Sampling the Ising Model

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History

- Proposed by Wilhelm Lenz to his student Ernst Ising
- 1924: Ernst Ising - *Beitrag zur Theorie des Ferromagnetismus*[1]

  "Es entsteht ... [durch] ... die Beschränkung der Wechselwirkung auf diejenige benachbarter Elemente [...] kein Ferromagnetismus."

- 1936: Rudolph Peierls - *On Ising's model of ferromagnetism*[2]

  "[...] for sufficiently low temperatures the Ising model in two [or more] dimensions shows ferromagnetism [...].

[1] Zeitschrift für Physik Februar–April 1925, Volume 31, Issue 1, pp 253-258
[2] Cambridge Philosophical Society 1936, Volume 32, Issue 03, Oct.

Lattice

Figure: Square Lattice in 1 dimension

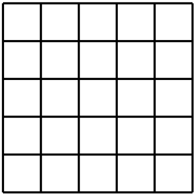

Figure: Square Lattice in 2 dimensions

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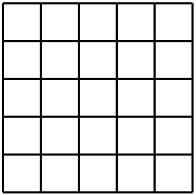

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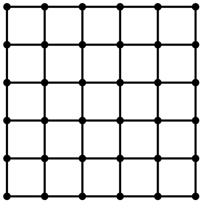

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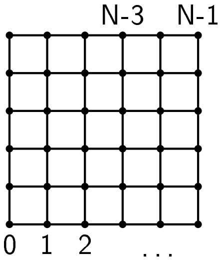

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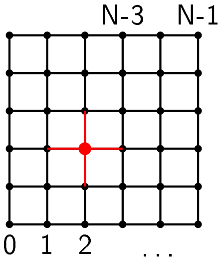

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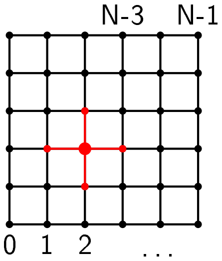

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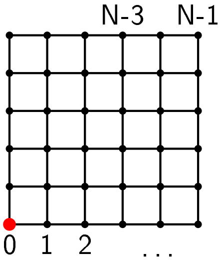

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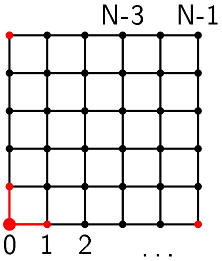

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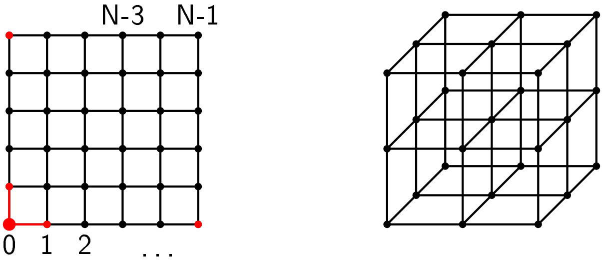
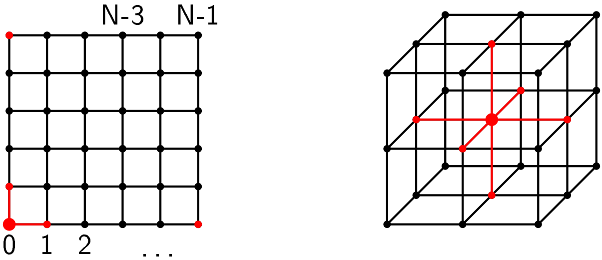


Figure: Square Lattice in 2 and 3 dimensions

Lattice

Figure: Square Lattice in 1 dimension



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Lattice Sites

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- Each site has a state $s_i = -1 \vee 1$
- Assignment of states $S = (s_0, s_1, s_2, \ldots, s_{N-1})$ to the lattice sites is called a configuration
- Therefore 2^N unique configurations for a lattice with N lattice sites.

Magnetization

- The magnetization of a configuration is calculated by

$$m_x = m(S_x) = \sum_i^N s_i \in [-N, N]$$

- usually the magnetization per spin is considered

$$M_x = \frac{m_x}{N} \qquad \in [-1, 1]$$

Energy

- Each configuration has a corresponding energy - the Hamiltonian.

$$E_x = E(S_x) = H(s_0, s_1, \ldots, s_{N-1}) = -J \sum_{<i,j>} s_i \cdot s_j - h \sum_{i} s_i$$

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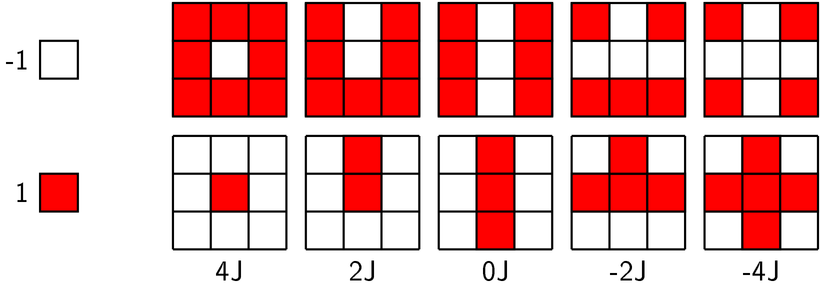

Figure: Energy contribution (nearest neighbor interaction) of the bonds connected to the central lattice site

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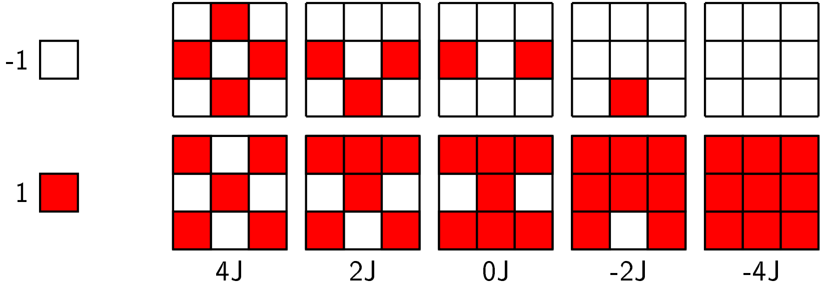

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Boltzmann distribution

Probability of system being in the state S is given by the Boltzmann distribution ($\beta = 1/kT$)

$$p_x = p(S_x) = \frac{e^{-\beta E_x}}{Z}$$

Z is the the partition function

$$Z = \sum_{i}^{2^N} e^{-\beta E_i}$$

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$\rightarrow$ *importance sampling*

Markov Chain

- Chain of iteratively created configurations $C_1, C_2, \ldots C_n$
- Resulting configurations correspond to the desired probability distribution p and span the entire state space.
- Configuration C_t only depends on C_{t-1} (Markov property).

Transitions in the Markov Chain

Probability for being in state A:	p_A
Transition probability for transition $S_A \rightarrow S_B$:	p_{AB}

If it fulfills *detailed balance* (it must!)

$$p_A \cdot p_{AB} = p_B \cdot p_{BA}$$

the following relation for the transition probability follows:

$$\frac{p_{AB}}{p_{BA}} = \frac{p_B}{p_A} = \left(\frac{Z}{Z}\right) \frac{e^{-\beta E_B}}{e^{-\beta E_A}} = e^{-\beta(E_B - E_A) = e^{-\beta \Delta E}}$$

Metropolis- Hastings Algorithm

- Configuration after t steps is C_t
- Flip one lattice site $\rightarrow C_t'$
  - has to be chosen randomly - suitable RNG necessary
- Calculate energy difference $\Delta E = E_t' - E_t$
- Calculate acceptance probability P

$$P = \min\left(1, e^{-\beta \cdot \Delta E}\right), \qquad \beta = 1/kT > 0$$

- Generate random number $r \in [0, 1[$
  - $r < P \rightarrow C_{t+1} = C_t'$
  - $r > P \rightarrow C_{t+1} = C_t$

Magnetization over time (MH- Algorithm)

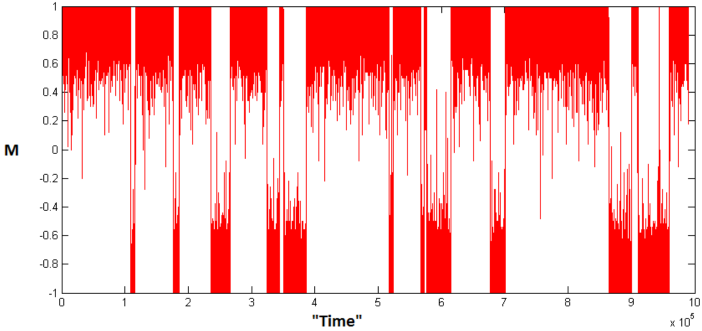


Figure: Not in physical time but Monte Carlo time steps.

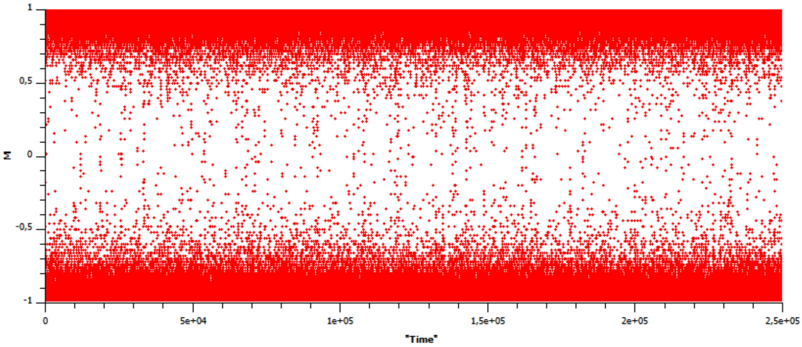
Swendsen- Wang Algorithm

- Search for clusters with equal spins
- Generate a bond between lattice sites in such a cluster with

$$p = 1 - e^{-2/T}$$

- Search for clusters connected by bonds
- Assign a random spin to each cluster.

Magnetization over time (SW- Algorithm)



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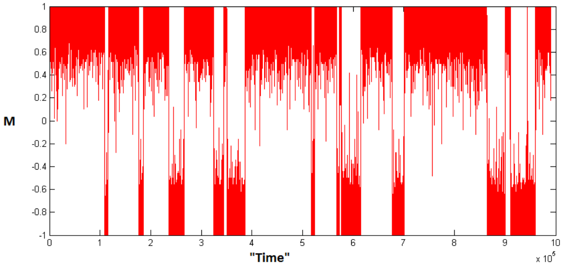
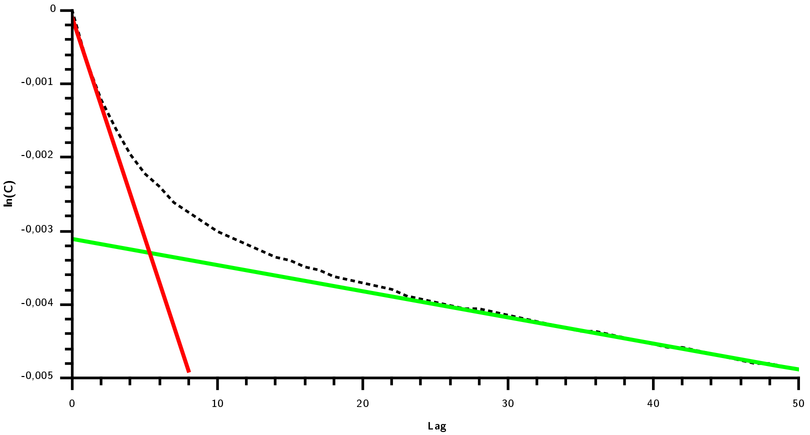
Autocorrelation

- Similarity of a function with a "lagged" version of itself.

$$C_M(t) = \frac{cov(M_n, M_{n+t})}{std(M_n)std(M_{n+t})} = \sum_i c_i e^{-t/\tau_i}$$





$$ln\left(C_M(t)\right) = \sum_i \left(ln(c_i) - \frac{t}{\tau_i}\right)$$

Effective Markov- chain length

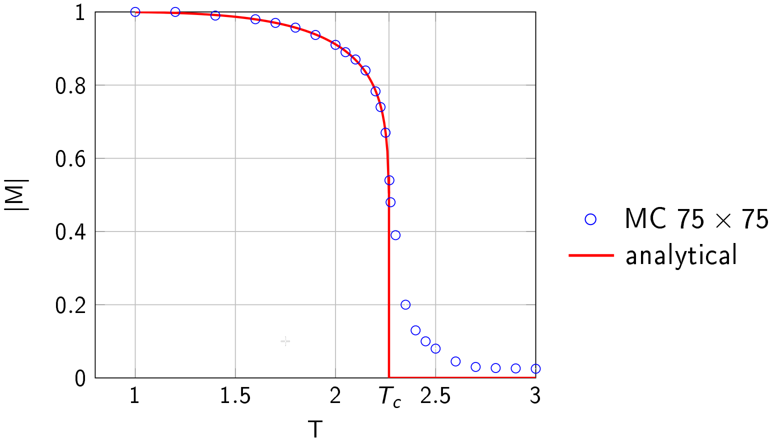
- naive error analysis leads to underestimated errors due to autocorrelation.

$$var(M) = \sigma_M^2 = \frac{\sum_i \left(M_i - \bar{M}\right)^2}{n}$$

- realistic error considers autocorrelation with smaller sample-size n_{eff}:

$$n_{eff} = \frac{n}{2\tau_{int}} \approx \frac{n}{2\sum_i c_i \tau_i}$$

Absolute magnetization per spin



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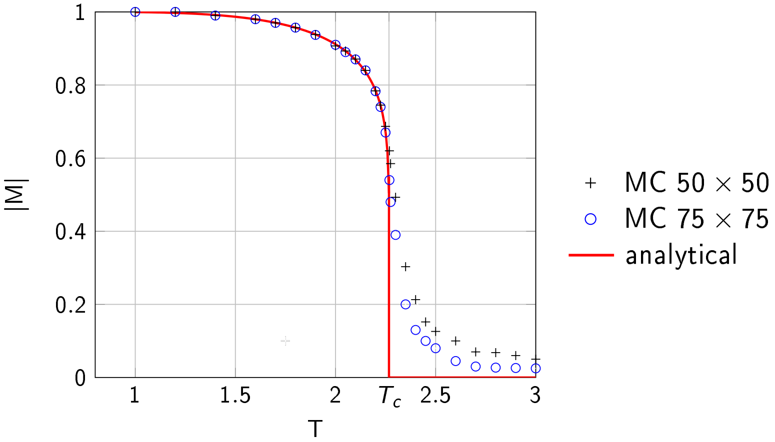

- Update algorithm must be chosen according to parameters.
- Sample size must be chosen big enough to compensate autocorrelation
- Right size of the lattice to adjust for finite size effects - depending on temperature.

Ambition

- Simulating flow of sediments in current
- Needed adjustments:
  - constant ”spin”- ratio and...
  - flowing and not random spawning/despawning of ”particles”
  - current in form of outer force
  - more states for a lattice site

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- Simulating flow of sediments in current
- Needed adjustments:
  - constant "spin"- ratio and... $\rightarrow$ Kawasaki Dynamics
  - flowing and not random spawning/despawning of "particles"
  - current in form of outer force $\rightarrow$ force term in Hamiltonian
  - more states for a lattice site $\rightarrow$ Potts Model

Kawasaki Dynamics

- Choose A-B bond
- Calculate ΔE for $A - B \rightarrow B - A$
- Accept with probability depending on energy difference

Behaviour:

- Spin- ratio (Magnetization) constant.
- Different spins get sorted (if coupling constant J is positive).

Current

$$H_G = -J \sum_{<i,j>} s_i s_j - \sum_j h_j \sum_{line_j} s_i$$

with

$$h_j = h_1 + j \frac{(h_L - h_1)}{L}$$

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Potts Model

- Generalized version of the Ising model.
- states not only $-1 \wedge 1$ but (discrete) angles.
- Energy usually in the form $H = -J_c \sum_{i,j} cos\left(\theta_i - \theta_j\right) + \ldots$

Thanks for your attention

- Sourcefiles and binaries on my github https://github.com/oerpli/Ising
  - currently only tested on Windows 7& 8.
  - Swendsen Wang Algorithm implemented with recursive DFS - accordingly stackoverflow error with big clusters (depending on configuration)