A Monte Carlo Simulation of the 2-D Ising Model Utilizing the Metropolis Algorithm

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Abstract

The 2-Dimensional Ising model is notoriously difficult to solve by hand, and thus in itself counsels us to make approximations and perform our experiments *in silico*. For the sake of efficiency a monte carlo algorithm, known as the Metropolis algorithm, was chosen. Through the use of the the programming interface, MATLAB , the algorithm was implemented and used to measure several thermodynamic variables over a range of relevant temperatures. Further, an attempt to demonstrate the accuracy of the simulation through the use of known "critical exponents" was made.

INTRODUCTION

Monte Carlo simulations, which take their name from the gambling mecca of southern france, utilize artificially created probabilities to evolve systems according to their given statistical models. Here, a well known Monte Carlo algorithm, known as the Metropolis algorithm is used to simulate the 2-D Ising model.

The Ising model is a statistical model of a magnetic, wherein the system is assumed to be a lattice composed of ions with intrinsic magnetic moments, each of which can occupy one of two positions: spin "up" or spin "down." Thus, the total energy of the 1-D system is,

$$E = -J\Sigma_i s_i s_{i+1} - H\Sigma_i s_i$$

Where J is the interaction energy of the two spins, and H is the magnetic field. In 2-D, the equation is the same, however there are two copies of the J term: one for horizontal and one for vertical neighbors. Here, it is assumed that only the nearest neighbors affect each spin. In a 2-D square lattice, this means that each spin has four neighbors: up, down, left and right. Further, it will be assumed that $H = 0$, *i.e.* that there is no external magnetic field, and that the long range spin-spin interactions are negligible. Thus, so long as we have a way to evolve the system, we can measure several thermodynamic variables of interest.

THE METROPOLIS ALGORITHM

The algorithm operates as follows:

1. Create an $N \times N$ lattice of spins, and impose boundary conditions
2. Choose a random spin somewhere in the lattice, and find its 4 nearest neighbors (top, bottom, left and right)
3. Calculate the change in energy that would result if the spin flipped (ΔE)
4. If the energy would decrease, then flip. If the energy would increase, then flip with the probability of: $p = e^{-\beta \Delta E}$
5. Repeat steps 2-3 many times, and record thermodynamic variables after allowing the system to equilibrate

Step 1 is accomplished through MATLAB by simply using the command: spinarr = ones(nrows,nrows). This initializes the system in uniform spin-up orientation. Next, periodic conditions were imposed by assigning the farthest right spins on the lattice "right side neighbors" of the far left spins of the same row, the farthest up spins "up neighbors" of the bottom spins of the same column, and *etc.* Step 3 is accomplished through the matlab command randi(nrows,1) which chooses a random integer between or equal to 1 and the number of rows. The same is dowe for the column. Then, using the above formula, the energy due to interaction with each of its neighbors is calculated and summed. $\Delta E = -2E$ since the spins can only be 1 or -1. Step 4 is performed by generating a random number between 0 and 1, and if that number is less than the "probability," p, for the given ΔE, then the change is accepted. The process is repeated for 100,000 steps of equilibration, then averages are taken over each spin in the lattice, the temperature is incremented, and the process repeats.

The Metropolis algorithm is a good choice because it keeps the lattice in likely microstates by keeping each spin it visits in likely states. This is known as *importance sampling*, and is an efficient way of ignoring the unlikely microstates, which have negligible contributions.

MEASURING THE THERMODYNAMIC VARIABLES

In order to measure thermodynamic variables over a range of temperatures, the system must be allowed to equilibrate, then the observable can be measured, the temperature incremented, and the process repeated. Observables are given by their Boltzmann-factor-weighted average values in the system, *i.e.* , for an observable, A:

$$\langle A \rangle = \frac{\Sigma_s A_s e^{-\beta E_s}}{\Sigma_s e^{-\beta E_s}}$$

It is perhaps worth noting that in order to sum over an entire state, only a sum over the direct neighbors is necessary, since long range interactions are ignored in this calculation.

Here, the following variables are measured: E, M, C and χ. E is the energy per spin, which is simply the sum of energies of each spin, divided by two to correct for the double counting performed in the summation. M is the magnetization per spin, which is simply the weighted-average spin. C and χ, the specific heat and magnetic susceptibility respectively, are slightly more difficult, since they are defined by partial derivatives. Thankfully, the

fluctuation dissipation theorem for zero external fields provides a solution to this dilemma:

$$\begin{aligned} C_V &= \frac{\partial \langle E \rangle}{\partial T} \\ &= -\frac{\beta}{T}\frac{\partial \langle E \rangle}{\partial \beta} \\ &= \frac{\beta}{T}\frac{\partial^2 \ln Z}{\partial \beta^2} \\ &= \frac{\beta}{T}\frac{\partial}{\partial \beta}\left(\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right) \\ &= \frac{\beta}{T}\left(\frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial \beta}\right)^2\right) \\ &= \frac{\beta}{T}\left(\langle E^2 \rangle - \langle E \rangle^2\right) \end{aligned}$$

Likewise,

$$\begin{aligned} \chi &= \frac{\partial \langle M \rangle}{\partial H} \\ &= \beta\left(\langle M^2 \rangle - \langle M \rangle^2\right) \end{aligned}$$

Therefore, if we simply keep track of E, M and their squares, we can also find C and χ.

THERMODYNAMIC RESULTS

All simulations were of 500×500 lattices, run for temperatures of 0.1 through 8.0 in natural units of J/k_B. After each temperature increment, the system was allowed to equilibrate for 100,000 steps, and then the averages were performed over the entire grid.

In all four plots, the phase transition from the ferromagnetic state, where magnetization is maintained even though there is no external magnetic field, and the paramagnetic state, where the temperature is high enough to render the spin-interactions insignificant, it readily observable. Once the critical temperature is reached, the spins have enough energy to overcome the barrier to flipping. Thus, the magnetization breaks down and oscillates about zero, since each spin is essentially equally likely to be spin up or down. The peak in susceptibility can be understood in the following way: first, there is no change in magnetization, because no spins have the energy to flip. Then, a high enough temperature is reached, and the spins that flip change the overall magnetization, increasing the susceptibility. This process

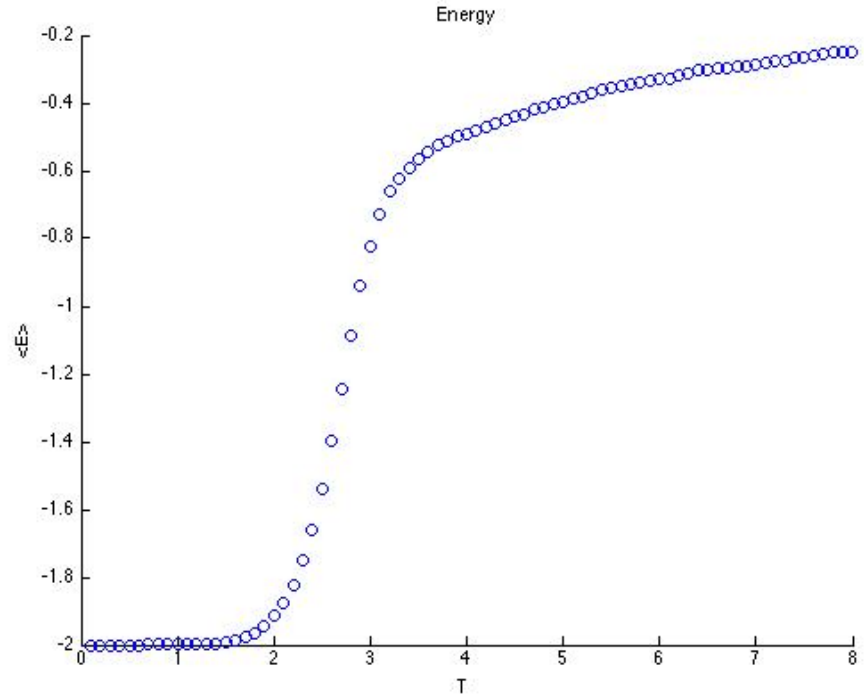

FIG. 1. The energy of the system

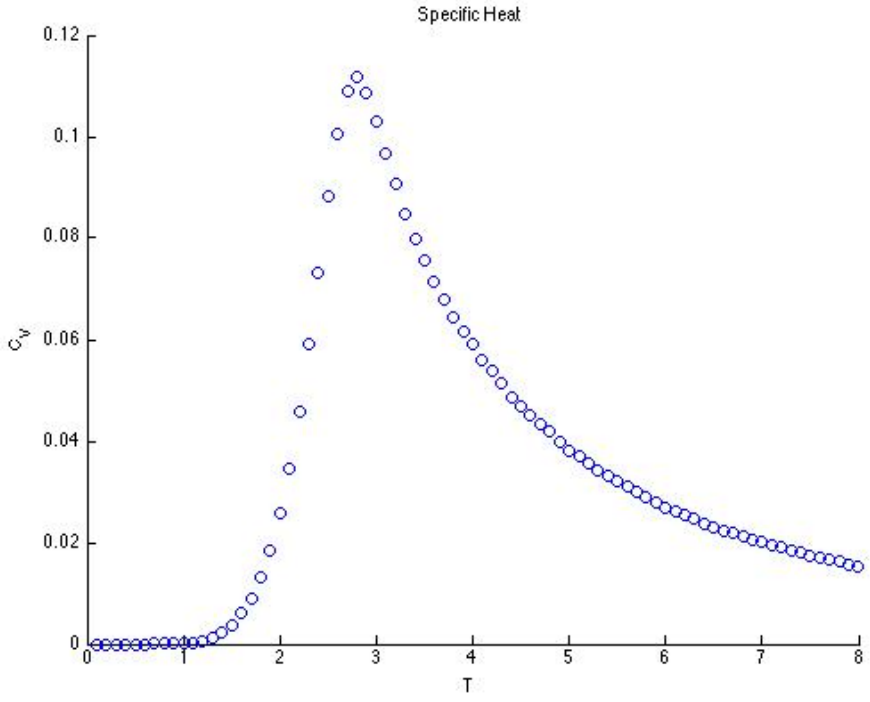

FIG. 2. The specific heat of the system

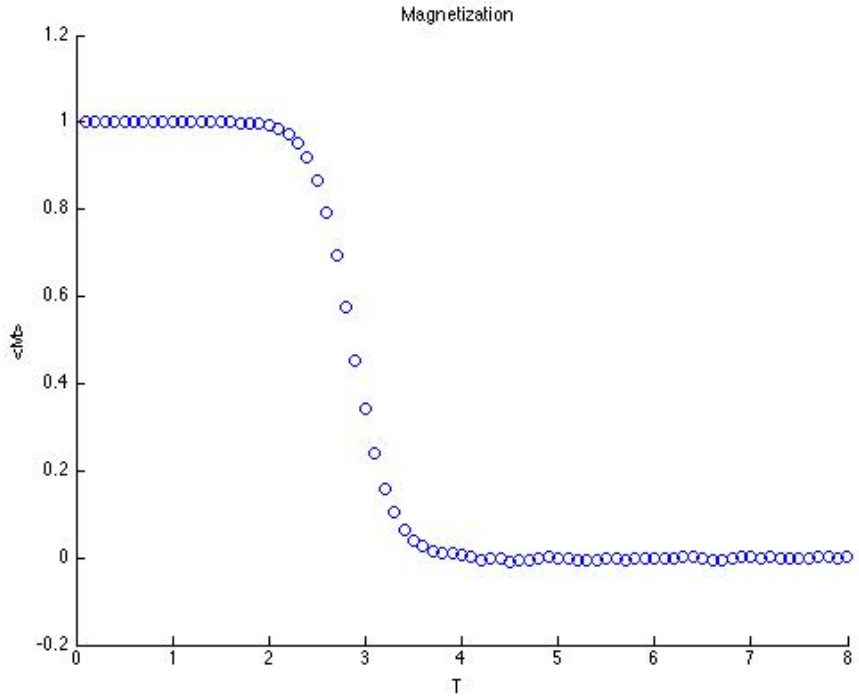

FIG. 3. The magnetization of the system

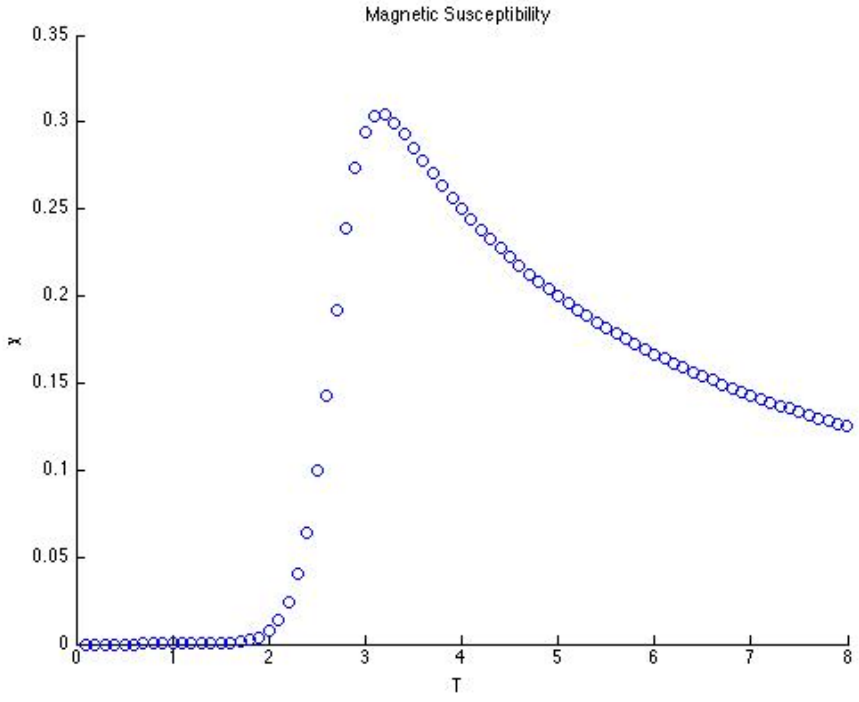

FIG. 4. The magnetic susceptibility of the system

continues until the phase transition at the critical temperature, at which point the kinetic energy due to temperature begins to dominate over the changing magnetization. The specific heat plot follows a similar narrative: at first no spins are flipping, so there is no change in energy; then, a high enough temperature is reached that they flip and more and more energy changes as temperature increases, until the phase transition at the critical temperature where temperature starts to dominate. Finally, the energy plot is a bit more subtle than the others. One might expect that it would oscillate about zero, as did the magnetization; however, it is important to recall that energy is only dependent on the direct neighbors of a spin, thus local pockets of unified spin persist and reinforce each other. Ultimately, one still expects that at a high enough temperature the energy will in fact oscillate about zero as intuitively expected.

Further, the plots can be seen to exhibit phase transitions right around 2.269 J/k_B, which we know to be the exact T_C from the Onsager solution.

CRITICAL EXPONENTS AS A MEASURE OF MACHINE ACCURACY

From the Onsager solution, approximated near $T \approx T_c$, we know the power rules obeyed by several thermodynamic variables, which are summarized in figure 5. Near the "critical temperature" each observable is described by some power of $\epsilon \equiv \frac{|T-T_c|}{T_c}$. Here we are interested in the correlation length, ξ. Since $\xi = \epsilon^{-\nu}$ and $\nu = 1$, ξ obviously diverges near T_c . Since the correlation length is a measure of the average distance over which one spin can affect another, this tells us that near T_c , ξ is infinite, and thus all spins affect all other spins, irrespective of their distance. Clearly, the simulation here is not of an infinite lattice; however, a good measure of the accuracy of our simulation would make use of the fact that $\xi \approx L$, where L is the width of the lattice, defines the limit of the computer's ability to simulate an infinite lattice.

If we rewrite the condition,

$$\xi \sim L \sim |T - T_c|$$

as:

$$|T - T_c| \sim L^{-1/\nu}$$

		values of the exponents		
quantity	singular behavior	$d = 2$ (exact)	$d = 3$	mean-field theory
specific heat	$C \sim \epsilon^{-\alpha}$	0 (logarithmic)	0.113	0 (jump)
order parameter	$m \sim \epsilon^{\beta}$	1/8	0.324	1/2
susceptibility	$\chi \sim \epsilon^{-\gamma}$	7/4	1.238	1
equation of state ($\epsilon = 0$)	$m \sim H^{1/\delta}$	15	4.82	3
correlation length	$\xi \sim \epsilon^{-\nu}$	1	0.629	1/2
correlation function $\epsilon = 0$	$G(r) \sim 1/r^{d-2+\eta}$	1/4	0.031	0

FIG. 5. A Table of the critical exponents in the Ising model, where $\epsilon \equiv \frac{|T-T_c|}{T_c}$ [1]

and then plug that into one of our variables, say ξ, then we have:

$$\chi(T = T_c) \sim \left(L^{-1/\nu}\right)^{-\gamma} \sim L^{\gamma/\nu}$$

Then we have a relationship between something we measure, χ, something we know, L, and a ratio of the critical exponents, in which we're interested. We know the exact solution of $\gamma/\nu = 7/4$, which holds for infinite length systems, so we can inspect the accuracy of our machine as a function of the size of the lattice we are simulating. This method is aptly named *finite size scaling*.

FINITE SIZE SCALING RESULTS

From the data, we see that the simulation missed the exact ratio of the critical exponents by about 31% for an 800×800 lattice. The dramatically slowed growth of the curve suggests that far more computational power than was available for this study would be required to approach "exact" values.

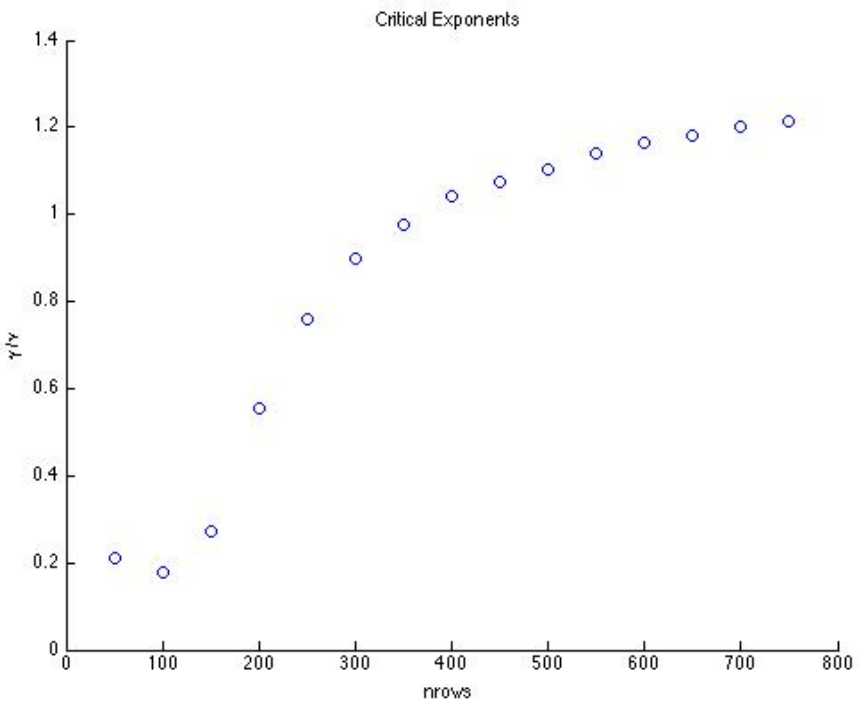

FIG. 6. Values of γ/ν, plotted for increasing lattice sizes

THE CODE

Code to sample thermodynamic variables over a range of temperatures

```
% 2D Ising model
% Written By Keith Zengel
% 9/14/2011


clear; close all; %take out the trash
hold off;
nrows = 500; % n x n grid size
nrows2 = nrows*nrows; % update plot every n^2 time through loop
equilibrated = 100000; % How many steps you want to allow the sample
                       % to equilibrate before taking data and how many
                       % steps to average data over
```