Cluster Monte Carlo Simulations of the Ising Model on a Cubic Lattice

# Introduction:

The Ising model is one of the most well-studied models in statistical mechanics and rightly so for the rich insights it provides, with the simple Hamiltonian.

|  |  |
| --- | --- |
|  | (1) |

Where represents the nearest-neighbor interaction strength, is the Bohr magneton, and is the magnetic field strength. The partition function for this system is then simply written as:

|  |  |
| --- | --- |
|  | (2) |

For many purposes, it is useful to define variables and so that we can refactor the Hamiltonian as

|  |  |
| --- | --- |
|  | (3) |

The constants and are unitless. For our analysis here, we set (no external magnetic field).

In one and two dimensions, the model has an analytic solution, which is to say the partition function can be written in terms of analytic functions.

# Mean-Field-Theory of the Ising Model and the Critical exponents

Mean field theory is done based on coarse-graining the system with an order parameter. Heuristically, we can determine the form of Hamiltonian based on this order parameter by forcing it to satisfy three constraints: locality, rotational symmetry, and symmetry in the variable .

The central idea of deriving the critical exponents is the Landau-Ginzburg Hamiltonian, which has the form:

|  |  |
| --- | --- |
|  | (4) |

We can further approximate this by considering expansions about the most likely configurations of the order parameter, which means can drop the gradient terms in the expansion as they are all zero in the ground state

|  |  |
| --- | --- |
|  | (5) |

Where V is the system volume and the subscript denotes the saddle point approximation. For large volumes, we can perform a saddle point approximation which requires us to look at the extremal values of:

|  |  |
| --- | --- |
|  | (6) |

As we are interested in behavior only near the critical point, we expect the overall magnetization to be small and hence we will also selectively drop higher order terms in our analysis.

The final form of the Landau free energy is then:

This form has a strong dependence on the sign of the coefficients. Below, we show a plot of the Landau free energy for several different cases:

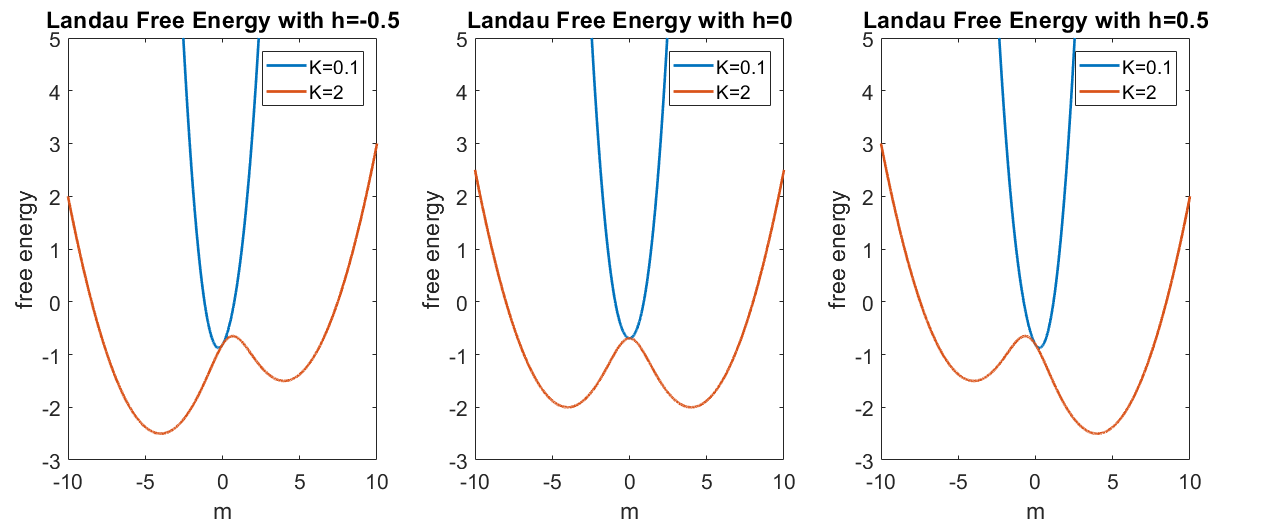


Figure : Landau Free Energy for different temperatures and different values of the magnetic field

Taking the derivatives of this leads us to solve an equation of the form:

|  |  |
| --- | --- |
|  | (7) |

First, we point out the fact that the parameter t has a specific importance, namely that . To see where this comes from, consider that we know the coefficients are all analytic functions of temperature and hence be expanded as a Taylor series about the critical point.

|  |  |
| --- | --- |
| Critical Exponent | Expression |
| Magnetization |  |
| Susceptibility |  |
| Correlation length |  |

Table : critical exponent expressions

It is these exponents which we wish to determine using the cluster Monte Carlo technique. Luckily, we can also analytically approximate the critical exponents using Mean field theory.

First, we know that can be solved by minimizing the Landau free energy:

|  |  |
| --- | --- |
|  | (8) |

First, the literature (or very exact results).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Dimension |  |  |  |  |
| 2 | 1/8 | 7/4 | 15 | 1 |
| 3 | 0.315 | 1.25 | 5 | 0.63 |
| 4 | 0.5 | 1 |  | 0.5 |
| 5 | 0.5 | 1 |  | 0.5 |

Table : critical exponents for different dimensions of the Ising model on a regular lattice

In fact, for , the predictions of mean field theory are exact. From an intuitive standpoint, this is due to the increasing number of nearest neighbors per site in higher dimensions.

# Cluster Monte Carlo:

The classic approach to simulating the Ising model is the Metropolis-Hastings algorithm which essentially proposes single spin flips, which makes it a local update algorithm. An alternative approach called the cluster Monte Carlo was proposed by Swendsen and Wang in 1987. Instead of proposing single spin flips, we now form clusters. The clusters are formed via bonds connecting nearest neighbors with the same spins. Each bond is formed only with probability .

All spins connected with the bond essentially form a cluster. A decision is made to either flip or retain the cluster with probability of one-half. Hence, in each step, we perform a global update of the lattice versus a local update.

One of the prime advantages of the SW algorithm is that it does not exhibit any slow-down as the system approaches a critical point. The updates have an autocorrelation time proportional to .

As a result, it becomes more difficult to generate configurations which are independent because the correlation length becomes longer and longer. However, the clusters, by connecting spins over larger distances effectively circumvents this problem.

Hence, the SW algorithm is much more efficient at generating estimations of critical exponents than the Metropolis-Hastings algorithm

We see that the cluster algorithm changes the spin configurations drastically in one step. We want to know that this algorithm satisfies the necessary conditions of all Monte Carlo algorithms: ergodicity and detailed balance.

Fortuin-Kasteleyn cluster decomposition

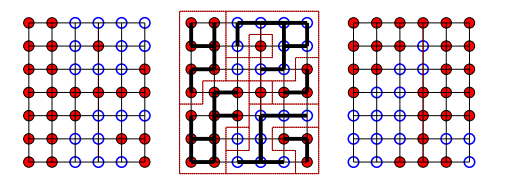


Figure : source: <http://www.helsinki.fi/~rummukai/simu/cluster.pdf>

Below, we validate our cluster Monte Carlo algorithm by showing a few snapshots of the Ising grid (below ) at different iterations during the algorithm

# Numerical Calculations of the Order Parameters

|  |  |
| --- | --- |
|  | (9) |

Where sum over sites. In the ordered phase, we expect the magnetization to be close to 1 but in the disordered phase, it should be close to 0.

For the susceptibility, we calculate:

|  |  |
| --- | --- |
|  | (10) |

Next is the spin correlation or the quantity

|  |  |
| --- | --- |
|  | (11) |

To measure correlation length, we have the expression:

|  |  |
| --- | --- |
|  | (12) |

To calculate energy, we can just directly read off the Ising Hamiltonian. For simplicity however, we first define the energy per site , which is:

|  |  |
| --- | --- |
|  | (13) |

The total energy is then just: , where the factor of comes from the fact that we are double counting bonds in our definition of .

Next is the heat capacity, which is defined from the energy

|  |  |
| --- | --- |
|  | (14) |

In practice, to calculate these order parameters, we will first ‘equilibrate’ the lattice by running 100 iterations without measuring any of the order parameters. After that we will run anywhere from 1000-10000 additional simulations and generate an average measurement for the given order parameters

# Finite Size Scaling

Finite size scaling phenomenon occur because the power laws we derive for the correlation length () are for an infinite volume (so it diverges as the temperature approaches the critical point). However, simulations we conduct are on finite sized lattices, hence the correlation length maxes out at whatever the scale of the lattice is.

Hence, we can say that system has an effective critical point, which is sometimes called a *pseudo-critical point.* We define

Finite size scaling does have drawbacks. It will usually provide a good estimate of the critical temperature, but usually fails

Use various volumes, we determine the maximum susceptibility. Then we do a power law fit to the maximum location of the susceptibility

The fit contains three parameters, one of which is the critical exponent.

# Numerical Results

## D = 2

For D=2, figures a,b,c show the plots

## D = 3

## D = 4

## D =5

# References

1. Swendsen and Wang, PRL 58 (1987) 86

# Source Code

<https://github.com/zhaonat/cluster_monte_carlo>