STUDY OF ISING SPIN SYSTEM USING THE MONTE CARLO METHOD

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Abstract. Ising model is a mathematical model used in statistical mechanics in order to study magnetic properties properties of matter, in which a magnetic substance is idealized by a discrete collection of quantities called 'spins', which can have only two values: +1 and -1. But the problem is that any macroscopic system must be thought of as a collection of huge number (of the order of 10^{23}) of such spins if one wants to calculate the properties of the system within any reasonable accuracy. So the number of all possible microstates of a system will be of the order of $2^{10^{23}}$. But the usual procedure of evaluating any macroscopic quantity as per the rules of statistical mechanics involves taking the weighted average of the quantity over all possible microstates, which will take billions of years to compute even with the fastest computers available today.

But here comes the Monte Carlo method in our rescue. Using this elegant method of simulation and an equally clever and efficient technique called the Metropolis algorithm, the magnetic properties of a lot of substances can be explained. In this project, the properties of a two-dimentional Ising spin system under various circumstances was studied.

1. A Brief Description of the Ising Spin Model:

In order to theoretically analyze magnetic properties of different kind of substances, somewhat simplified models are often used, because the actual atomic machinery responsible for those properties are very complicated to analyze mathematically and they might not even be completely understood yet. Ising model is such an abstract model. In this model, any substance is assumed to have a lattice-like structure so that at each lattice-point a variable called the 'spin' has either of these values: +1 or -1. The total macroscopic magnetisation S is the absolute value of the sum of those spins:

$$S = |\sum_i S_i| \tag{1.1}$$

The energy E of an Ising spin system without the presence of any external magnetic field is:

$$E = -J \sum_{\langle i,j \rangle} S_i S_j \tag{1.2}$$

Here the brackets indicate that the sum is done over adjacent spins only. J is a constant characteristic of the material whose value depends on the nature and strength of the interaction between adjacent spins.

- If J $>$ 0 the interaction is called ferromagnetic.
- If J $<$ 0 the interaction is called antiferromagnetic.
- If J = 0 the spins are noninteracting.

In this project, we will deal with ferromagnetic systems only, i.e. systems in which J>0. Basically those systems has low energy when its adjacent spins are aligned in the same direction.

If + and - spins are interchanged, equation (0.2) remains unchanged. So normally an Ising spin system is completely symmetric under the interchange of + and - spins. But in the presence of an external magnetic field B, individual spins interact with that B field and the system is biased in favored to one direction of S. The equation of energy now becomes:

$$E = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i \tag{1.3}$$

It can be readily observed that when the individual spins are aligned in the direction of the B field, the system has low energy.

Now at a certain temperature, such a system with lattice size of $n \times n$ can be in any of the 2^{n^2} possible configurations. The probability P(C) of the system being in a configuration C is given by the **Boltzmann distribution**:

$$P(C) \propto e^{-E(C)/kT} \tag{1.4}$$

Where E(C) is the energy of the microstate C, k=the Boltzmann constant and T = the temperature.

So any arbitrary macroscopic property Q of the system is the weighted average of the property taken over all microstates. For example the magnetisation S of the system will be:

$$S = \sum_C S(C)P(C) \tag{1.5}$$

S(C) being the magnetisation of the configuration C.

1.1. **Phase Transition in Ising Spin Systems:** Phase transition, i.e. the transition of magnetic materials from ferromagnetic to paramagnetic phase with increase of temperature is a very intersting physical phenomena. At low temperature, the entropy of the system is low. So the no. of microstates available to the system is small. So the system, on the average, stays in the microstates for which the energy is lower. According to equation (0.2), clearly that happens when most of adjacent pair of spins are aligned in the same direction. But at high temperature, the system has high entropy, so rather than settling for a handful of microstates with minimum energy, it has lot more microstates available to it. In other words, at low temperature Ising spin systems with positive value of J are ferromagnetic but at sufficiently higher temperature they become paramagnetic. Generally, this transition occurs very sharply at a temperature called the critical temperature.

Ernst Ising solved the model for the 1D case in his 1925 PhD thesis. In one dimension, the solution admits no phase transition. On the basis of this result, he incorrectly concluded that this model does not exhibit phase transition in any dimension. But Onsager solved the 2-D case analytically in 1944 and showed that indeed phase transition occurs there.

2. Use of Monte Carlo Methods in the Study of Ising Systems:

In principle, any macroscopic property of the substance can be calculated if the value of the property for all the microstates are known. Given a physical model, we could evaluate the energies E(C) for each of the possible microstates, and equation (0.3) would then give the probabilities of these states. To evaluate any "average value" function of the system, we need only perform the sum in equation (0.4). However, the number of terms in summation in equation (0.4) is incomprehensibly large. (If we could somehow use all computing resources on the planet for one full year we could only evaluate equation (0.4) for "trivially simple" problems).

Since it is practically impossible to carry out the sum in equation (0.4), the only statistically proven alternative is taking a relatively small sample of microstates and taking the average over those microstates only. One can observe after looking at the sum in equation (0.4) carefully that the value of the sum does not deviate significantly if some of terms in which P(C) is very small is omitted. In other words, one can minimize the error incurred due to sampling by choosing those microstates for which P(C) is high. But how to ensure that only those "important" samples are taken without losing too much of computational time?

The Monte Carlo method does just that. Using random numbers and some suitable sampling techniques it can simulate even most complicated physical processes for which using deterministic algorithms is not a viable options due to large computational time required. As in gambling, random numbers play an important role in this technique, hence it is named after the famous district of Monte Carlo in Monaco. This method is widely used in varius fields such as physics,mathematics,biology and even economics.

This method coupled with a brilliant sampling technique called the Metropolis algorithm dramatically brings down the time of computation whereas not compromising too much on accuracy.

2.1. **The Metropolis Algorithm:**

This algorithm can determine any property of an Ising spin system by the method of iterations. The algorithm is as follows:

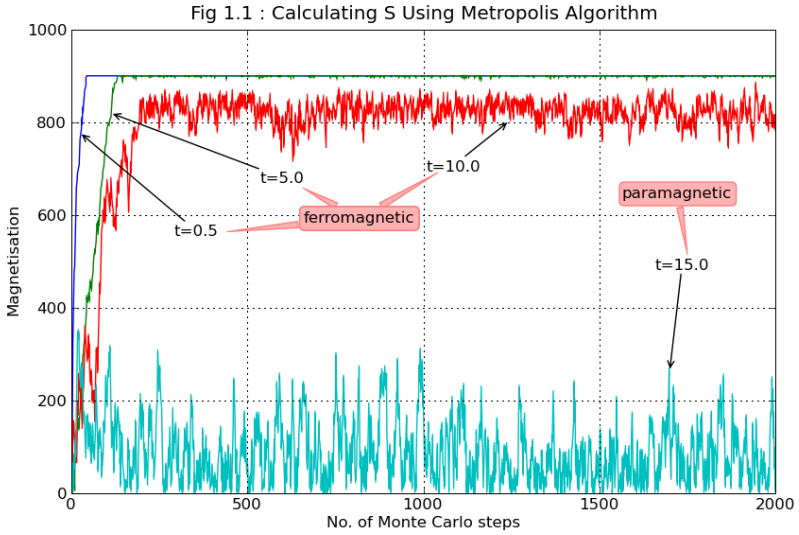
(1) At first, all the lattice points are assigned random spin values.
(2) Then one lattice-point is chosen randomly. The change in the energy $\triangle H$ of the system if that particular spin is inverted is calculated according to the equation:

$$\triangle H = 2JS_i \times (Sum\, of\, neighbouring\, spins) \tag{2.1}$$

(3) Let $\alpha = e^{-\triangle H/kT}$.
  (a) If $\triangle H \leq 0$: The inversion of spin at that lattice point is allowed.
  (b) If $\triangle H > 0$: An random number β between 0 and 1 is picked uniformly.
    (i) If $\alpha \geq \beta$, still the inversion is allowed.
    (ii) If $\alpha < \beta$, the inversion is not allowed.
(4) Step 2 and step 3 are repeated.

When this routine is performed as many times as the number of spins in the system, one says that one *Monte Carlo step* has been performed. It is really impressive that this deceptively simple algorithm produces quite accurate result within 2000 Monte Carlo steps, which takes merely *a few seconds* for a 30×30 lattice in a common desktop computer with 3.0 GHz Intel processor. Another beautiful thing about this algorithm is that it being iterative in nature, one can achieve higher and higher

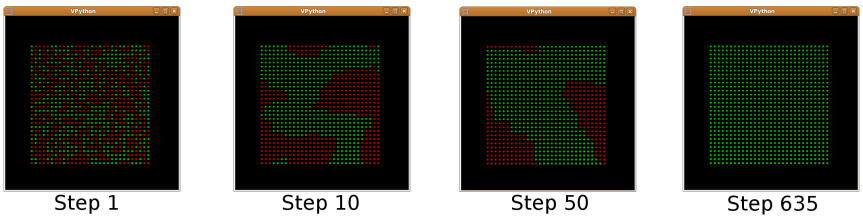
degree of accuracy by simply increasing the number of iterations. The following plot illustrates how rapidly the value of net magnetisation of a 30×30 Ising spin system converges while using this algorithm in a program written in the programming language python:



In fact carrying out the program till 2000 Monte Carlo steps was an overkill here! The plot clearly shows that for all temperatures, 1000 iterations would have produced almost equally accurate result. High value of magnetisation of the system at low temperatures implies that it is in ferromagnetic state. But at higher temperature (15.0 in this case), it has almost zero magnetisation, which means that phase transition has already occured and the system is now in paramagnetic state. It is also evident from the plot that at low temperature, the value of S stabilizes pretty quickly. Whereas at high temeperatures, it takes many more Monte Carlo steps to do so.

In order to understand how the algorithm works, we can actually make our program produce visual representations of the system at each step, thanks to a nifty python module called vpython also known as visual python. Basically what happens is that the program generates an 'image' of the system following some pre-defined rules to represent +ve and -ve spins. Each time a spin gets flipped, the image is also updated. So the user basically *sees* an animation of the changes the system undergoes with each Monte Carlo step. A few images generated by this program is shown below:

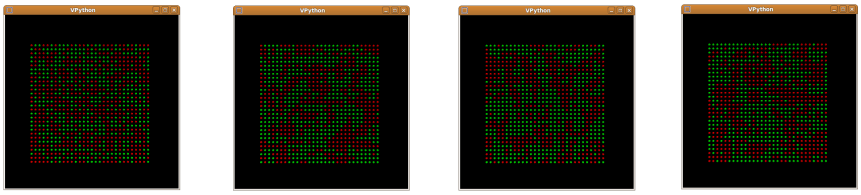
Fig 1.2 : A Few Microstates Generated by The Metropolis Algorithm for Ferromagnetic Material



In these images, green spheres represent +ve spins and red ones represent -ve spins. This series of images clearly shows that initially the spins are completely at random, which is of course expected from our algorithm. At step 10, seperate chunks of +ve and -ve spins have formed. But still, sum total of +ve spins is almost equal to that of -ve spins. At step 50, +ve spins start to gain an edge over the -ve ones. In the last image, all spins are +ve and the system has reached equillibrium.

However, the system can reach equillibrium in this fashion only if it is in ferromagnetic state. What happens in the paramagnetic case is illustrated below:

Fig 1.3 : A Few Microstates Generated by The Metropolis Algorithm For Paramagnetic material



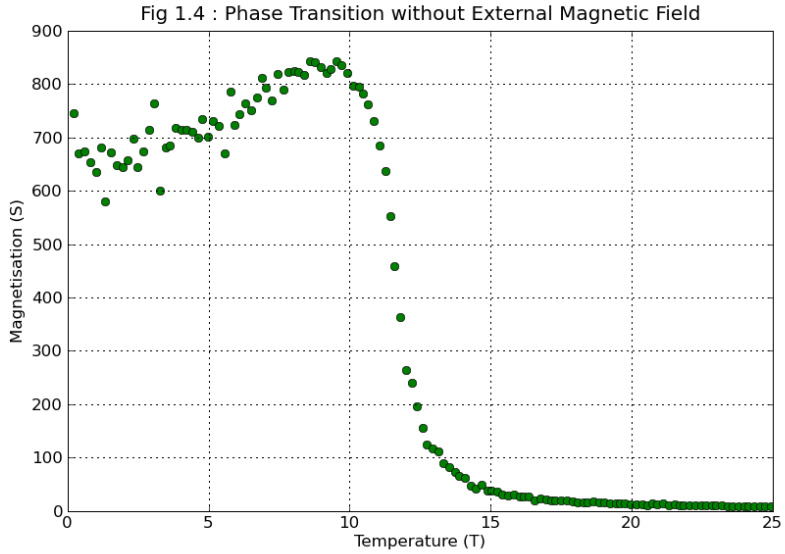
The system starts from a state pretty much similar to the initial step for the ferromagnetic case. But as the algorithm progresses, instead of a few big chunks of similar spins we see numerous small 'domains' of similar spins. Apart from the size, these domains are different from their ferromagnetic counterpart in another respect: these domains have smaller subdomains of opposite spins inside them. And of course, the system does not stabilize at all in this case.

3. Studying the Phase Transition:

Armed as we are now with the Metropolis algorithm, studying phase transition is not a difficult task at all. All we need to do is use our algorithm repeatedly to evaluate the magnetisation value S for various temperatures. To be extra cautious, we evaluated S values 100 times for each tempearatures and then took the average.

3.1. **With No External Magnetic Field:**

The plot of the S values vs. the corresponding temperatures is presented without further ado :



As expected, there is a sharp decline in the value of S between T=10 and T=15. But why is the behaviour of S between 0 and 10 so erratic? Moreover, the value of S seems to be *higher* at t=10 than that at t=0.2! This does not tally with the experimental results at all.

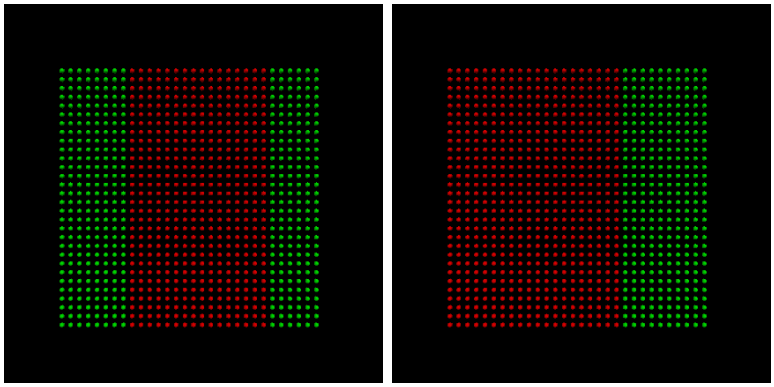
3.1.1. *A Startling Drawback of the Metropolis Algorithm:* In order to investigate the cause of the baffling behaviour of the plot at low temperatures, at first the program was modified so that it performs 1000 Monte Carlo steps for a specific temperature, prints the final value of S and repeats the same task a few times. When the program was run for T=0.2, the following numbers came up on the screen:

900,900,900,180,900,900,900,900,900,300,120,240,180,240,900,900,900,360,900,60,
900,900,900,900,900,900,900,900,120,900,240,900,900,900 etc.

The occurences of numbers like 60,180,240,300,360 in the list above is definitely most unexpected. At such a low temperature like 0.2 , the system should invariably stabilize well within 1000 Monte Carlo steps and the S value should be 900 in almost all cases. It is also noteworthy that all such numbers deviating from 900 are multiples of 30, the length of the square lattice.

To understand what really is going on, again we took recourse to the admirable vpython module. We set the temperature to some very low value and watched the visual representation of the system as it was changing as per the rules of Metropolis algorithm. On executing the program for the first time, all the spins became aligned in the same direction pretty quickly, as expected. We kept running the same program repeatedly. Although we did not exactly expect something dramatic to happen, suddenly in one execution of the program we noticed a peculiar thing: a ribbon-like structure was formed, consisting of alternate bands of +ve and -ve spns. The trouble was that the system did not come out of that configuratin, even after as many as 5000 Monte Carlo steps.

Fig 1.3 : A Couple of Examples of the Ribbon-like Structures



On further investigation, it was revealed that such *bands* or *ribbons* form only at low temperature and once they are formed, the system *always* gets stuck at that configuration. Moreover, the frequency of the formation of such bands decrease with increase in temperature. So now we get to understand what is actually happening in that temperature interval: for very low values of T, more number of iterations yielded ribbon structures. The ribbon structure having lower magnetisation than a perfectly uniform one, the contribution due to those ribbons pulled down the average value of the magnetisation for those temperatures. With relatively little increase of temperature (within 10), the frequency of formation of such ribbons decrease, which accounts for the initial increase in S with increase in T.

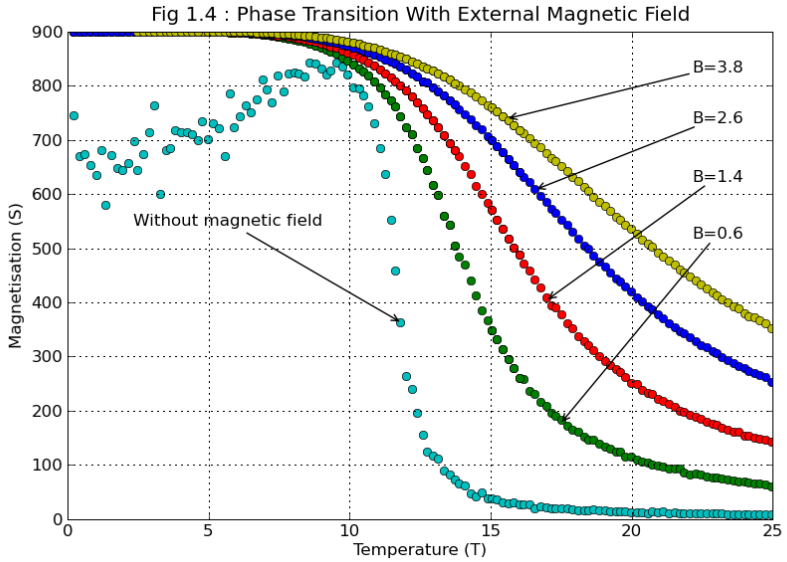
But of course, when the value of T crosses the critical value for phase transition, the system does not stabilize at all. Neither the ribbon nor the perfectly uniform structure is formed anymore. Everytime we end up with the domains of +ve and -ve spins then. So the ribbon effect no longer remains significant.

3.1.2. *Reasons of Formation of the Ribbon:* Although the formation of the ribbon is a rather unexpected incident, it is not that difficult to explain. In any ribbon structure, every spin at a +ve/-ve border has 3 neighbours of same spin and 1 neighbour of opposite spin. So according to equation 2.1, $\triangle H = 2JS_i \times 2S_i = 2JS_i^2 = 2J > 0$. So $\alpha = e^{-\triangle H/kT} = e^{-2J/kT}$, which has very small value for small values of T. Therefore in the next step when a random number β between 0 and 1 is chosen, there is a very high probability of α being smaller than β and therefore the spin remaining the same.

So we see that the ribbon structure is very stable so far as Ising model goes. Now the question is: does this kind of ribbon structure get formed in nature also? Then of course we should see increase in net magnetisation with temperature for some temperature range. Whether that happens or not can only be verified experimentally and hence is beyond the scope of the project. But available data from experiments done already lacks any such evidence.

Or it is possible that the ribbon structure is not stable in the long run. Maybe the system will come out of those ribbon structures if we wait long enough. That explains why the same effects are not observed in nature: evidently Nature finds the stablest configuration of ferromagnetic substances at a much faster rate than our computers do, despite being helped with the mighty Metropolis algorithm. In that case, Metropolis algorithm is not suitable for studying the characteristics of magnetic substances at low temperatures.

3.2. **With External Magnetic Field:** First the plot of net magnetisation Vs. temperature is presented for different values of magnetic field intensity. The one for no magnetic field is also presented for sake of comparisn :



The first thing to be noticed in this plot is that on application of an external magnetic field, the M Vs. T plot has become smoother. In the case without an external magnetic field, there was a sharp downfall in S near phase transition. But the change is less sharp if magnetic field is present.

Another important feature of the plot is that at any specific value of T, the value of S is higher for higher magnetic field. This implies that the system has higher net magnetism for higher values of external magnetic field, which is in accordance with experimental facts.

A very noticeable deviation of these plots from the one for the no magnetic field case is in the absence of the wiggliness of the plot for low temperatures in the cases where magnetic field was present. From this we may presume that the aforementioned ribbon structures are not forming if magnetic field is present. A saving grace it obviously is for the Metropolis algorithm and it is not difficult to understand why.

In the case without any magnetic field, +ve and -ve spins were equivant: none had any special privileges. But with the introduction an external magnetic field, the system is getting biased. So any spin in the system has the tendency to get aligned with the external field. So the ribbon is not at all such a stable structure here. Mathematically speaking, the main reason for the ribbons getting formed were the low values of $\alpha = e^{-\triangle H/kT}$. Now the expression of $\triangle H$ has one additional term: $2BS_i$. This addisional term will help increase the value of α, effectively eliminating the possibility of the system getting stuck at such a ribbonlike configuration.