Sampling the Ising Model

Abraham Hinteregger

University of Vienna

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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

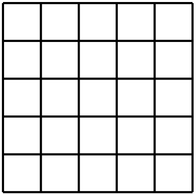

Figure: Square Lattice in 2 dimensions

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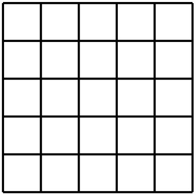

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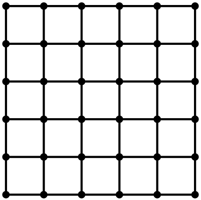

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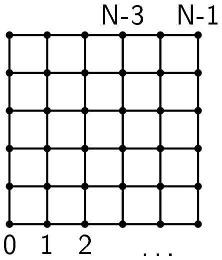

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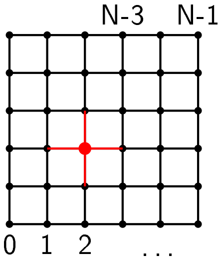

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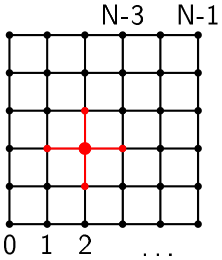

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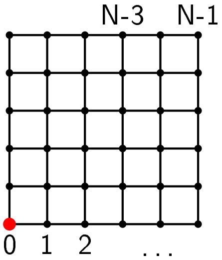

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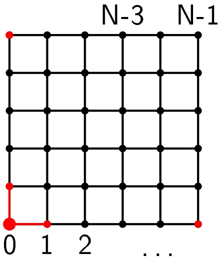

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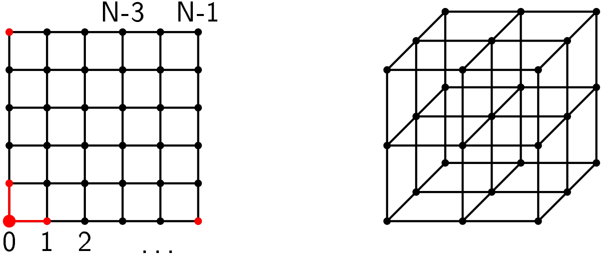
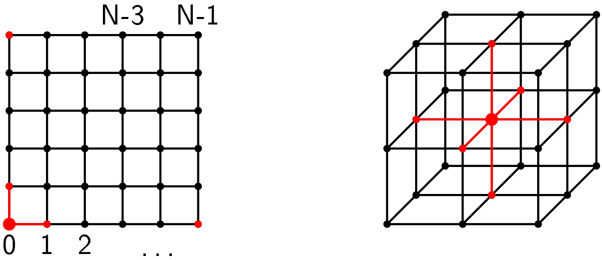


Figure: Square Lattice in 2 and 3 dimensions

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

$$M_S = M(S) = \sum_i^N s_i \in [-N, N]$$

- The squared magnetization is an indicator for the degree of order

$$M_S^2 = \sum_i s_i^2 \in [0, N]$$

Energy

- Each configuration has a corresponding energy - the Hamiltonian.

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

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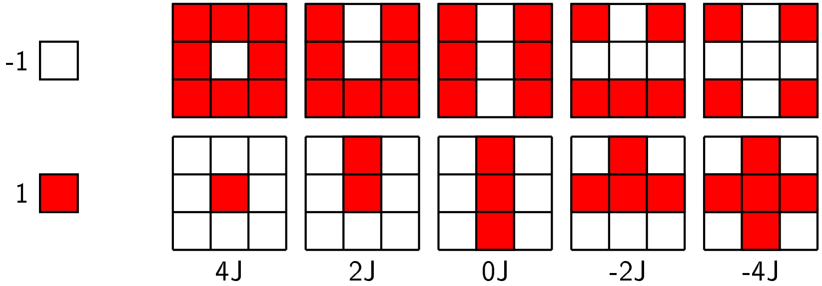

Figure: Energy contribution (nearest neighbor interaction) of the bonds connected to the central lattice site

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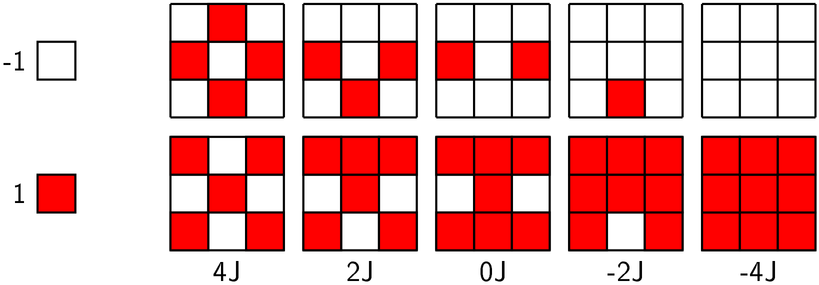

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Boltzmann distribution

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

$$p_S = p(S) = \frac{e^{-\beta E_S}}{Z}$$

Z is the the partition function

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

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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 $S_A \to S_B$: 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:

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

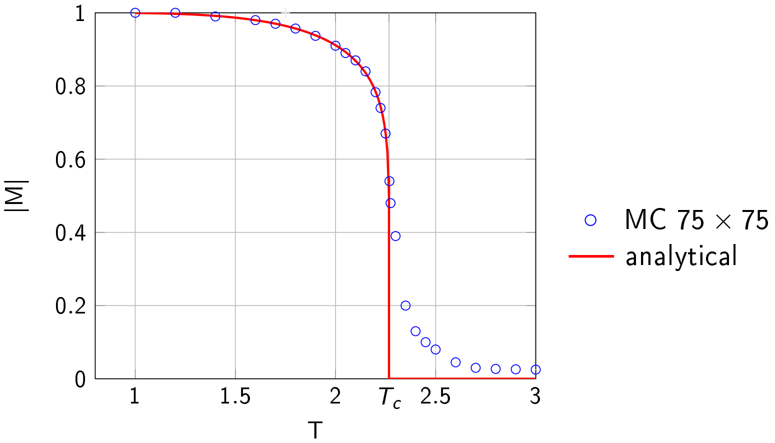
Metropolis- Hastings Algorithm

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

Absolute magnetization per spin



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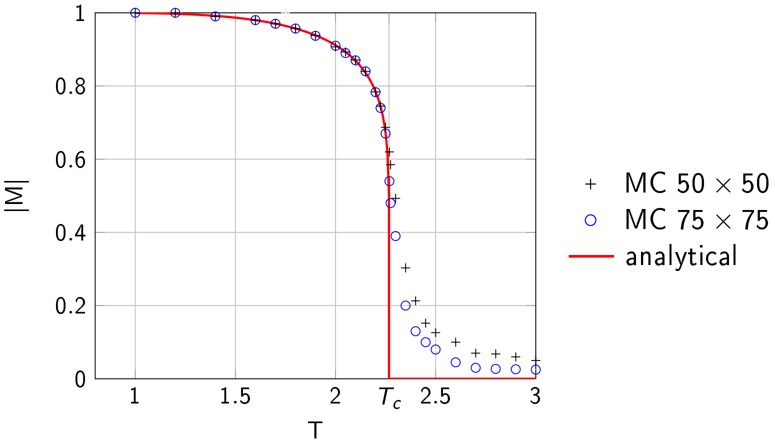

Magnetization over time

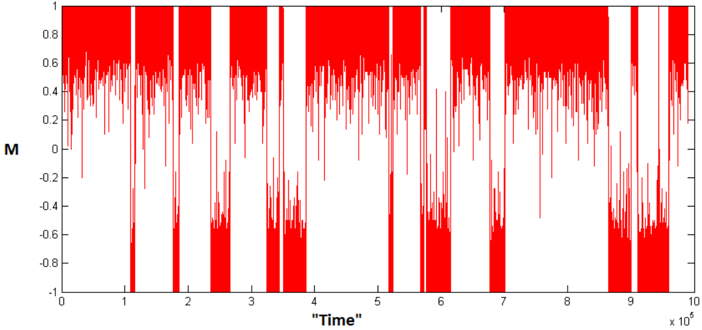

Figure: M per spin plotted over time (Monte Carlo steps)

Properties of a configuration s

- Energy – Hamiltonian: $E(s) = H(s)$
- Internal energy (per spin): $e(s) = E/N \in [-2, 2]$
- Magnetization: $M(s) = \sum_i^N s_i$
- Magnetization (per spin): $m(s) = M/N \in [-1, 1]$

Temperature

Temperature in the Ising Model

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

- $\Delta H < 0 \rightarrow P = 1$
- high temperature leads to higher acceptance probability $\rightarrow$ unordered (low magnetization, Curie Temperature T_c)
- critical temperature T_c when $\left\langle \sum_i^N s_i \right\rangle / N \approx 0$

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  - $kT_c/J = 2.269$

Cluster Flip Algorithms

Summary - Ising Model

- molecules on a lattice - each with with one of two possible states
- (magnetic) moments prefer to align
- low temperatures: ordered
- high temperatures: disordered

Different Models

- Single value obtained from one configuration hasn't much significance
- Average from many (n) configurations instead:

$$\bar{E} = \frac{1}{n}\sum_{i}^{n} E_{S_i} \qquad \bar{M} = \frac{1}{n}\sum_{i}^{n} M_{S_i} \qquad \ldots$$

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- Sampling from completely random configurations does not work well for ordered configurations seen in ferromagnets.