Cluster algorithms for the Ising model

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

Ising model - Why?

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

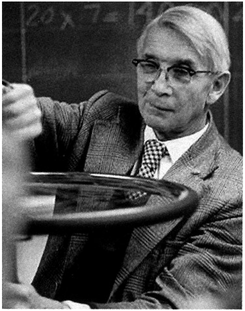

Figure : Ernst Ising (1900 - 1998)

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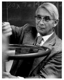

Figure : Ernst Ising (1900 - 1998)

Figure: Ernst Ising, lived from 1900 to 1998

1. Phase transitions are important
2. The Ising model is one of the simplest statistical models that shows a phase transition.
3. Ising model can be used to simulate magnetic systems (ferromagnetic and antiferromagnetic), opinion models and binary mixtures.
4. Ising model invented by Wilhelm Lenz (1888 - 1957) (the same as the Lenz in the Laplace-Runge-Lenz vector) in 1920, his student Ernst Ising solved it in the one-dimensional case 1924.
5. Wolfgang Pauli (1900 - 1958), at whom the road outside is named after, was an assistant of Lenz.
6. Also Otto Stern (1888 - 1969) from the Stern-Gerlach experiment was an assistant of Lenz.

Ising model - Definition

- Lattice with N sites
- Discrete integer spins $\sigma_i = \pm 1$ on each lattice site
- $$\mathscr{H}(\sigma) = -J \sum_{i,j} \sigma_i \sigma_j - \mu H \sum_i \sigma_i$$
- J: interaction, H: external field
- $$p(\sigma, T) = \frac{e^{-\beta \mathscr{H}(\sigma)}}{\mathscr{Z}(T)}, \qquad \beta = \frac{1}{k_B T}$$
- $$\langle M \rangle_T = \sum_\sigma M(\sigma) p(\sigma, T)$$

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1. Sum over nearest neighbours.
2. More favorable for the spins to be aligned!
3. J_{ij} in general case, $J > 0$: ferromagnetic, $J < 0$: antiferromagnetic
4. Configuration probability given by boltzmann distribution, Z partition function, given as

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

5. So we are looking at a canonical system with constant temperature T.
6. Measurement value of a function, e.g. magnetization, is given by the sum over all states of the measurement value at the configuration times the configuration probability.

Ising model - Monte Carlo I

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- We can't sample equally distributed over energy.
- Solution: Biased sampling using Metropolis ($M(RT)^2$) algorithm.

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1. Why not? $\rightarrow 2^N = 2^{L^d}$ e.g. $L = systemSize = 15$ in 2 dimensions: $2^{15^2} = 2^{225} = 5 \cdot 10^{67}$
2. We can't compute the exact expectation value of an observable. But that's what we're interested in.
3. Because the distribution of the average energy gets sharper with increasing size $\left(\alpha \sqrt{L^d}\right)$.

Single spin flip metropolis - Algorithm

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

1. Choose on site.
2. Calculate energy difference.
3. Accept new configuration with transition probability above.

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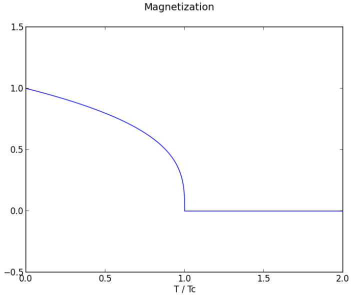
2. Calculate energy difference.
3. Accept new configuration with transition probability above.

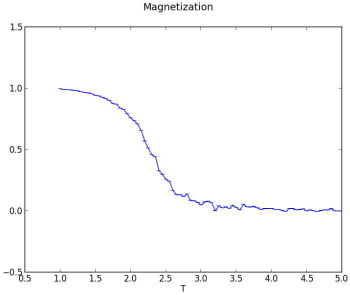
If energy decreases, always accept. If energy increases, accept with probability $e^{-\beta \Delta E}$.Blazingly fast (Troells: 2 flips/ns?), easy to implement.

1. New state given by spinflip at this site.

Single spin flip metropolis - Results

Spontaneous magnetization $M_s(T) = \left\langle \frac{1}{N} \sum_{i=1}^{N} \sigma_i \right\rangle$





Questions

Wolff or Swendsen-Wang?

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

A sample slide

A displayed formula:

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}$$

An itemized list:

- itemized item 1
- itemized item 2
- itemized item 3

Theorem

In a right triangle, the square of hypotenuse equals the sum of squares of two other sides.