Ising Model

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(Dated: March 27th, 2019)

The Ising Model is a simple yet highly useful model in many areas in physics. Here, we use it to model a two-dimensional $N \times N$ lattice of particles, all interacting due to each of their magnetic spins. We use a Monte Carlo Markov Chain technique to perform the simulation. Having experimentally found a critical temperature T_c of [CRITICAL TEMP] that's [ERROR] away from the theoretical value of 2.269, we are satisfied with our results. In addition, we calculate the values of five critical exponents, finding [CRITICAL EXPONENTS].

CONTENTS

I. INTRODUCTION

A. Motivation and theory

The Ising Model consists of a d-dimensional square lattice of nodes, each in one of two possible states. Given the generality of the model, it is useful in many fields. In physics, it is most natural to call each node a "particle" and to let each particle have a magnetization of either up or down (representing its "spin"). We'll let the particles interact with their nearest neighbors with strength J and be coupled to an external magnetic field of strength B. The Hamiltonian for a lattice of side-length N is

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{I.1}$$

where $\sigma_i = \pm 1$ denotes the i-th spin state and $\langle i, j \rangle$ denotes a sum over nearest neighbors.

The particular novelty of the Ising Model is that, despite its simplicity, it exhibits a phase transition (for $d \geq 3$). In this lab, we'll explore the $d = 2$ case, which will exhibit a phase transition at zero applied field and at a temperature of T_c. For $T \ll T_c$, the spins align, and the lattice develops a uniform magnetization. For $T \gg T_c$, thermal fluctuations dominate, and no overall magnetization is expected. When T is near T_c, spins are expected to align in chunks, such that one area of the lattice may be uniformly up, while another area is uniformly down. These three cases are depicted in Figure I.1.

B. Simulation

[WRITE ABOUT MOTIVATION BEHIND MCMC SIMULATION TECHNIQUE]

C. Observations

The theory for the Ising Model is simplest in the limit $N \to \infty$. Although we cannot simulate the limit, we'll use this theory and be satisfied with an appropriately large lattice (discussed in sec REF).

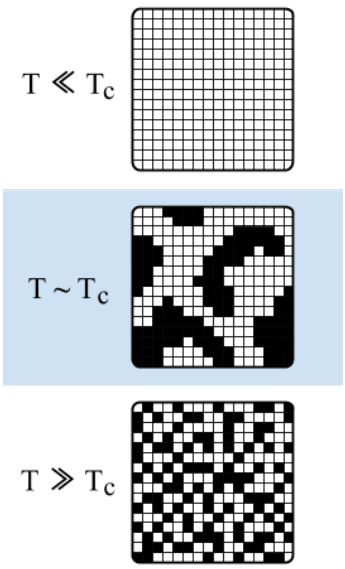

Figure I.1. The three temperature regimes for a lattice with $d = 2$. A white square represents a particle with spin $+1$ and a black square represents a particle with spin -1. Above T_c, the spins of the particles are somewhat random, leading to an expected average magnetization of 0. Near T_c, the lattice breaks into groups, all with particles of the same spin. Below T_c, all of the particles are either spin $+1$ or spin -1.

1. Energy

The energy per lattice site is

$$E(T) = -2\tanh\left(\frac{1}{T}\right) - \frac{\sinh^2(2/T)-1}{\sinh(2/T)\cosh(2/T)}\left[\frac{2}{\pi}K_1(\kappa)-1\right] \tag{I.2}$$

where

$$\kappa = 2\frac{\sinh(2/T)}{\cosh^2(2/T)} \tag{I.3}$$

and

$$K_1(\kappa) = \int_0^{\pi/2} \frac{\mathrm{d}\phi}{\sqrt{1-\kappa^2\sin^2\phi}} \ . \tag{I.4}$$

2. Magnetization

For $T > T_c$, we expect the average magnetization $\langle M \rangle$ to be zero, because the spins of the sites are approximately random. When $T < T_c$, though, we expect

$$|\langle M \rangle| = \left(1 - \left[\sinh(2/T)\right]^{-4}\right)^{1/8} \ . \tag{I.5}$$

These equations - Equation I.2 and Equation I.5 - both serve as preliminary tests of good data. If the respective parts of a set of data (from a single simulation) is fit well by of these equations, then it is appropriate to continue with the analysis.

Of greater interest than the above theoretical fits, are the so-called critical exponents of the 2-dimensional Ising Model. If we define a reduced temperature t as

$$t = \frac{T - T_c}{T_c} \ , \tag{I.6}$$

then it turns out many system state quantities scale as some power law in t. For example, theoretically,

$$|M| \propto |t|^{\beta} \ . \tag{I.7}$$

β is the critical exponent in this case, and has a theoretical value of 1/8. While a fit, such as Equation I.2, is characteristic of the specific Ising Model, these critical exponents are characteristic of the critical point T_c itself, and thus have greater generality.

3. Specific Heat

For specific heat c_V, the critical exponent relation is

$$c_V \propto |t|^{-\alpha} \ , \tag{I.8}$$

and α has a theoretical value of 0. A graph of the theoretical curve for specific heat as a function of final temperature is shown in Figure I.2.

4. Susceptibility

For magnetic Susceptibility, the critical exponent relation is

$$\chi \propto |t|^{-\gamma} \ , \tag{I.9}$$

and γ has a theoretical value of 7/4.

5. Correlation Functions

Thermodynamic fluctuations in the model can be probed by spatial correlation functions, which measure how closely two separate lattice sites are correlated. We'll consider the function

$$R(x) = \langle \sigma(0)\sigma(x) \rangle \ , \tag{I.10}$$

which measures how likely two spins separated by a distance x are aligned. $R(x) \sim 1$ indicates high correlation, while $R(x) \sim 0$ indicates low correlation. Generally, $R(x)$ dies off exponentially;

$$R(x) \sim e^{-x/\xi} \ , \tag{I.11}$$

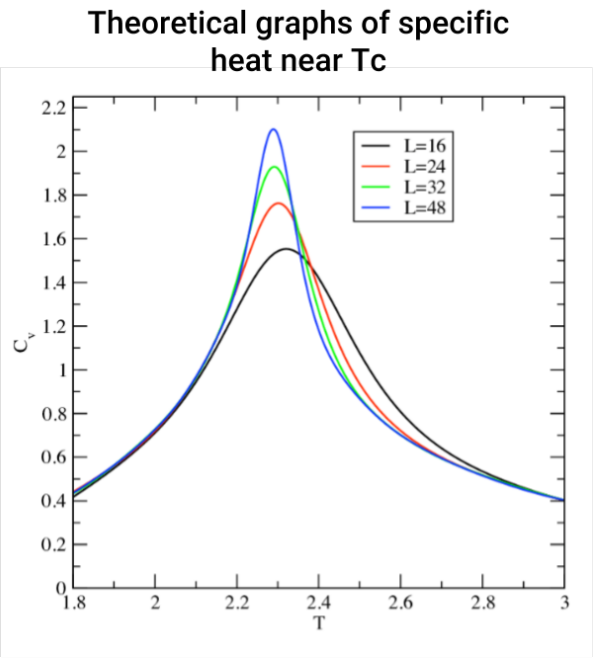

Figure I.2. Theoretical specific heat curve for lattice sizes of $N = 16, 24, 32, 48$ [3].

where ξ is the correlation length of the system and is dependent on T. Finally, we introduce our final critical exponent, η. When $\ll \xi$,

$$R(x) \sim \frac{1}{|x|^{d-2+\eta}} \tag{I.12}$$

where d is the dimension of the system (2, in this case). In our analysis, we'll examine ξ for various temperatures and find η near the phase transition.

II. EXPERIMENTAL METHOD

A. Preparation

We made two modifications to the Ising Model code. First, we changed the array of final T values to be denser around a guess of 2.269 for the critical temperature [2]. This will give greater resolution in the area of interest, while maintaining efficiency. Secondly, we added calculations of specific heat c_V and χ (and their respective standard deviations). We used the following equations for these calculations [2]:

$$c_V = \frac{\beta}{T}\left(\langle E^2\rangle_T - \langle E\rangle_T^2\right) \tag{II.1}$$

and

$$\chi = \beta\left(\langle M^2\rangle_T - \langle M\rangle_T^2\right) \ . \tag{II.2}$$

To reduce the negative effect of correlation between consecutive data points, we randomly re-ordered the list of

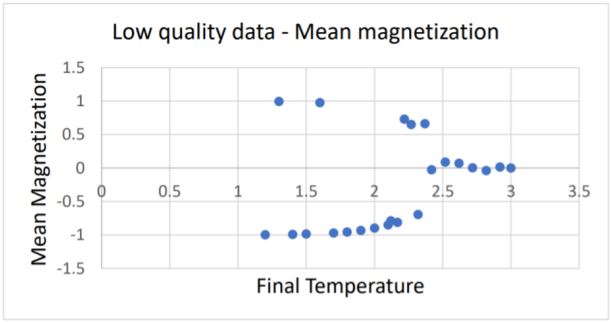

Figure II.1. An example of low quality data generated by a simulation on a 20×20 grid with too few annealing, burn-in, and sample steps.

energy and magnetization values collected for each final temperature, and then split the list into 10 bins. We then stored the standard deviation for each bin, and calculated c_V and χ from there.

B. Parameters and Data Quality

When running a simulation, there are about a dozen parameters to specify. A balance between rigor and time efficiency must be struck. Low quality data is exemplified in Figure II.1, which was the results of a simulation with a lattice size of 20×20, a temperature step size of .1 away from T_c and .05 close to T_c, 3000 annealing steps, 2000 burn-in steps, and 5000 sample steps. The chart does not have nearly enough resolution to gather a sense of where T_c falls.

An improved choice of parameter values will improve the quality of data. We found that our best simulations were simply those whose parameters were as large (or as small, in the case of the temperature step) as possible. In practice, we took these limits to be $N = 150$, $T_stepp = .001$ (and .0005 near T_c), and all three of annealing, burn-in, and sample steps to be 50000. An example of a data set created from a simulation with these values is shown in **??**.

1. *Parameters Explained*

[TABLE OF PARAMETERS WE MODIFIED] [Explanation of what they do]

2. *Optimal Data Parameters*

[TABLE OF FINAL PARAMETERS] [MAGNETIZATION CURVE OF FINAL DATA]

C. Data Analysis

The majority of our data analysis consisted of finding the best fits of our theoretical curves on our data. From these optimal fits, we were able to derive best fit parameters and compare them against accepted values.

First, we were able to directly test the validity of the analytic fits we were given for the entirety of our Energy and Magnetization curves through a χ^2_ν analysis. Then, we were able to derive estimates for T_c and the aforementioned critical exponents with uncertainty for each of the power law fits for $|M|$, c_V, χ, and the correlation length function, as described in section I C.

By comparing these estimates to theoretical predictions and plotting the residuals of each optimal fit and our data, we were able to gauge the consistency of our data with theory.

1. Reduced χ^2_ν Minimization

To obtain a quantitative measure of the deviation of our data from theoretical predictions we used the χ^2_ν metric. The χ^2_ν measure is a reflection of the distance of our data from a curve constructed through theoretical predictions. Specifically, we calculate the χ^2_ν as follows:

$$\chi^2_\nu = \frac{1}{\nu} \underbrace{\sum_{i=1}^{N} \frac{(y_i - f(x_i, \alpha))^2}{\sigma_i}}_{\chi^2} \tag{II.3}$$

where y_i are our N simulated data points, $f(x_i, \alpha)$ are the y values of our theoretical curve given parameter set α, and σ_i is the uncertainty in our simulated data y_i. In addition, $\nu = N - p$ is the number of data points N minus number of parameters p we are free to change. This ν is a measure of the true degrees of freedom in our fit. By reducing our χ^2 by ν, we obtain a normalized χ^2_ν which is much easier to make sense of than our original χ^2. We also see that a larger χ^2 is acceptable if our ν, number of degrees of freedom, is larger.

Our goal is to find the set of parameters α that minimize our χ^2_ν for each fit. In our earlier analysis, we traversed a grid of parameter choices for each fit. Then, by finding the minimum of the χ^2_ν values calculated for each point on our parameter grid, we were able to ascertain the optimal parameters that minimized the χ^2_ν of our fit. However, we discovered the SciPy Python module from which we imported *scipy.optimize.curve_fit* [1]. This function allowed us to find the optimal parameter set that minimized our χ^2_ν over a range of parameter values for each parameter in our set. This function also returns a covariance matrix from which we are able to calculate one standard deviation errors on each of our parameters. This standard deviation error calculation is equivalent to starting at our optimal parameters point in our parameter grid and finding the minimum distance we have to travel down the relevant parameter axis to double our minimum χ^2_ν value, which is the classic method of calculating optimal fit parameter error.

Once we have calculated our minimum χ^2_ν, we can begin to interpret the quality of our fit. Namely, if our $\chi^2_\nu << 1$, then we have either overestimated our errors or over-fitted and if our $\chi^2_\nu >> 1$, then we have either underestimated our errors or discovered a discrepancy between our data and what is expected by theory reflecting the inaccuracy of our model.

2. Residuals

Another method of fit analysis is a residuals calculation. Here, we subtract our optimal fit curve from our data normalized by the error bars in our data.

The residual for data point y_i is:

$$\epsilon_i(x_i) = \frac{y_i - f(x_i, \alpha^*)}{\sigma_i} \tag{II.4}$$

where $f(x_i, \alpha^*)$ is the theoretical value at x_i using the best fit parameter set α^*, as determined by our χ^2_ν minimization and σ_i is the error bar of data point y_i.

The residuals add in quadrature to yield our minimum χ^2 value, and while minimizing this sum is important, it is also important that our residuals reflect roughly randomly distributed data around our theoretical predictions. Ideally, the resulting curve should resemble normally distributed noise with mean zero and standard deviation 1. A reasonable residuals curve and minimum χ^2_ν value are strong indications of data that is consistent with theory.

3. Parameter Estimates and Ranges

While our analytic fits for Energy and Magnetization, stated in section I C 1 and section I C 2 respectively, have no free parameters to fit, our power law fits in section I C 3, section I C 4, and section I C 5 have free parameters to fit, as depicted in Table II.1. We used the theoretical values for our critical exponents to help us set parameter estimates and center our parameter ranges. The relevant theoretical curves exhibit discontinuities or otherwise identifiable behaviour around T_c. For this reason, we often derived the T_c parameter range through visual inspection of our data.

4. Fitting Techniques

While many of these power law fits are only valid near T_c, they also exhibit discontinuities at $T \approx T_c$. For example, we found that the range of temperatures we vary

Critical Exponent	Defination	Theoretical Value
α	$c_V \propto \lvert t\rvert^{-\alpha}$	0
β	$\lvert M\rvert \propto \lvert t\rvert^{\beta}$	1/8
γ	$\chi \propto \lvert t\rvert^{-\gamma}$	7/4
ν	$\xi \propto \lvert t\rvert^{-\nu}$	1
η	$R(x) \propto \lvert x\rvert^{-d+2-\eta}$	1/4
Parameter		
c_V	specific heat	
M	magnetization	
χ	magnetic susceptibility	
ξ	correlation length	
t	reduced temperature	$(T - T_c)/T_c$
T_c	critical temperature	2.269

Table II.1. Table of critical exponents and parameters, and their theoretical values when appropriate.

our free parameter T_c between must be outside the range of temperatures we are attempting to fit for our specific heat curve. This is because of a discontinuity inherent in the power law fit at T_c. As depicted in section III, similar nuances of our other power law fits compelled us to only fit data near T_c, but never at T_c. Because the range of data we aimed to fit depended on our estimate of T_c, the analysis of some of these curves was an iterative process in which we gradually improved our parameter estimate ranges for T_c until we were satisfied with the resulting minimum χ^2_ν and residuals curve.

[1] community, T. S. (2019), "scipy.optimize.curve_fit," .

[2] Stewart, D. (2019), "Phys 382 Ising Model Lab," .

[3] Viot, P. (2011).