2-D Ising Model

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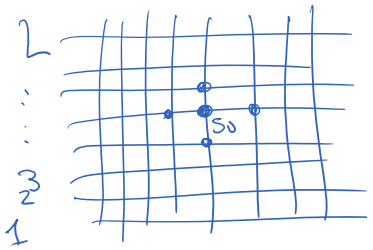
Consider: A system of N spins $\nu = 1, \ldots N$ $S_\nu = \pm 1$ which interact depending on their spatial separation.

Consider a d-Dimensional grid with constant grid spacing for the arrangement of these spins.



$d = 2$

$N = L^d$

Hamiltonian (Energy)

$$H = -J \sum_{n,\nu} S_n S_\nu - B \sum_\nu S_\nu$$

$\sum_{n,\nu}$: over interacting neighbors only

$\sum_\nu$: External Magnetic Field

The product $S_n S_\nu$ is either $+1$ or -1

$+1$: aligned -1: anti-aligned

If $J > 0$ Ferromagnetic System

$J < 0$ Antiferromagnetic

For $J > 0$ all the spins want to align themselves to minimize the total Energy (all terms in the sum are positive)

For the 2-d Ising Model ($d = 2$, $B = 0$) an exact solution was obtained by L. Onsager 1944. The Ising model has a critical point at temperature T_c which is given by

$$\frac{J}{k_B T_c} = -\frac{1}{2} \log\left(\sqrt{2} - 1\right) \sim 0.44069$$

k_B is the Boltzmann Constant and has dimensions of energy per unit temperature.

For our simulations we will set this to 1. It defines our unit system and can be rescaled if needed.

At $T = T_c$ we have a phase transition (of 2nd order).

Above T_c the magnetization of the system vanishes

$$M = \sum_\nu S_\nu \qquad \langle m \rangle = \frac{\langle M \rangle}{N}$$

below T_c a spontaneous magnetization takes place which is given by

$$\langle m \rangle \equiv \frac{\langle M \rangle}{N} \sim (T_c - T)^\beta \quad , \beta = 1/8$$

This exact Onsager solution can be used later to test the correctness of our simulated system.

MONTE CARLO SIMULATION

It is a path through configuration space. The configuration space is the space of all possible states of the system. For Ising model we have 2^N configurations.

A path through configuration space is given by $C_1, C_2, C_3, \cdots$

This sequence is constructed as a Markov process which means that the probability of reaching C_s is given solely by the preceding n configurations in the path,

$$C_{s-1}, C_{s-2}, \cdots C_{s-n}$$

an order n Markov process.

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$$\langle F \rangle = \frac{1}{S} \sum_{i=1}^{S} g(C_i) F(C_i)$$

$F(C_i)$ is the physical property of the system in configuration C_i, e.g., energy or magnetization.

S is the total number of steps carried out, $g(C_i)$ is a weighting factor of how strongly a given configuration influenced the physical property $F(C_i)$.

We want systems in equilibrium also we will set $g(C_i) = 1$.

Consider a transition probability from one configuration to another: $W(C \to C')$.

We want this to be such that the probability of obtaining any particular configuration C_i is

$$p(C_i) \sim e^{-\beta E_i} \qquad \beta \equiv \frac{1}{k_B T}$$

Equilibrium!

this constraint forces:

$$e^{-\beta E_i} W(C_i \to C_j) = e^{-\beta E_j} W(C_j \to C_i)$$

Condition of detailed balance.

E.g. suppose one step is 10^{-16} s

for $L = 12$ $\quad 2^{L^2} = 2^{144} = 10^{17}$ s

which is longer than the age of the universe

Metropolis algorithm:

Pick a single spin S_v and decide if it should flip.

$+S_v \to -S_v$?

$\Delta E = E(-S_v) - E(+S_v)$

other $N-1$ spins stay the same.

We call this a "Move".

$$\Delta E = 2 J S_v \sum_{(v)} S$$

(v) Neighbors of v

Detailed Balance:

$$\frac{W(+S_v \to -S_v)}{W(-S_v \to +S_v)} = e^{-2\beta J S_v u_v}$$

$$u_v \equiv \sum_{(v)} S$$

$$W(+S_v \to -S_v) = \min\left(1, \exp(-\beta \Delta E)\right)$$

$$W(-S_v \to +S_v) = \min\left(1, \exp(\beta \Delta E)\right)$$

Algorithm:

1. Pick spin S_v
2. Calculate ΔE
3. If $\Delta E < 0$ ——— $S_v = -S_v$
4. else: $\Delta E \geq 0$
   - 4a. Pick a random number $0 \leq r < 1$
   - 4b. If $r < \exp(-\beta \Delta E)$ ——— $S_v = -S_v$

Use a periodic grid

use Black or white pixels for

+, − Sv.

Start with a high temperature and visualize what happens

$\langle m \rangle$ $T > T_c$ $\langle m \rangle = 0$

disordered

Correlated spins for $T < T_c$

Order $\langle m \rangle \neq 0$.