# Cluster algorithms for the Ising model

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

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▶ Phase transitions

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

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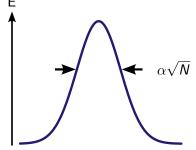
$$p(\sigma, T) = \frac{e^{-\beta \mathscr{H}(\sigma)}}{\mathscr{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$

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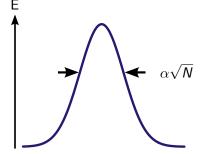
$$p(\sigma, T) = \frac{e^{-\beta \mathcal{H}(\sigma)}}{\mathcal{Z}(T)}, \quad \beta = \frac{1}{k_B T}$$
$$\langle M \rangle_T = \sum_{\sigma} M(\sigma) p(\sigma, T)$$

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

- ▶ We can't compute all configurations (2<sup>N</sup>)
- ► We can't sample uniformely distributed over energy



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► Solution: Importance sampling using Metropolis algorithm

1. Choose one site (uniformly randomly)

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

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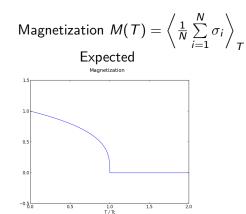
Magnetization 
$$M(T) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \sigma_i \right\rangle_T$$

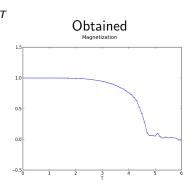
Magnetization 
$$M(T) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \sigma_i \right\rangle_T$$
Expected

Magnetization

1.0 T / Tc

-0.5





# Ising model - 2 spins

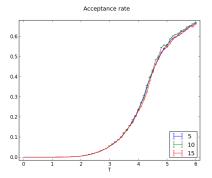
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$$\mathscr{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

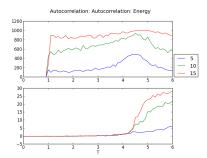
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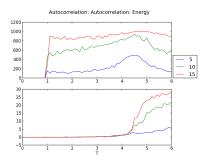


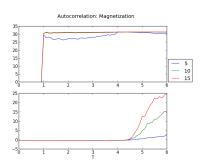
$$\phi_{A}(t) = rac{\langle A(t_0)A(t) \rangle - \langle A \rangle^2}{\langle A(t_0)^2 \rangle - \langle A \rangle^2}$$

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



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#### Binning analysis I

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

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

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

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

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

### Binning analysis II

$$\begin{split} A_i^{(I)} &= \frac{1}{2} \left( A_{2i-1}^{(I-1)} + A_{2i}^{(I-1)} \right) \\ \Delta^{(I)} &= \sqrt{\mathsf{Var} A^{(I)} / M^{(I)}} \overset{I \to \infty}{\to} \Delta = \sqrt{(1 + 2\tau_A) \mathsf{Var} A / M} \\ \tau_A &= \lim_{I \to \infty} \left( \frac{2^I \mathsf{Var} A^{(I)}}{\mathsf{Var} A^{(0)}} - 1 \right) \end{split}$$

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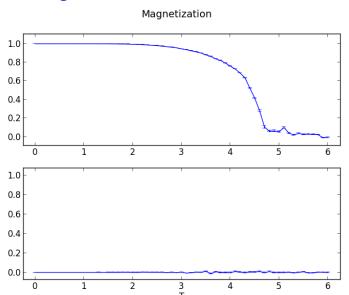
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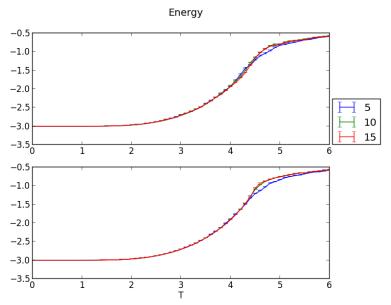
$$P(\sigma_x, \sigma_y) = 1 - \min\left(1, e^{2\beta\sigma_x\sigma_y}\right)$$

- 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

#### Wolff or Swendsen-Wang?

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