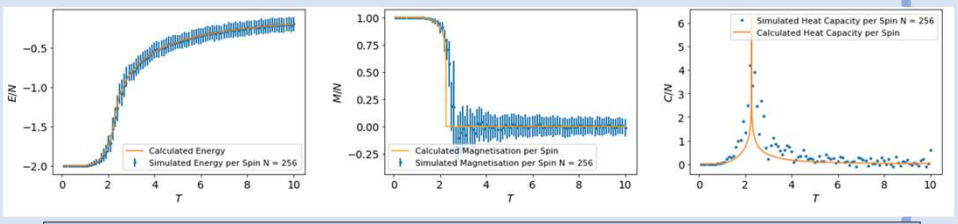
- On a *D*-dimensional lattice there are *N* nodes. At each one of these node, a spin is contained. Each one of these spins can either be in an up state, or a down state. This is represented by the spin value being either +1 or -1.
- The Hamiltonian that describes the total energy of the system is defined as the following:

$$H = -J\sum_{(i,j)}^{N} s_i s_j - h\sum_{i=1}^{N} s_i$$

- By solving the partition function, the exact solution for the thermodynamic quantities can be found.

$$Z_N = \sum_i e^{-\beta H(i)} = \sum_i e^{-\beta E_i} \qquad Z_N = \sum_{s_1=\pm 1}\cdots\sum_{s_N=\pm 1} e^{\sum_{\langle i,j\rangle}^{N} s_i s_j - h\sum_{i=1}^{N} s_i}$$

$$E = \frac{\partial \ln Z_N}{\partial \beta} \qquad C = \frac{\partial E}{\partial T}$$



Two Dimensional Ising Model:

- The two dimensional Ising model is set up as an *NxN* lattice of N^2 nodes. Each spin on the lattice now has four nearest neighbours.
- Solving the two dimensional Ising model is extremely difficult. By following Peierls argument, in which the number of spins on the lattice pointing in a given direction is bounded, it can be shown that a phase transition must occur at low temperatures. Onsager solved this model in 1944, with his paper being just over 30 pages long! The solutions are:

$$E = -2NJ\tanh 2\beta J - NJ\frac{\sinh^2 2\beta J - 1}{\sinh 2\beta J \cosh 2\beta J}\left[\frac{2}{\pi}K_1(\kappa) - 1\right] \qquad C = Nk_B\frac{4}{\pi}(\beta J\coth 2\beta J)^2\left[K_1(\kappa) - E_1(\kappa) - (1-\tanh^2 2\beta J)\left(\frac{\pi}{2} + (2\tanh^2 2\beta J - 1)K_1(\kappa)\right)\right] \qquad T_c = \frac{2}{\ln(1+\sqrt{2})}$$

- The results above were produced using the Metropolis algorithm, on a lattice size of 16x16, from *T*=0.1 to *T*=10 in increments of 0.1. As can be seen, the results lie within error range of the exact solution
- The magnetisation stays around zero for high temperatures. It then suddenly acquires a non-zero magnetisation at lower temperatures. This indicates the phase transition between the paramagnetic and ferromagnetic phases. The heat capacity has a divergence at the critical temperature, due to an infinite sensitivity in the energy caused by the drastically different behaviours of the two phases. Due to the finite size of the lattice in the simulation, the divergence cannot be simulated. This can be used, however, to determine where the simulated critical temperature occurs, since this is where the maximum of the heat capacity will be.

Methodology:

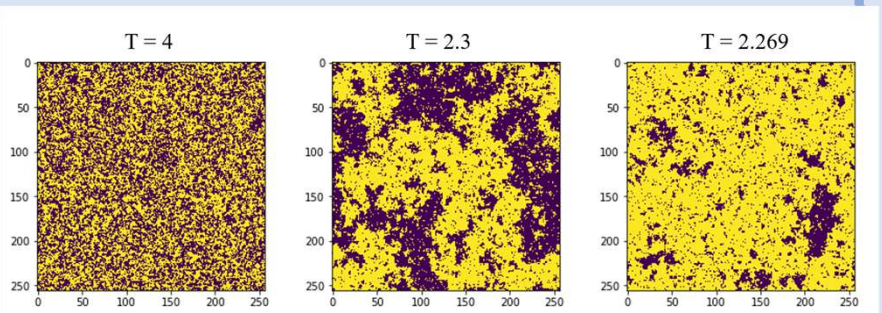
- The two algorithms used in the project, the Metropolis and Wolff algorithms, are examples of Markov chain, Monte Carlo methods.
- The Metropolis algorithm is a local sampling technique, which means that it is efficient for smaller lattice sizes, and when not close to the critical temperature. This is the algorithm used for the majority of the calculations in the project.
- The Wolff algorithm builds clusters of spins in a single iterations, causing it to not suffer from critical slowing down, when close to the critical temperature, as much as the Metropolis algorithm. This algorithm is useful when simulating large lattice sizes.

Metropolis Algorithm:

- The steps of the Metropolis algorithm are the following:
  1. An initial microstate of *N* spins is generated, the state corresponding to infinite temperature is useful since the spins can be randomised.
  2. A random node is chosen, and the spin at this node is flipped.
  3. If the energy of the lattice is decreased, the new microstate is accepted. If the energy is increased, the new state is accepted with probability $p = e^{-\beta\Delta E}$.

Wolff Algorithm:

- The steps of the Wolff algorithm are the following:
  1. An initial microstate of *N* spins is chosen in the same way as before.
  2. A random node is chosen. Its direction, *d*, is noted, and the spin is added to the cluster, *C*.
  3. For each of the spins neighbours, if their spin direction equals *d*, then the spin is added to *C* with probability $p = 1 - e^{-2\beta}$
  4. Each of the new spins added to the cluster have their neighbours searched over.
  5. The algorithm terminates when no new spins are added to the cluster.



Correlation Length:

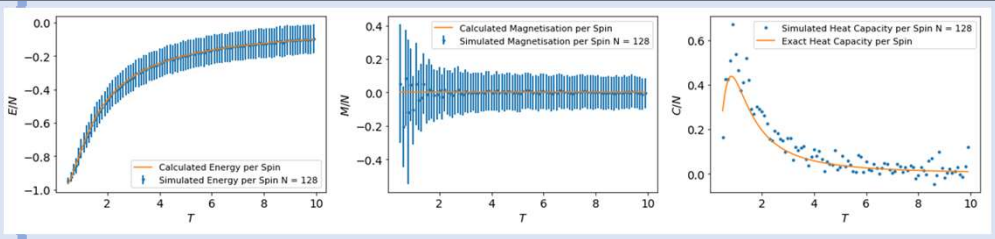
- As the temperature is decreased near the critical temperature, the correlation length diverges i.e all spins are correlated with each other. This causes the creation of domains of spins to be formed just above the critical temperature, seen above at *T*=2.3, and then the majority of spins in the lattice to take on the same value, such as *T*=2.269. This also causes scale invariance in he system i.e there will be domains of all sizes.

One Dimensional Ising Model:

- By using the transfer matrix method, the free energy per spin can be found. By differentiating this with respect to the external field gives the magnetisation. And by solving the partition function, the energy and heat capacity equations can be found.

$$m = -\frac{\partial f}{\partial h} = \frac{\sinh\beta h}{\left(\sinh^2\beta h + e^{-4\beta J}\right)^{1/2}} \qquad E = -NJ\tanh\beta J \qquad C = Nk_B(\beta J)^2(\operatorname{sech}\beta J)^2$$

- As the external field goes to zero, the magnetisation goes to zero for a finite temperature. Therefore, the one dimensional Ising model does not demonstrate a finite temperature phase transition.
- The results below were produced using the Metropolis algorithm on a chain size of 128 nodes. The results are within error range of the exact solution to the model.
- The heat capacity results were produced using the numerical derivative of the energy with respect to the temperature, which is why there is a lot of noise on the results.



Conclusion and Perspectives:

- In this report, it has been demonstrated both analytically and numerically that the one dimensional Ising model contains no phase transition at a finite temperature, and the two dimensional Ising model has a finite temperature, second order phase transition between the paramagnetically and ferromagnetically ordered phases.
- The Ising model may seem like an incredibly focused exercise, since the model deals with a specific area of magnetism, demonstrating a specific form of phase transition. However, this is not the case. This Ising model can have applications in almost all areas of science.
- The Ising model can be used as a testbed for new computational techniques, since it is a solvable model that can be simulated using widely used methods.
- It can lead into more sophisticated techniques like the renormalisation group.
- By replacing the spins in the Hamiltonian with Pauli matrices, the model becomes the Quantum Ising model. This can lead into the more complex study of quantum phase transitions, and also quantum criticality.

References:

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