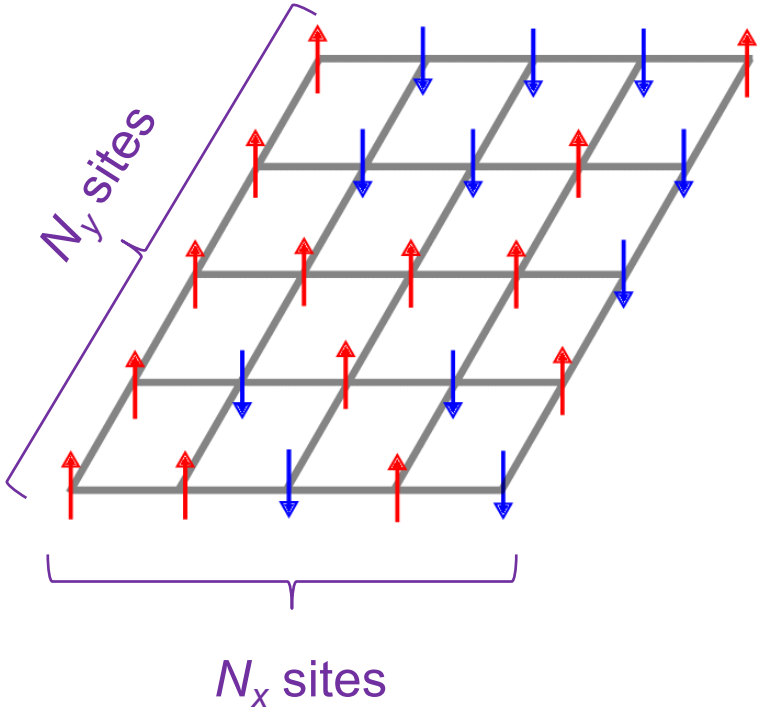
Course 12/1

Monte Carlo simulation of 2D spin systems

- Model of spins in 2D
- Physical quantities of interest
- Physics of Ising model
- Application of Metropolis algorithm
- Trial move and computational effort
- Numerical problems

Model of spins in 2D



System

Two-dimensional grid of N spins: $N = N_x \times N_y$

In every site α, there is one spin: $S_\alpha = \pm 1$

Periodic boundary conditions

Configurations

Number of configurations: $2 \times 2 \times \ldots \times 2 = 2^N$

Example: for $N_x = N_y = 16$, this gives $2^{256} \approx 10^{77}$

A configuration is denoted $\vec{S} = \{ S_\alpha \}_{\alpha = 1,\ldots N}$

Energy of a configuration

$$\mathcal{H} = -J \sum_{\langle \alpha \beta \rangle} S_\alpha S_\beta \quad -B \sum_{\alpha} S_\alpha$$

spin-spin interaction

interaction with external field

sum over nearest neighbors only

$J > 0$ ferromagnetism is preferred locally ↑↑, ↓↓

$J < 0$ antiferromagnetism is preferred locally ↑↓, ↓↑

Canonical averages

$$\langle A \rangle = \frac{\sum_{\vec{S}} A(\vec{S}) \exp\left[-\beta \mathcal{H}(\vec{S}) \right]}{\sum_{\vec{S}} \exp\left[-\beta \mathcal{H}(\vec{S}) \right]}$$

$$\beta = \frac{1}{kT}$$

$$= \sum_{\vec{S}} A(\vec{S})\, \omega(\vec{S})$$

where

$$\omega(\vec{S}) = \frac{\exp\left[-\beta \mathcal{H}(\vec{S}) \right]}{\sum_{\vec{S}} \exp\left[-\beta \mathcal{H}(\vec{S}) \right]}$$

Physical quantities of interest

- Average magnetization

$$M = \sum_{\vec{S}} \omega(\vec{S}) \left(\sum_{\alpha} S_{\alpha} \right)$$

Importance sampling with weight function

- Average energy

$$E = \sum_{\vec{S}} \omega(\vec{S}) \mathcal{H}(\vec{S})$$

Importance sampling with weight function

- Magnetic susceptibility

$$\chi = \frac{\partial M}{\partial B}$$

?

- Heat capacity

$$C = \frac{\partial E}{\partial T}$$

?

Magnetic susceptibility

$$\chi = \frac{\partial M}{\partial B} = \frac{\partial}{\partial B} \left(\frac{\sum_{\vec{S}} \left(\sum_{\alpha} S_\alpha \right) \exp\left[-\beta \mathcal{H}(\vec{S}) \right]}{\sum_{\vec{S}} \exp\left[-\beta \mathcal{H}(\vec{S}) \right]} \right)$$

$$= \frac{1}{\mathcal{Z}} \sum_{\vec{S}} \left(\sum_{\alpha} S_\alpha \right) \left(\sum_{\beta} S_\beta \right) \exp\left[-\beta \mathcal{H}(\vec{S}) \right]$$

$$- \frac{1}{\mathcal{Z}^2} \sum_{\vec{S}} \left(\sum_{\alpha} S_\alpha \right) \exp\left[-\beta \mathcal{H}(\vec{S}) \right] \sum_{\vec{S}'} \left(\sum_{\beta} S'_\beta \right) \exp\left[-\beta \mathcal{H}(\vec{S}') \right]$$

$$= \beta \left[\sum_{\vec{S}} \left(\sum_{\alpha} S_\alpha \right)^2 \omega(\vec{S}) - M^2 \right]$$

Variance of the magnetization

Importance sampling with weight function

Heat capacity

$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\left(\frac{\sum_{\vec{S}} \mathcal{H}(\vec{S}) \exp[-\beta \mathcal{H}(\vec{S})]}{\sum_{\vec{S}} \exp[-\beta \mathcal{H}(\vec{S})]} \right)$$

$$= \frac{\sum_{\vec{S}} \mathcal{H}(\vec{S})\, \mathcal{H}(\vec{S}) \exp[-\beta \mathcal{H}(\vec{S})]}{\sum_{\vec{S}} \exp[-\beta \mathcal{H}(\vec{S})]} \frac{k}{(kT)^2}$$

$$\frac{\partial}{\partial T}(-\beta) = \frac{k}{(kT)^2}$$

$$- \frac{1}{\mathcal{Z}^2} \sum_{\vec{S}} \mathcal{H}(\vec{S}) \exp[-\beta \mathcal{H}(\vec{S})] \sum_{\vec{S}'} \mathcal{H}(\vec{S}') \exp[-\beta \mathcal{H}(\vec{S}')] \frac{k}{(kT)^2}$$

$$= \frac{k}{(kT)^2}\left[\sum_{\vec{S}} [\mathcal{H}(\vec{S})]^2 \omega(\vec{S}) - E^2 \right]$$

Importance sampling with weight function

Variance of the energy

Physics of Ising model

Case $B = 0$ and $J > 0$ (ferromagnetic)

$$\mathcal{H} = -J \sum_{\langle \alpha \beta \rangle} S_\alpha S_\beta$$

For $N_x \to \infty$ and $N_y \to \infty$, an exact analytical solution is available (Ising model).

Nevertheless, there is an interest for a numerical approach, since more complicated interactions can be studied.

The energy is invariant for a global spin flip: all $S_\alpha \to -S_\alpha$

Ising model: Low and high temperature regimes

$$\mathcal{H} = -J \sum_{\langle \alpha \beta \rangle} S_\alpha S_\beta$$

Low temperature ($\beta \to \infty$)

All the spins are aligned to minimize the energy.

There two equivalent states because of the global spin flip invariance.

One spin flip involves an important energy difference and is thus unlikely:

$$r = \exp (-8J / kT) \to 0$$

High temperature ($\beta \to 0$)

All Boltzmann factors become 1: $\exp [-E / (kT)] \to 1$.

Every spin remains an equivalent amount of time up and down.

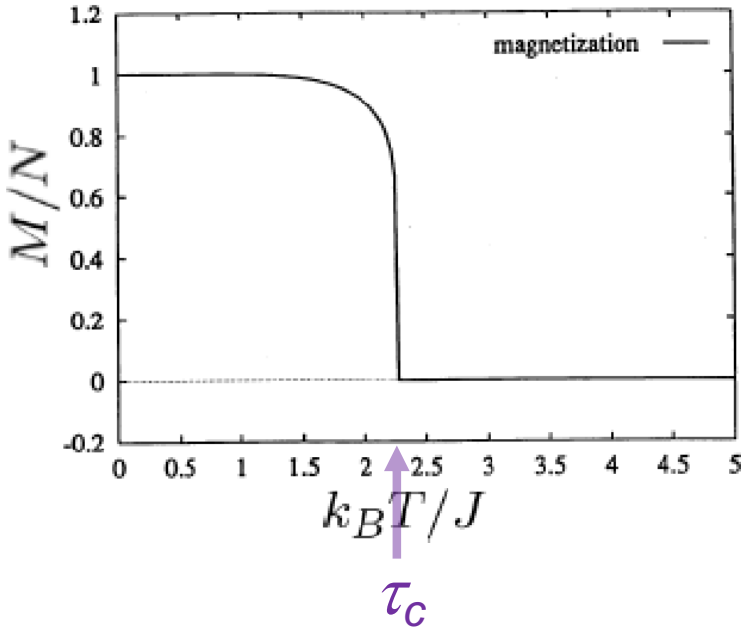
The average magnetization is vanishing.

Ising model: Magnetization

Two possibilities

- Analytic connection between the low and high temperature limits.
- Non-analytic connection between the low and high temperature limits.

  Phase transition



Critical reduced temperature

$$\tau_c = \frac{kT_c}{J} = 2.269$$

https://www.semanticscholar.org/paper/MATH-505-Project-%3A-Ising-model—-Phase-transition-Wu-Li/de75b1ed085ada344a8fe3e28307bbe52ac73b83

Application of Metropolis algorithm

Initial configuration — Random choice for each S_α (appropriate for high T)

Trial move

- Random choice of one spin S_α^n
- Spin flip: $S_\alpha^t = -S_\alpha^n$

Calculation of r

$$r = \frac{\omega(\vec{S}_t)}{\omega(\vec{S}_n)} = \frac{\exp[-\beta \mathcal{H}(\vec{S}_t)]}{\exp[-\beta \mathcal{H}(\vec{S}_n)]}$$

Algorithm

1

$r \geq 1$  Accepted $\vec{S}_{n+1} = \vec{S}_t$

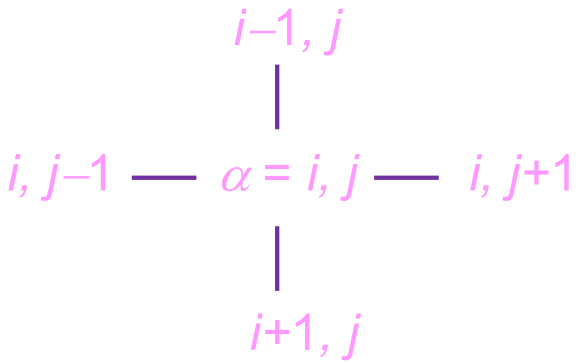
$r < 1$ A random number $\eta \in (0,1)$ is extracted.

2

$\eta \leq r$  Accepted $\vec{S}_{n+1} = \vec{S}_t$

$\eta > r$  Rejected $\vec{S}_{n+1} = \vec{S}_n$

Trial move and computational effort



$$r = \exp\left(-\beta \Delta\mathcal{H} \right)$$

$$\Delta\mathcal{H} = \mathcal{H}(\vec{S}_t) - \mathcal{H}(\vec{S}_n)$$

unchanged for $\alpha \neq (i,j)$

$$= -J S_\alpha^t \left(S_{i+1,j}^t + S_{i-1,j}^t + S_{i,j-1}^t + S_{i,j+1}^t \right) - B S_\alpha^t$$

$$+ J S_\alpha^n \left(S_{i+1,j}^n + S_{i-1,j}^n + S_{i,j-1}^n + S_{i,j+1}^n \right) + B S_\alpha^n$$

Let us define: $f = S_{i+1,j}^n + S_{i-1,j}^n + S_{i,j-1}^n + S_{i,j+1}^n$

Then $\Delta\mathcal{H} = -\left(S_\alpha^t - S_\alpha^n \right)\left(J f + B \right)$

Trial move and computational effort

$$\Delta\mathcal{H} = -\left(S_\alpha^t - S_\alpha^n \right)\left(J f + B \right)$$

For a trial move consisting of a single spin flip: $S_\alpha^t = -S_\alpha^n$

$$\Delta\mathcal{H} = -2S_\alpha^t \left(J f + B \right)$$

only nearest neighbor information

$$r = \exp\left(-\beta \Delta\mathcal{H} \right) = \exp\left[2\beta S_\alpha^t \left(J f + B \right) \right]$$

5 possible values of f : $\{ -4, -2, 0, +2, +4 \}$; 2 possible values of S_α^t : $\{ -1, +1 \}$

$\Rightarrow$ 10 possible values of r (only 5 possible values if $B = 0$).

These values are stored rather than calculated for achieving maximum speed.

Note the advantage of using a trial move consisting of a single spin flip.

Numerical problems

- Finite vs infinite

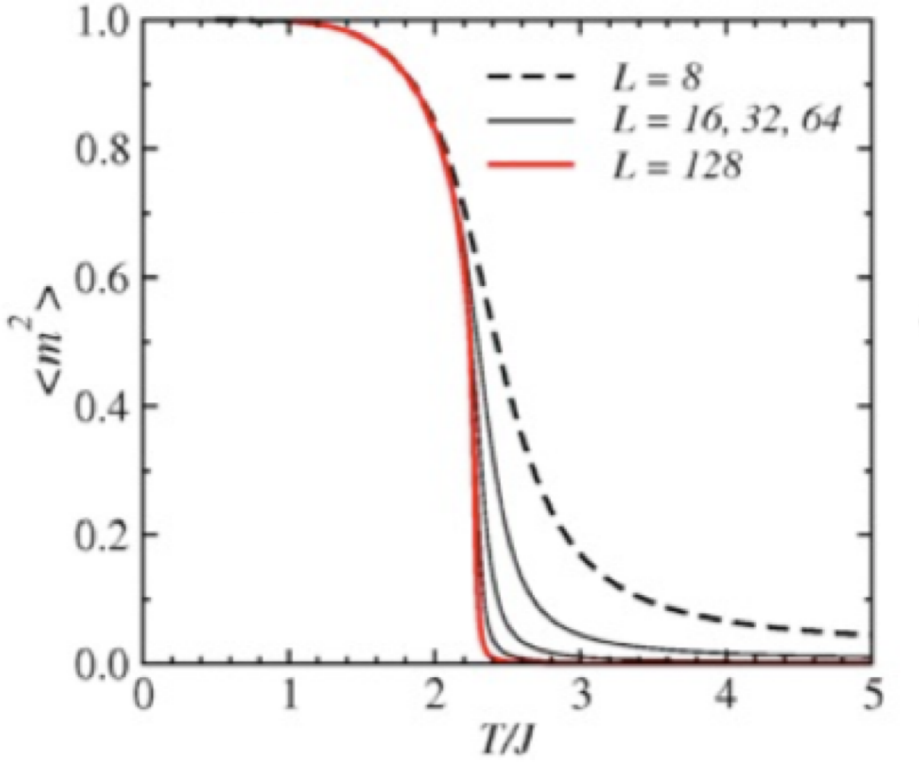
Numerical simulations concern a finite number of spins.

This leads to a continuous curve and the phase transition is not seen.

The limit $N \to \infty$ can only be approached.

Theories have been developed to address the finite-size scaling

http://indico.ictp.it/event/a14246/session/17/contribution/28/material/5/0.pdf

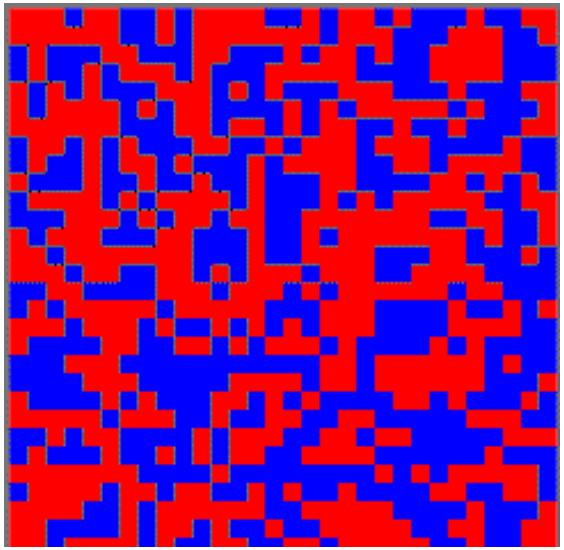


Numerical problems

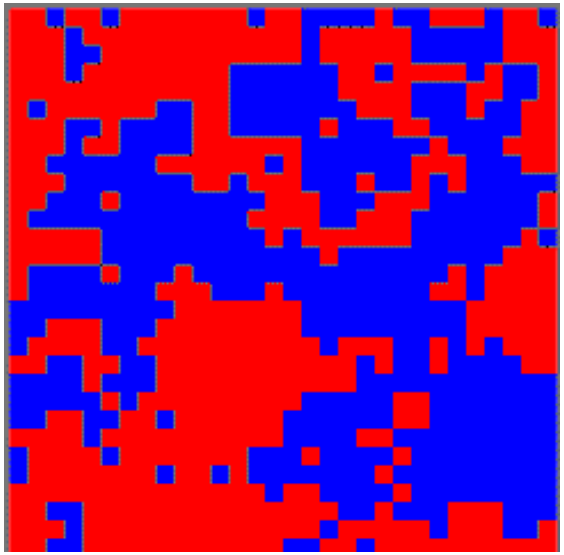
- Limitation associated to single spin-flips

  When starting from a high-T configuration, it might take a long time to reach an ordered state upon crossing the critical temperature.

http://pages.physics.cornell.edu/sss/ising/ising.html



spins at high T



spins near T_c

The slowing down is associated to the trial moves:

Full domains need to be reversed, flipping one spin is an unlikely event.

→ Rejections ↑, correlation time ↑, correlation length ↑

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