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

Phase transitions

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- Magnetic systems, opinion models, binary mixtures

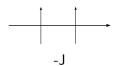
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Figure : Ernst Ising (1900 - 1998)

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

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Ising model - Canonical ensemble

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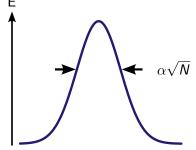
$$p(\sigma, T) = \frac{e^{-\beta \mathscr{H}(\sigma)}}{\mathscr{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$

Ising model - Canonical ensemble

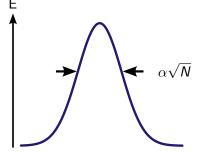
$$p(\sigma, T) = \frac{e^{-\beta \mathcal{H}(\sigma)}}{\mathcal{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$
$$\langle M \rangle_T = \sum_{\sigma} M(\sigma) p(\sigma, T)$$

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

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► Solution: Importance sampling using Metropolis algorithm

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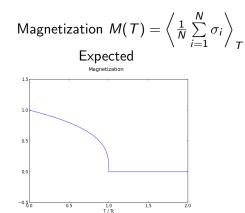
Magnetization
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Expected

Magnetization

1.0 T / Tc

-0.5



Obtained Magnetization 1.5 1.0 0.5 0.0 1.2 3 4 5 6

Ising model - 2 spins

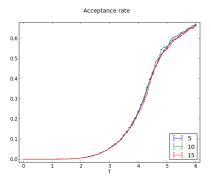
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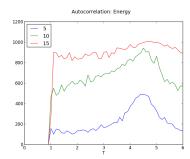
$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$



$$\phi_{\mathcal{A}}(t) = rac{\langle \mathcal{A}(t_0)\mathcal{A}(t)
angle - \langle \mathcal{A}
angle^2}{\langle \mathcal{A}(t_0)^2
angle - \langle \mathcal{A}
angle^2}$$

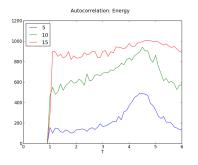
$$\phi_{\mathcal{A}}(t) = rac{\langle \mathcal{A}(t_0)\mathcal{A}(t) \rangle - \langle \mathcal{A} \rangle^2}{\langle \mathcal{A}(t_0)^2 \rangle - \langle \mathcal{A} \rangle^2} \propto \mathrm{e}^{-\frac{t}{\tau_{\mathcal{A}}}}$$

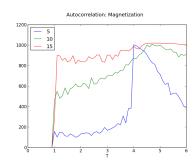
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Autocorrelation time

$$\phi_{A}(t) = rac{\langle A(t_0)A(t)
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$$Var X := E\left[X^2\right] - E\left[X\right]^2$$

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 $(\Delta X)^2 = rac{\mathsf{Var} X}{N} \left(1 + 2 au_X
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$$A_i^{(I)} = \frac{1}{2} \left(A_{2i-1}^{(I-1)} + A_{2i}^{(I-1)} \right)$$

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$$\tau_A = \lim_{I \to \infty} \left(\frac{2^I \mathsf{Var} A^{(I)}}{\mathsf{Var} A^{(0)}} - 1 \right)$$

What really happens in the System

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

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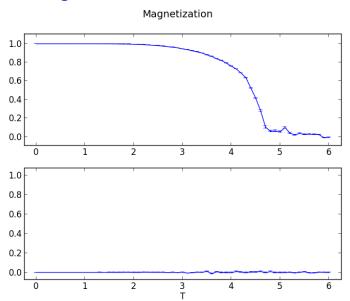
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- 2. Flip its spin and add it to the cluster

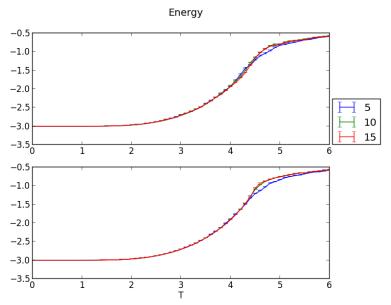
$$P(\sigma_x, \sigma_y) = 1 - \min\left(1, e^{2\beta\sigma_x\sigma_y}\right)$$

- 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

Magnetization

Magnetization squared

Computation time per spin flip

Swendsen-Wang

Questions

Binning analysis in detail

$$VarX := E[X^{2}] - E[X]^{2}$$

$$(\Delta X)^{2} = \frac{1}{N^{2}} \sum_{i,j=1}^{N} \left(E[X_{i}X_{j}] - E[X]^{2} \right)$$

$$= \frac{VarX}{N} + \frac{1}{N^{2}} \sum_{i \neq j} \left(E[X_{i}X_{j}] - E[X]^{2} \right)$$

$$= \frac{VarX}{N} + \frac{2}{N^{2}} \sum_{i=1}^{N} \sum_{t} \left(E[X_{i}X_{i+t}] - E[X]^{2} \right)$$

$$:= \frac{VarX}{N} (1 + 2\tau_{X})$$

Wolff or Swendsen-Wang?

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