Monte Carlo Simulation of the 2D Ising Model

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Project Presentation
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7 Jan 2014

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Hello everyone, my name is Onur Kaplan.Welcome to my advanced physics lab. project presentation I explain Monte Carlo Simulation of the 2D Ising Model.

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Let me start by giving an outline of my talk.
Firstly, i will describe Monte Carlo method and then i will make a little introduction to Ising Model. Then, i will show the results of simulation of 2D Ising model with Metropolis algorithm. Finally, i specify problems at phase transition and how to pass it.

Monte Carlo Method

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Statistical approach

- to compute integrals by sampling function values:
  Useful for large dimensional integrals
- for statistical physics problems:
  to analyze properties of large systems with using limited states of the system
- requires generation of pseudo-random numbers

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Statistical approach
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  Useful for large dimensional integrals
- for statistical physics problems:
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Monte Carlo method is a statistial approach to compute large dimensinal integrals by using sampling function values and it is also used to simulate statistical physics problems, to analyze properties of large systems with using limitied states of the system. It requires generation of pseudo-random numbers to sample states.

Estimation of Expected Value

For Maxwell-Boltzmann dist. expected value of Q;

$$\langle Q \rangle = \frac{\sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}} \qquad \beta = 1/kT \tag{1}$$

Sampling the following probability with the Monte Carlo method

$$P_{\mu} = Z^{-1} e^{-\beta E \mu}, \qquad Z = \sum_{\mu} e^{-\beta E_{\mu}} \tag{2}$$

the estimator of the above expected value is;

$$Q_M = \frac{1}{M} \sum_{i=1}^{M} Q_{\mu i} \tag{3}$$

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If we want to calculate expected value of a property of a system, which obeys MB dist., we should consider all states of system. But, it is hard to do for large systems.
Monte Carlo method estimates expected value of this quantity with choosing states of system in a proba. dist. P mu. Also, it is obvious that if Pmu is in the form of MB dist, we get better approx as in (2). Z is a normalization cst. and it is called canonical partition fnct. In this case, estimation of expected value is (3).

Markov Process and Equilibrium Prob. Dist.

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- Transition probability $P(\mu \to \nu)$ depends only on μ and ν:

$$\sum_{\nu} P(\mu \to \nu) = 1 \tag{4}$$

- Markov Chain: Repeated Markov Processes.
  By choosing $P(\mu \to \nu)$ obtain the desired distribution in a long run
- Equilibrium condition:

$$\sum_{\nu} P_{\mu} P(\mu \to \nu) = \sum_{\nu} P_{\nu} P(\nu \to \mu) \tag{5}$$

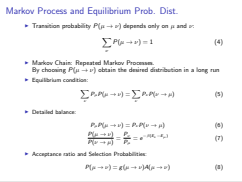
- Detailed balance:

$$P_{\mu} P(\mu \to \nu) = P_{\nu} P(\nu \to \mu) \tag{6}$$

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{P_{\nu}}{P_{\mu}} = e^{-\beta(E_{\nu} - E_{\mu})} \tag{7}$$

- Acceptance ratio and Selection Probabilities:

$$P(\mu \to \nu) = g(\mu \to \nu) A(\mu \to \nu) \tag{8}$$



To generate states obeying MB dist, we can use Markov Chain sampling. Suppose that, we are in a state mu and we consider a move to another state nu, then probability to move from mu to nu is called transition prob. and it only depends on these 2 states. Also, it is logical that sum of probs. to move another state and staying same state is 1. This move between states is called MARKOV PROCESS: If we repeat MPR, we get MARKOV CHAIN. When MCR runs for long enough, we generate states which obey MB dist. However, we have to define some conditions for it.
Firstly, if we want to get a stable distribution at the end of MCR, we should achieve equilibrium.Equilibrium condition states that, transitions into a state and out of that state must be equal and it means that our probability distribution of states after equilibrium is achieved will be a stable distribution, because after equilibrium, probability distribution will not change on average. Also, to achieve desired MB distribution after getting a stable distribution, we have to satisfy detailed balance condition in (6). If we look at detailed balance condition, it also includes equilibrium condition. Hence, if detailed balance is satisfied, then equilibrium condition will also be satisfied.
Hence, if we satisfy equation (4) and (7), we will create states with MB dist.

The Ising Model

- Model of magnetization of a material.
- Spins are +1 or -1.
- Hamiltonian is,

$$\mathrm{H} = -J \sum_{<i,j>} s_i s_j - H \sum_i s_i \qquad (9)$$

Ising model is a model of magnetization of a material. Magnetization is formed by spins in the material which can be up(1) or down(-1). In the model spins are interacting with each other. In our case: Interaction occurs in only nghd spins. Hamiltonian of the model is (12).
// yok // J is interaction energy. s_i is a spin of system. $< i, j >$ represents sum of nghd spins. We can see that interaction occurs in only nghd spins. H is external magnetic field on spins.

1. Wait a period of time called equilibration time, τ_{eq}.
2. Analyze with independent samples. Autocorrelation function falls of exponential,
$$\chi(t) \sim e^{-t/\tau} \tag{10}$$
3. Define errors in calculations.

- Blocking Method: Data is divided into several blocks.
$$\sigma = \sqrt{\frac{1}{n-1}(\langle q^2 \rangle - \langle q \rangle^2)} \tag{11}$$
- Jackknife Method: Using n-1 data.
$$\sigma = \sqrt{\sum_{i=1}^{n}(q_i - q)^2} \tag{12}$$

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To analyze system's properties, firstly we have to wait to get equilibration. Secondly, we should use states which are independent from each other for analyze of system properties. To get independent states, we have to wait a period of time between two independent state, this period of time is called Correlation time τ. We can find correlation time with using autocorrelation function , $\chi(t)$. It is in the form of (11) for early times.
Finally, errors in our calculations should be defined. To calculate errors in our calculation, there are a lot of method exist. But we look at only 2 of them:
Blocking Method: // anlat sadece denklemi acklama
In the Blocking Method, data is divided in to several blocks with several samples and for each block, mean of that quantity is calculated in each block which is labelled as q in equation. n is block number
Jackknife: // anlat sadece denklemi acklama
When calculating a quantity, n independent samples are used. In the Jackknife method, that quantity is calculated again with using n-1 samples by removing first, second, ... ith independent sample, respectively, if quantities are labeled as qi with ith sample removed. q is the quantity calculated with n samples.

Structure of Metropolis Algorithm

A single-spin-flip algorithm.
Selection probability is same for all accessible N states,

$$g(\mu \to \nu) = \frac{1}{N} \qquad (13)$$

Then, to satisfy detailed balance condition,

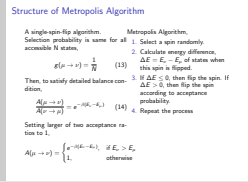
$$\frac{A(\mu \to \nu)}{A(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)} \qquad (14)$$

Setting larger of two acceptance ratios to 1,

$$A(\mu \to \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)}, & \text{if } E_\nu > E_\mu \\ 1, & \text{otherwise} \end{cases}$$

Metropolis Algorithm,

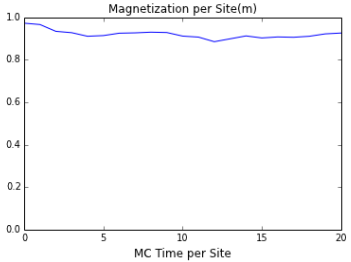
1. Select a spin randomly.
2. Calculate energy difference, $\Delta E = E_\nu - E_\mu$ of states when this spin is flipped.
3. If $\Delta E \leq 0$, then flip the spin. If $\Delta E > 0$, then flip the spin according to acceptance probability.
4. Repeat the process



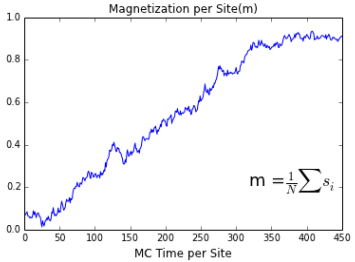
Metropolis algorithm is a single-spin-flip algorithm. It means that in each step of Metropolis algorithm, we try to flip only 1 spin.
For Ising model, which has N spins, probability to create any state is same for all accessible states. To satisfy detailed balance condition and to create states with MB dist. eq (14) should be satisfied.
We want to accept states as much as possible. Hence, to maximize acceptance ratios, we set larger of the acceptance ratios to 1.
In Metropolis algorithm, after defining initials spins, we select a spin randomly and we calculate energy difference between states when spin is flipped and we flip the spin according to acceptance probability. Then, we repeating this procedure, we get a succession of states.
// en alttaki fonksiyonu acklama sadece en yuksek olmas iin bu sekilde olmal de.

Equilibration Time

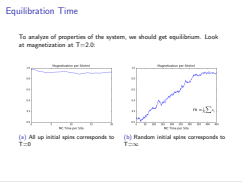
To analyze of properties of the system, we should get equilibrium. Look at magnetization at T=2.0:



(a) All up initial spins corresponds to T=0



(b) Random initial spins corresponds to T=∞



Let's look at equilibration times at T=2.0. If we start simulation with all spins up, which corresponds to T=0 case, we will reach equilibrium after about 5 MC time per site. Also, if we start simulation with random spins which corresponds to T=∞ case, we will reach equilibrium after about 350 MC time per site. Therefore, we can see that if our initial temperature, that we start the simulation, is close to our systems temperature we will get equilibrium faster.

Autocorrelation Function and Correlation Time

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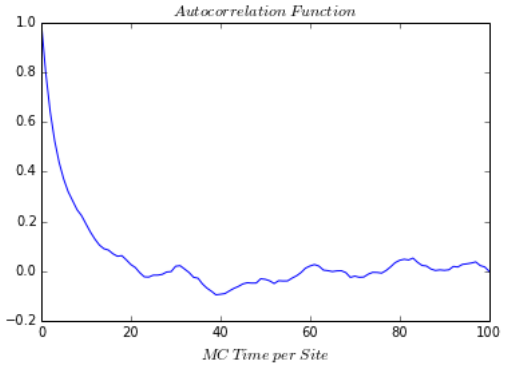
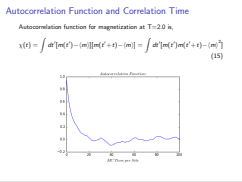
Autocorrelation function for magnetization at T=2.0 is,

$$\chi(t) = \int dt'[m(t')-\langle m\rangle][m(t'+t)-\langle m\rangle] = \int dt'[m(t')m(t'+t)-\langle m\rangle^2] \quad (15)$$





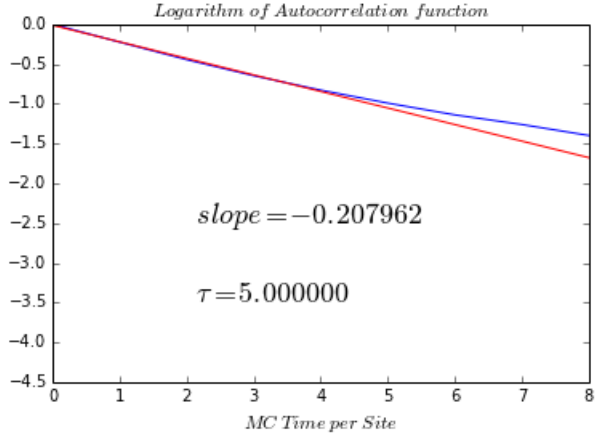
To find correlation time, we should look at autocorrelation function. Autocorrelation function gives correlation of two different values of magnetization with t time difference. We can see that if time between states is small, magnetizations are same and fluctuations are in the same direction. Hence, with summing them for all times, we get high positive autocorrelation value. And if t is large, it means that we change a lot of spins between these 2 calculations, hence, magnetizations are different and fluctuations of magnetizations are different. Hence, autocorrelation is around 0. If autocorrelation function is not equal to 0 the fluctuations are correlated, on average.

// autocorrelation function acklama. sadece 2 propertnin fluctuationlar arasndaki correlation verir de.

//Actually, autocorrelation is calculated by integrating over an infinite time. //ama yok infinite gibi yapmak iin son magnetization degerlerini //bastakiler ile iliskilendirdik. bu yuzden sonlarda autocorrelation artt //tekrar.

Fitting autocorrelation function for early times,

$$\chi(t) \sim e^{-t/\tau} \qquad log(\frac{\chi(\tau)}{\chi(0)}) = \frac{-t}{\tau} \tag{16}$$

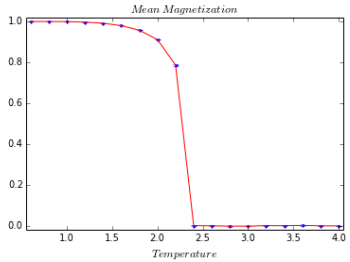


We know that autocorrelation is exponentially decaying function. Hence, if we normalize it, taking logarithm of it we can find correlation time by fitting a line.

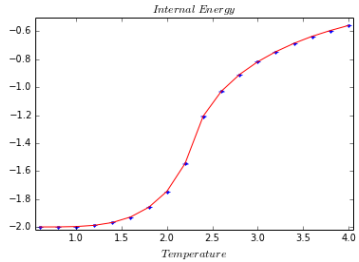
System Properties

$$\langle m \rangle = \frac{1}{N} \left\langle \sum_i s_i \right\rangle \qquad (17)$$

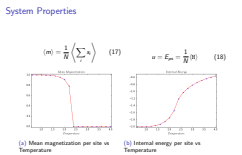
$$u = E_{ps} = \frac{1}{N} \langle \mathrm{H} \rangle \qquad (18)$$



(a) Mean magnetization per site vs Temperature

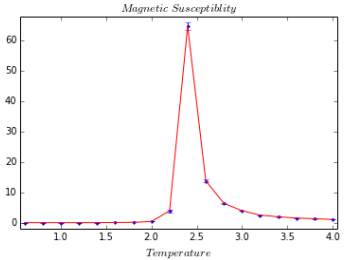


(b) Internal energy per site vs Temperature

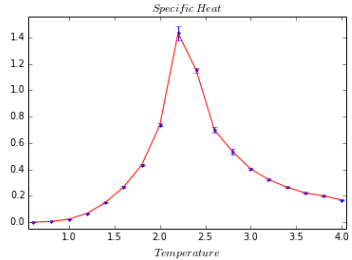


If we look at the plot, mean magnetization is 1 when T=0 and 0 when T= as we expected. Also, if we increase the temperature from 0, we see that magnetization is about 1 until T is around 2.2. Also, if we keep on increasing the temperature, we will see a sharp decrease in magnetization to 0. This sharp change around when T is around 2.2 is called Phase Transition. Again, we see that a change in internal energy of the system when T is around 2.2. This is also caused by phase transition.
// direkt sharp olacakt ama finite size.

$$\chi = \beta N[\langle m^2 \rangle - \langle m \rangle^2] \qquad (19) \qquad c = k\beta^2 N[\langle E_{ps}^2 \rangle - \langle E_{ps} \rangle^2] \qquad (20)$$



(a) Magnetic suscept. vs Temperature



(b) Specific heat vs Temperature

Lets look at fluctuations in magnetization and energy, which are magnetic susceptibility and specific heat of the system.
We can see that fluctuations in the magnetization and energy is diverged at the temperature of phase transition. Hence, we see a peak at that temperature.
Also, because of this increased fluctuations at the phase transition and increased correlation times at phase transition our error bars are increased

Look at correlation times:

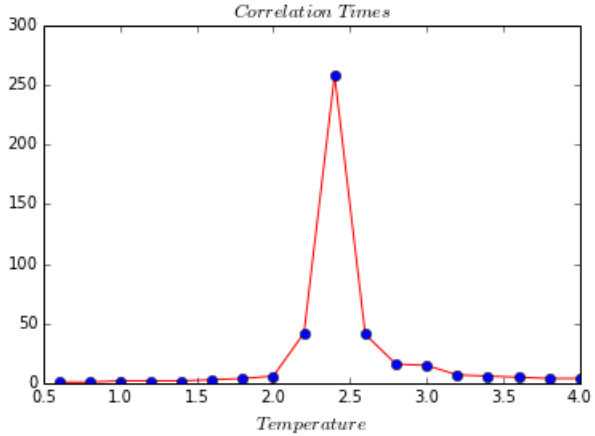


Figure : Correlation time vs Temperature

When phase transition occurs, our correlation times, states times between independent states, are diverged. Hence, because of that it is hard to simulate system around phase transition. Because, to get a lot of independent samples, we have to wait for a long time. Also, these increase in correlation time causes us to get a small number of independent samples; hence,causes increased error bars at the phase transition.
correlation time artar az veri ve fluctuationdan dolay hata artar.

Occurs at Critical temperature T_c.
For 2D Ising model, $T_c \approx 2.269$
Property of Ising Model
Causes critical fluctuations
When we approach to phase transition correlation length increases.
Reduced temperature, t, is

$$t = \frac{T - T_c}{T_c} \tag{21}$$

For Ising model, divergence of correlation length near phase transition goes like

$$\xi \propto |t|^{-\nu} \tag{22}$$

ν is critical exponent. Correlation Time per site

$$\tau \propto |t|^{-z\nu} \propto \xi^z \tag{23}$$

z is dynamic exponent.

Now, suppose we are at high temperatures where spins are random and uncorrelated. If we decrease temperature, interaction between spins forces spins to be in same direction. Hence, spins become correlated. Spin groups which are correlated because of these effect are called clusters and size of clusters are , correlation length. This is because of the nature of the Ising model.
Hence, when we flip a spin at critical temperature, these clusters will flip, because spins inside it are correlated, hence, we see fluctuations in magnetization and energy. and one of the error sources in critical region is these fluctuations.
When T is closer to critical temperature large regions of spins are in same direction. This regions are called domains. When T = Tc, there is about 3 percent chance to flip a spin inside a domain. Therefore, for Metropolis algorithm it is difficult to flip a spin because it tries to flip spin by spin. Because of that, correlation time is getting bigger at phase transition, this is called critical slowing down. Hence, other error source in critical region is correlation time.
Hence, we can find a way to decrease correlation times to increase accuracy. We define reduced temperature, absolute value of it gives how much we differ

Wolff Algorithm

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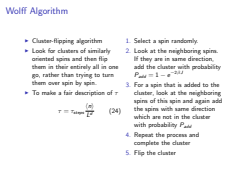
- Cluster-flipping algorithm
- Look for clusters of similarly oriented spins and then flip them in their entirely all in one go, rather than trying to turn them over spin by spin.
- To make a fair description of τ

$$\tau = \tau_{steps} \frac{\langle n \rangle}{L^d} \qquad (24)$$

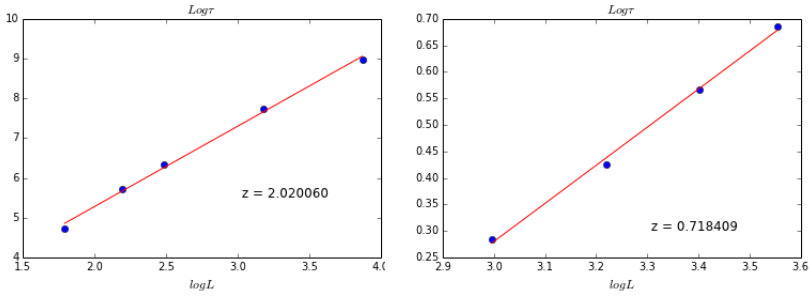
1. Select a spin randomly.
2. Look at the neighboring spins. If they are in same direction, add the cluster with probability $P_{add} = 1 - e^{-2\beta J}$
3. For a spin that is added to the cluster, look at the neighboring spins of this spin and again add the spins with same direction which are not in the cluster with probability P_{add}
4. Repeat the process and complete the cluster
5. Flip the cluster



In metropolis algorithm we flip only 1 spin and at critical temperature it is hard to flip a spin inside domain. But, chance of flip a spin at the edge of a domain is high because it has opposite spins in its neighbourhood, hence lower energy cost. The basic idea of Wolff algorithm is to look for clusters of similarly oriented spins and then flip them in their entirely all in one go, rather than trying to turn them over spin by spin. Hence, with using Cluster algorithms we can reduce critical slowing down.
// algoritmay oku zaman kalrsa
In Wolff algorithm we flip spins in a cluster. If there is n spins in a cluster, we flip n spins. Also, in Metropolis algorithm we flip 1 spin. Hence, to make a fair description of correlation time, this difference must be considered.
To make a fair description of tau –¿ we can calculate correlation times in the form of eqn (24)

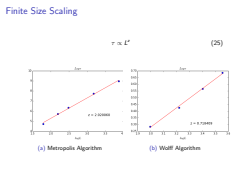
Finite Size Scaling

$$\tau \propto L^z \tag{25}$$



(a) Metropolis Algorithm

(b) Wolff Algorithm



At T=Tc, cluster size diverges, but we are in a finite size system. Hence max. value of cluster size is L. Then correlation time is in the form of eq (25) at phase transition.

We found that z = 2.02 for metropolis algorithm and z=0.72 for wolff algorithm. hence we can expect that correlation time can be decreased with using a cluster size algorithm.