

Cluster algorithms for the Ising model

Monte Carlo methods which overcome the problem of critical slowing down close to second order phase transitions

Contents

- ▶ Ising model
- ▶ Single spin flip metropolis
- ▶ Autocorrelation, Binning Analysis
- ▶ Wolff algorithm
- ▶ Swensen-Wang algorithm

Ising model

Ising model

- ▶ Phase transitions

Ising model

- ▶ Phase transitions
- ▶ One of the simplest statistical models that show a phase transition

Ising model

- ▶ Phase transitions
- ▶ One of the simplest statistical models that show a phase transition
- ▶ Magnetic systems, opinion models, binary mixtures

Ising model

- ▶ Phase transitions
- ▶ One of the simplest statistical models that show a phase transition
- ▶ Magnetic systems, opinion models, binary mixtures

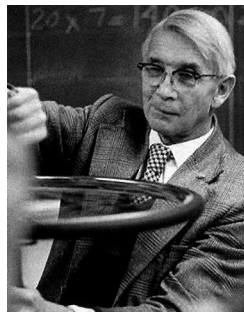


Figure : Ernst Ising (1900 - 1998)

Ising model - Definition

Ising model - Definition

- ▶ Discrete integer spins $\sigma_i = \pm 1$ on each lattice site

Ising model - Definition

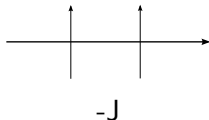
- Discrete integer spins $\sigma_i = \pm 1$ on each lattice site

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$$

Ising model - Definition

- Discrete integer spins $\sigma_i = \pm 1$ on each lattice site

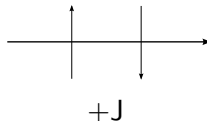
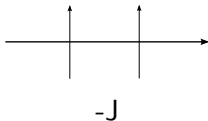
$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$$



Ising model - Definition

- Discrete integer spins $\sigma_i = \pm 1$ on each lattice site

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$$



Ising model - Canonical ensemble

Ising model - Canonical ensemble

$$p(\sigma, T) = \frac{e^{-\beta \mathcal{H}(\sigma)}}{\mathcal{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$

Ising model - Canonical ensemble

$$p(\sigma, T) = \frac{e^{-\beta \mathcal{H}(\sigma)}}{\mathcal{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$

$$\langle M \rangle_T = \sum_{\sigma} M(\sigma) p(\sigma, T)$$

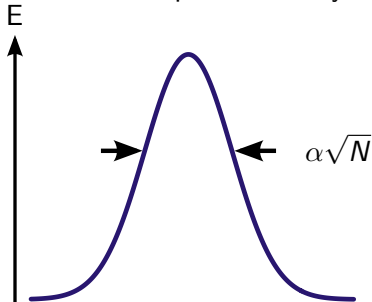
Ising model - Monte Carlo

Ising model - Monte Carlo

- ▶ We can't compute all configurations (2^N)

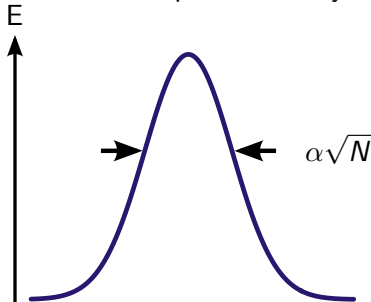
Ising model - Monte Carlo

- ▶ We can't compute all configurations (2^N)
- ▶ We can't sample uniformly distributed over energy



Ising model - Monte Carlo

- ▶ We can't compute all configurations (2^N)
- ▶ We can't sample uniformly distributed over energy



- ▶ Solution: Importance sampling using Metropolis algorithm

Single spin flip metropolis - Algorithm

Single spin flip metropolis - Algorithm

1. Choose one site (uniformly randomly)

Single spin flip metropolis - Algorithm

1. Choose one site (uniformly randomly)
2. Generate new trial configuration Y by flipping spin

Single spin flip metropolis - Algorithm

$$A(X \rightarrow Y) = \min \left(1, \frac{p(Y)}{p(X)} \right)$$

1. Choose one site (uniformly randomly)
2. Generate new trial configuration Y by flipping spin
3. Accept new configuration with transition probability above

Single spin flip metropolis - Algorithm

$$\begin{aligned} A(X \rightarrow Y) &= \min \left(1, \frac{p(Y)}{p(X)} \right) \\ &= \min \left(1, e^{-\beta[E(Y) - E(X)]} \right) \end{aligned}$$

1. Choose one site (uniformly randomly)
2. Generate new trial configuration Y by flipping spin
3. Accept new configuration with transition probability above

Single spin flip metropolis - Results

Single spin flip metropolis - Results

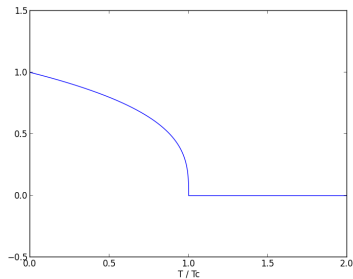
$$\text{Magnetization } M(T) = \left\langle \frac{1}{N} \sum_{i=1}^N \sigma_i \right\rangle_T$$

Single spin flip metropolis - Results

$$\text{Magnetization } M(T) = \left\langle \frac{1}{N} \sum_{i=1}^N \sigma_i \right\rangle_T$$

Expected

Magnetization

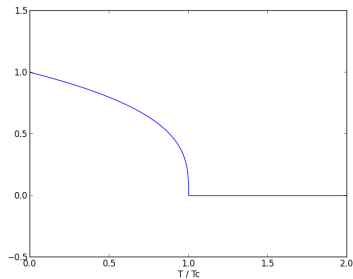


Single spin flip metropolis - Results

$$\text{Magnetization } M(T) = \left\langle \frac{1}{N} \sum_{i=1}^N \sigma_i \right\rangle_T$$

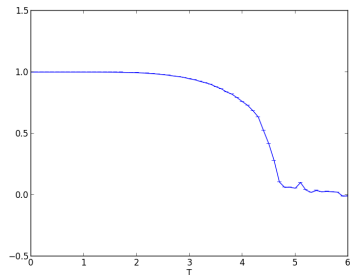
Expected

Magnetization



Obtained

Magnetization



Ising model - 2 spins

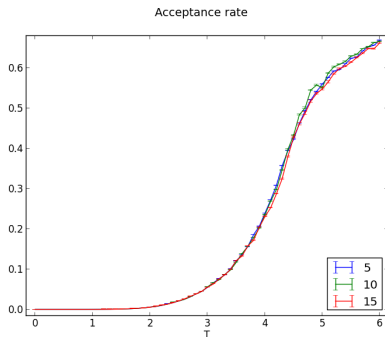
Single spin flip metropolis - To flip or not to flip

Single spin flip metropolis - To flip or not to flip

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

Single spin flip metropolis - To flip or not to flip

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$



Autocorrelation time

Autocorrelation time

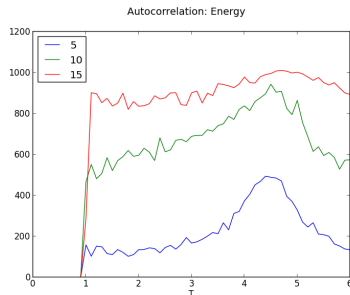
$$\phi_A(t) = \frac{\langle A(t_0)A(t) \rangle - \langle A \rangle^2}{\langle A(t_0)^2 \rangle - \langle A \rangle^2}$$

Autocorrelation time

$$\phi_A(t) = \frac{\langle A(t_0)A(t) \rangle - \langle A \rangle^2}{\langle A(t_0)^2 \rangle - \langle A \rangle^2} \propto e^{-\frac{t}{\tau_A}}$$

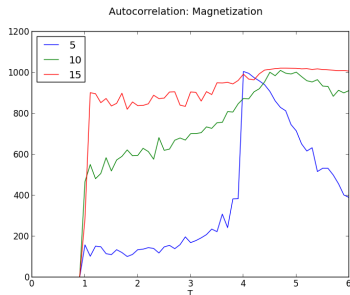
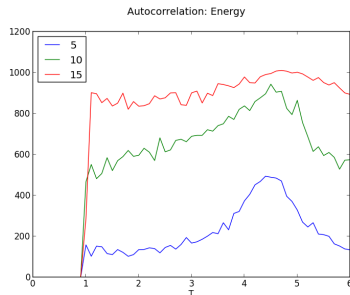
Autocorrelation time

$$\phi_A(t) = \frac{\langle A(t_0)A(t) \rangle - \langle A \rangle^2}{\langle A(t_0)^2 \rangle - \langle A \rangle^2} \propto e^{-\frac{t}{\tau_A}}$$



Autocorrelation time

$$\phi_A(t) = \frac{\langle A(t_0)A(t) \rangle - \langle A \rangle^2}{\langle A(t_0)^2 \rangle - \langle A \rangle^2} \propto e^{-\frac{t}{\tau_A}}$$



Binning analysis I

Binning analysis I

$$\text{Var}X := E[X^2] - E[X]^2$$

Binning analysis I

$$\text{Var}X := E[X^2] - E[X]^2$$

$$(\Delta X)^2 = \frac{\text{Var}X}{N} (1 + 2\tau_X)$$

Binning analysis II

Binning analysis II

$$A_i^{(l)} = \frac{1}{2} \left(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)} \right)$$

Binning analysis II

$$A_i^{(l)} = \frac{1}{2} \left(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)} \right)$$

$$\Delta^{(l)} = \sqrt{\text{Var} A^{(l)} / M^{(l)}} \xrightarrow{l \rightarrow \infty} \Delta = \sqrt{(1 + 2\tau_A) \text{Var} A / M}$$

Binning analysis II

$$A_i^{(l)} = \frac{1}{2} \left(A_{2i-1}^{(l-1)} + A_{2i}^{(l-1)} \right)$$

$$\Delta^{(l)} = \sqrt{\text{Var}A^{(l)} / M^{(l)}} \xrightarrow{l \rightarrow \infty} \Delta = \sqrt{(1 + 2\tau_A) \text{Var}A / M}$$

$$\tau_A = \lim_{l \rightarrow \infty} \left(\frac{2^l \text{Var}A^{(l)}}{\text{Var}A^{(0)}} - 1 \right)$$

What really happens in the System

Cluster algorithms: Wolff algorithm

Cluster algorithms: Wolff algorithm

1. Choose one site (uniformly randomly)

Cluster algorithms: Wolff algorithm

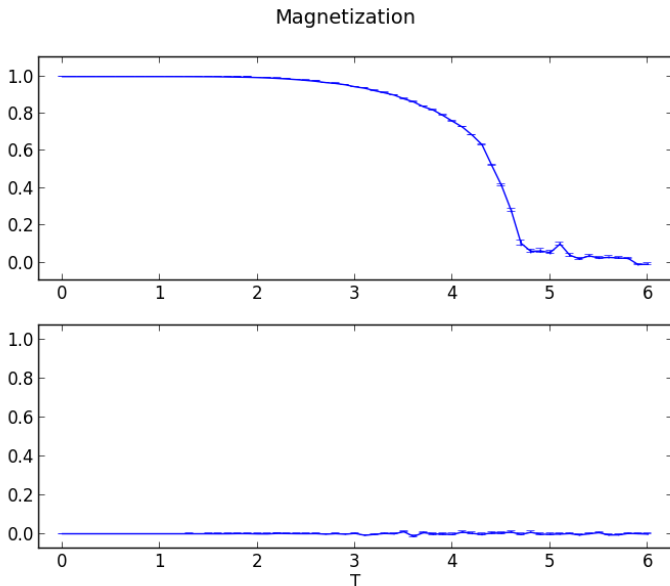
1. Choose one site (uniformly randomly)
2. Flip its spin and add it to the cluster

Cluster algorithms: Wolff algorithm

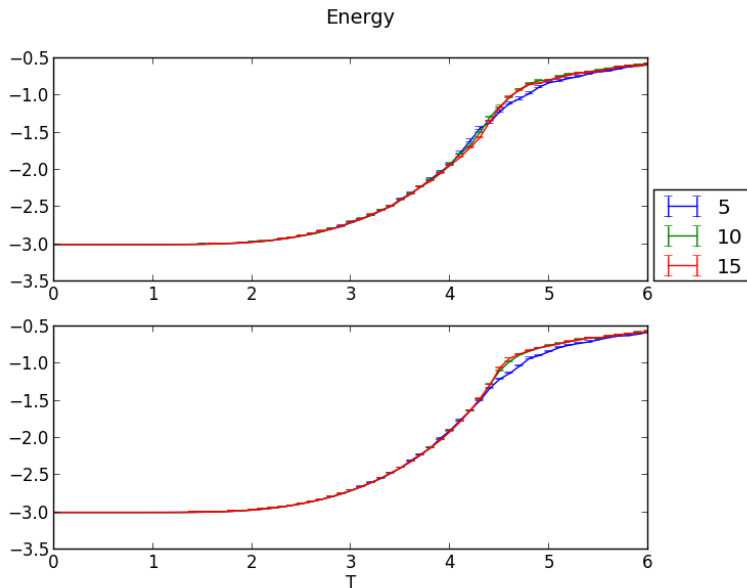
$$P(\sigma_x, \sigma_y) = 1 - \min \left(1, e^{-2\beta\sigma_x\sigma_y} \right)$$

1. Choose one site (uniformly randomly)
2. Flip its spin and add it to the cluster
3. For all sites in the cluster:
 - 3.1 Visit every unknown neighbour, flip its spin and add it to the cluster with probability given above

Why cluster algorithms are better

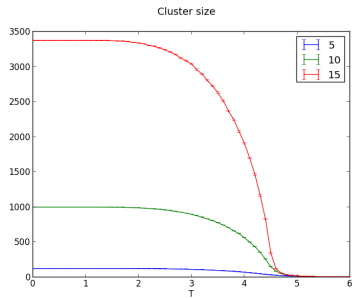


Energy

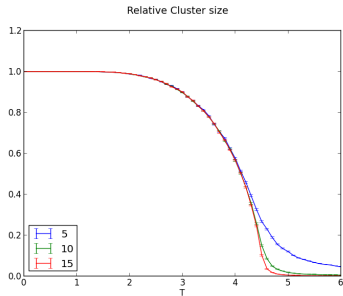
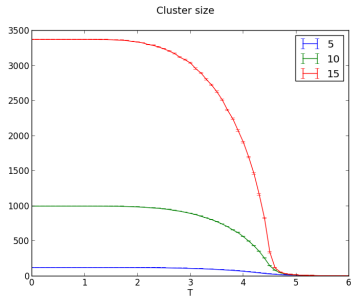


Cluster size

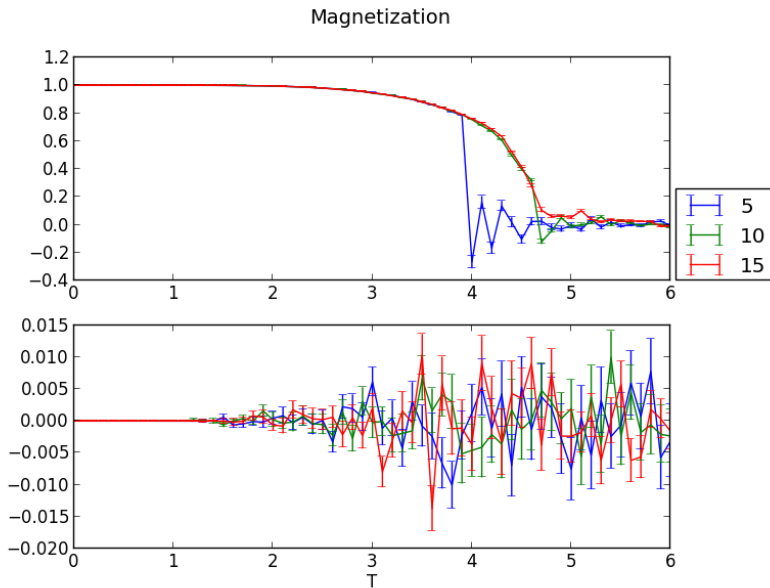
Cluster size



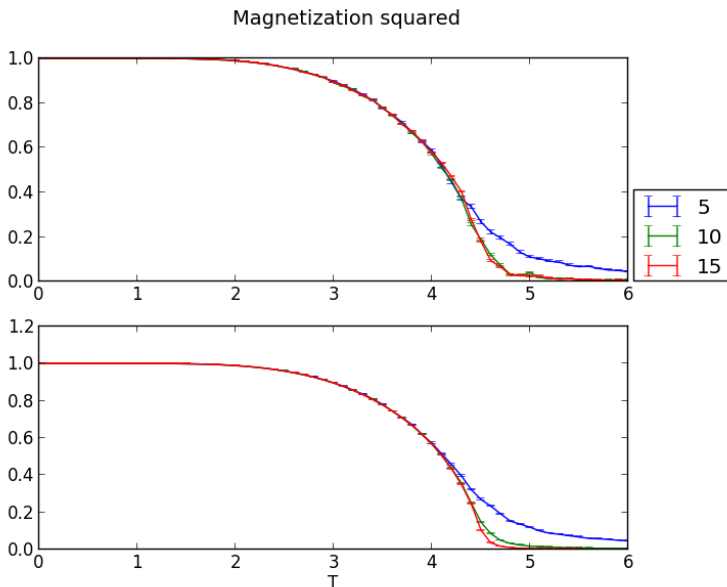
Cluster size



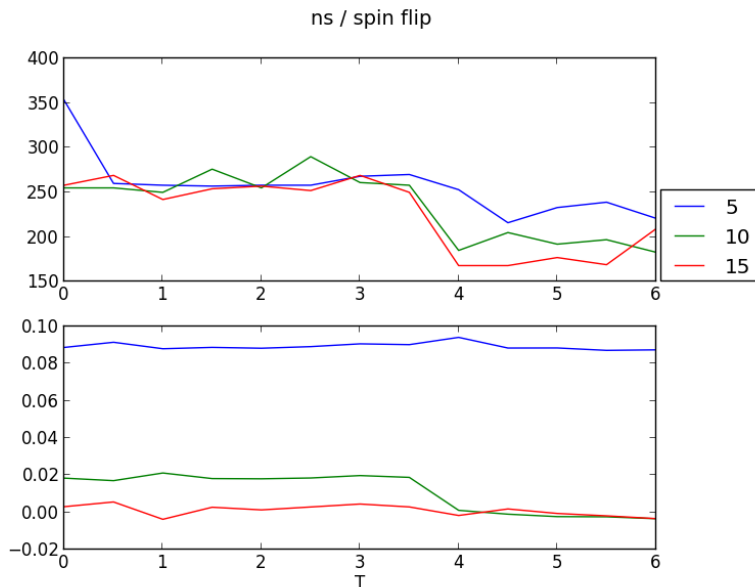
Magnetization



Magnetization squared



Computation time per spin flip



Similar to Wolff, but:

Similar to Wolff, but:

- ▶ Partitions the whole lattice in clusters

Similar to Wolff, but:

- ▶ Partitions the whole lattice in clusters
- ▶ Randomly chooses a new (same) spin for every cluster

Similar to Wolff, but:

- ▶ Partitions the whole lattice in clusters
- ▶ Randomly chooses a new (same) spin for every cluster
- ▶ Always touches every spin

Questions

Binning analysis in detail

$$\text{Var}X := E[X^2] - E[X]^2$$

$$\begin{aligned}(\Delta X)^2 &= \frac{1}{N^2} \sum_{i,j=1}^N \left(E[X_i X_j] - E[X]^2 \right) \\&= \frac{\text{Var}X}{N} + \frac{1}{N^2} \sum_{i \neq j} \left(E[X_i X_j] - E[X]^2 \right) \\&= \frac{\text{Var}X}{N} + \frac{2}{N^2} \sum_{i=1}^N \sum_t \left(E[X_i X_{i+t}] - E[X]^2 \right) \\&:= \frac{\text{Var}X}{N} (1 + 2\tau_X)\end{aligned}$$

Wolff or Swendsen-Wang?

Swendsen-Wang better for parallelization because it touches the whole lattice.