Modelling of Complex Systems

Phase transitions

Simulation of the Ising model

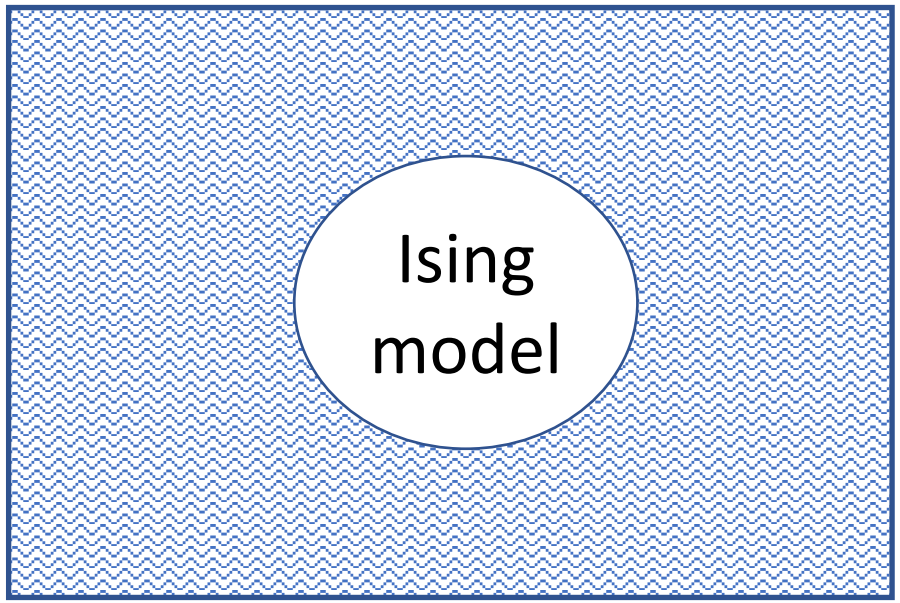
The Metropolis algorithm

Relaxation dynamics

Finite-size effects and fluctuations

Introduction

Let us consider the that our system of spins (Ising model) is in contact with a thermal reservoir.



The system's state is fully characterized by the configuration of the spins

$$\vec{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_N)$$

where $\sigma_n = \pm 1$, and N is the number of spins.

Introduction

The interaction between the system and the bath results in a sequence transitions from one microstate (spin configuration) to another microstate.

Let us numerate these microstates by the index $i = 1,2,3, \ldots$.

We have the sequence (random walks in the space of spin configurations):

$$\vec{\sigma}^{(1)} \rightarrow \vec{\sigma}^{(2)} \rightarrow \ldots \rightarrow \vec{\sigma}^{(i)} \rightarrow \ldots$$

Given a physical quantity $A(\vec{\sigma})$ that depends on the spins σ_n (for example, energy, magnetization, susceptibility, etc), we can calculate its mean value averaging over the microstates:

$$\langle A \rangle = \frac{1}{M} \sum_{i=1}^{M} A(\vec{\sigma}^{(i)})$$

where M is the number of visited microstates.

Introduction

For example, the magnetization (mean magnetic moment) is:

$$\langle m \rangle = \left\langle \frac{1}{N} \sum_{n=1}^{N} \sigma_n \right\rangle = \frac{1}{M} \sum_{i=1}^{M} \left(\frac{1}{N} \sum_{n=1}^{N} {\sigma_n}^{(i)} \right)$$

$$= \frac{1}{N} \sum_{n=1}^{N} \left(\frac{1}{M} \sum_{i=1}^{M} {\sigma_n}^{(i)} \right) = \frac{1}{N} \sum_{n=1}^{N} \langle \sigma_n \rangle$$

In equilibrium (with the bath), we can find the probability $P(\vec{\sigma})$ that the system is in a microstate $\vec{\sigma}$. This probability is proportional to the number of times that the system visits the microstate, $N(\vec{\sigma})$:

$$P(\vec{\sigma}) = \lim_{M \to \infty} \frac{N(\vec{\sigma})}{M} = \frac{e^{-\frac{E(\vec{\sigma})}{k_B T}}}{Z}$$

where $E(\vec{\sigma})$ is the energy of the microstate, and Z is a normalization factor, the so-called partition function.

Introduction

Then, for the average of a quantity $A(\vec{\sigma})$ we can write:

$$\langle A \rangle = \frac{1}{M} \sum_{i=1}^{M} A(\vec{\sigma}^{(i)}) = \frac{1}{M} \sum_{\{\vec{\sigma}\}} N(\vec{\sigma}) A(\vec{\sigma})$$

$$= \sum_{\{\vec{\sigma}\}} P(\vec{\sigma}) A(\vec{\sigma}) = \sum_{\{\vec{\sigma}\}} \frac{e^{-\beta E(\vec{\sigma})}}{Z} A(\vec{\sigma})$$

where $P(\vec{\sigma}) = \frac{N(\vec{\sigma})}{M}$, and $N(\vec{\sigma})$ is the number of times the system visited microstate $\vec{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_N)$.

Introduction

A sidenote: Why is $P(\vec{\sigma}) \propto e^{-\beta E(\vec{\sigma})}$?

If the system consists of two parts A and B, then the microstate of the system

$$\vec{\sigma}_{A+B} = (\vec{\sigma}_A, \vec{\sigma}_B).$$

Moreover, if A and B do not interact with each other, then we expect

$$E(\vec{\sigma}_{A+B}) = E(\vec{\sigma}_A) + E(\vec{\sigma}_B),$$

and

$$P(\vec{\sigma}_{A+B}) = P(\vec{\sigma}_A)P(\vec{\sigma}_B).$$

Assuming the probability of a microstate only depends on the energy

$$P(\vec{\sigma}_{A+B}) = P\big(E(\vec{\sigma}_{A+B})\big) = P\big(E(\vec{\sigma}_A)\big)P\big(E(\vec{\sigma}_B)\big).$$

For this equation to be satisfied the probability $P(E)$ must be an exponential function of the energy E, that is:

$$P\big(E(\vec{\sigma})\big) = \frac{e^{-\beta E(\vec{\sigma})}}{Z}$$

Detailed balance

Let us denote by $w_{\alpha\to\alpha'}$ the probability of a transition from the microstate α to the microstate α'.

Then, the transition from α to α' occurs at the frequency $P(\alpha)w_{\alpha\to\alpha'}$.

The detailed balance condition assumes that in equilibrium (with the thermal reservoir) frequency of transitions from α to α' is equal to the frequency of transitions from α' to α. That is

$$P(\alpha)w_{\alpha\to\alpha'} = P(\alpha')w_{\alpha'\to\alpha}.$$

Then, we can express the ratio of probabilities as

$$\frac{w_{\alpha\to\alpha'}}{w_{\alpha'\to\alpha}} = \frac{P(\alpha')}{P(\alpha)} = \frac{e^{-\beta E_{\alpha'}}}{e^{-\beta E_{\alpha}}} = e^{-\beta\left(E_{\alpha'}-E_{\alpha}\right)} = e^{-\beta\Delta E_{\alpha\to\alpha'}}$$

The detailed balance condition is satisfied as long as the transition probabilities follow this ratio, which is determined by the energy difference

$$\Delta E_{\alpha\to\alpha'} = E_{\alpha'} - E_{\alpha}.$$

Metropolis algorithm

The simplest way to achieve detailed balance between transition frequencies is given by the Metropolis algorithm.

First, this algorithm proposes a new microstate picked at random. Then it accepts the new state with the following probability

$$w_{\alpha\to\alpha'} = \begin{cases} 1 & \text{if } E_{\alpha'} \le E_{\alpha}, \\ e^{-\beta \Delta E_{\alpha\to\alpha'}} & \text{if } E_{\alpha'} > E_{\alpha}. \end{cases}$$

Notice that, the acceptance probability for the reverse transition $\alpha' \to \alpha$ is

$$w_{\alpha'\to\alpha} = \begin{cases} e^{-\beta \Delta E_{\alpha'\to\alpha}} & \text{if } E_{\alpha'} < E_{\alpha}, \\ 1 & \text{if } E_{\alpha'} \ge E_{\alpha}. \end{cases}$$

Therefore, these acceptance probabilities satisfy detailed balance condition:

$$\frac{w_{\alpha\to\alpha'}}{w_{\alpha'\to\alpha}} = e^{-\beta \Delta E_{\alpha\to\alpha'}}.$$

Metropolis algorithm

In the limit of an infinite number of transitions, the probability distribution over microstates will be the Boltzmann distribution because

$$\frac{P(\alpha')}{P(\alpha)} = \frac{w_{\alpha\to\alpha'}}{w_{\alpha'\to\alpha}} = e^{-\beta\left(E_{\alpha'}-E_{\alpha}\right)},$$

$$\Rightarrow P(\alpha)e^{\beta E_{\alpha}} = P(\alpha')e^{\beta E_{\alpha'}} = \text{const.}$$

$$\Rightarrow P(\alpha) \propto e^{-\beta E_{\alpha}}$$

Then the probability of finding the system in state α is

$$P(\alpha) = \frac{e^{-\beta E_{\alpha}}}{Z},$$

where the partition function $Z = \sum_{\alpha} e^{-\beta E_{\alpha}}$.

Metropolis algorithm

Furthermore, the basic process in a spin system is the rotation of a single spin:

$$(\sigma_1, \sigma_2, \dots, \sigma_n, \dots, \sigma_N) \longrightarrow (\sigma_1, \sigma_2, \dots, -\sigma_n, \dots, \sigma_N).$$

That is, we assume transitions between microstates are only due to the local change of the state of one spin: $\sigma_n \longrightarrow -\sigma_n$.

This idea is based on the notion that the simultaneous rotation of multiple spins is a very unlikely event.

Thus, our algorithm generates candidates for the next microstate by rotating a single spin on the current microstate.

Transitions between two microstates that differ by more than one spin state are not allowed, which is also a form of detailed balance:

$$P(\alpha)w_{\alpha\to\alpha'} = P(\alpha')w_{\alpha'\to\alpha} \Rightarrow P(\alpha)\times 0 = P(\alpha')\times 0$$

Dynamics

Assuming that every configuration has the same mean duration τ_0, we can introduce time as $t = \tau_0 M$, where M is the number of transitions.

The time scale τ_0 is determined by interaction between the thermal reservoir and the system of spins.

This allows us to analyse the relaxation dynamics and find the relaxation time t_r, which determines the rate at which the system approaches equilibrium:

$$\Delta m \propto e^{-\frac{t}{t_r}},$$

where Δm is the deviation of the magnetic moment from its value at equilibrium.

There is, however, an exception to this kind exponential relaxation.

Dynamics

Theoretical analysis of the relaxation time shows that when a magnetic system approaches the critical temperature T_c the relaxation time diverges as

$$t_r \propto \frac{1}{|T - T_c|}.$$

This phenomenon is known as *critical slowing down*.

Exactly at the critical point we have $t_r = \infty$, which mean that the system relaxes not exponentially, but following a power-law

$$\Delta m \propto \frac{1}{t^z},$$

where z is a dynamical exponent.

These results mean that the closer we are to T_c the longer the system will take to reach the equilibrium state.

Dynamics

The effect of critical slowing down leads to deviations of the simulations from the theoretical formulas that were derived for an infinite number of microstates, especially near the critical point.

Therefore, this phenomena should be taken into account in our simulations by increasing the number of microstates (that is, the number of Monte Carlo steps) when approaching the critical temperature.

Additionally, the *burn-in* period (initial number of samples that are discarded) might also need to be increased.

Finite size effects

All of our analytical results are obtained in the thermodynamic limit, that is the limit of infinite number of spins, $N \to \infty$.

In this limit, there is a critical temperature T_c above which the system is in the disordered state with zero magnetization, and below which the system is in the ordered state with spontaneous magnetization (for $D > 1$).

The divergence of the susceptibility χ signals the continuous phase transition.

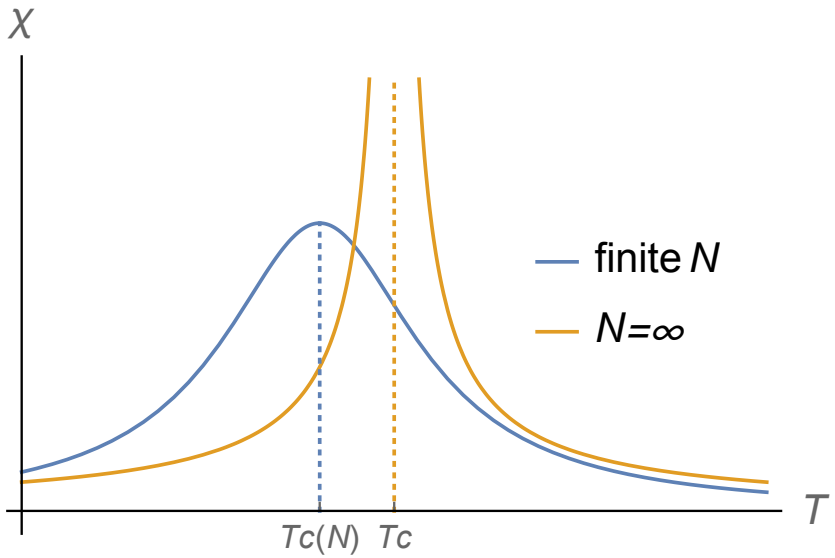
Below T_c the system spends an infinite time in either a state with $m > 0$ (majority of spins up) or in a state $m < 0$ (majority of spins down).

Finite size effects

However, if the number of spins N is large but finite, then the lifetime of these states is also large but finite.

This means that the system can spontaneously jump from the state with up magnetization ($m > 0$) to the state with down magnetization ($m < 0$).

In finite systems, the susceptibility does not really diverge at the critical point, instead it has a maximum. Furthermore, the critical point (i.e. position of this maximum) is shifted to the left, that is, $T_c(N) < T_c(\infty)$.



It is the fluctuations of the magnetization that break down the phase transition

Fluctuations

Recall that we defined the susceptibility as $\chi \equiv \frac{d\langle m \rangle}{dH}$ (i.e., as a response function). However, we can show that it has a deeper meaning: χ actually quantifies the fluctuations of the magnetization $\langle m^2 \rangle - \langle m \rangle^2$.

$$\frac{d\langle m \rangle}{dH} = \frac{d}{dH} \sum_{\{\vec{\sigma}\}} \frac{m(\vec{\sigma}) e^{-\frac{E(\vec{\sigma},J,H)}{T}}}{Z} = \sum_{\{\vec{\sigma}\}} \left[-\frac{dE}{dH} \frac{m\, e^{-\frac{E}{T}}}{TZ} - \frac{m\, e^{-\frac{E}{T}}}{Z^2} \frac{dZ}{dH} \right]$$

$$= \left[\sum_{\{\vec{\sigma}\}} N \frac{m^2 e^{-\frac{E}{T}}}{TZ} \right] - \frac{\langle m \rangle}{Z} \frac{dZ}{dH} = \frac{N}{T} (\langle m^2 \rangle - \langle m \rangle^2)$$

$$\Rightarrow \quad \chi = \frac{N}{T} (\langle m^2 \rangle - \langle m \rangle^2)$$