a) Ising Model

b) Metropolis algo.

c) Glauber algo or dynamics.

(Heat bath dynamics)

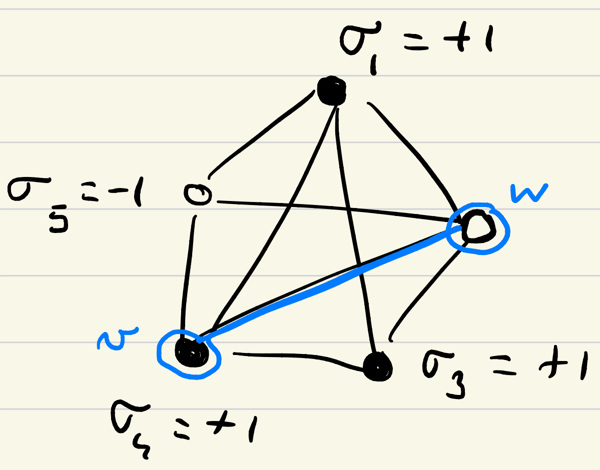
$G = (V, E)$. $\qquad V = \{1, 2, 3, \dots N\}$.

binary alphabet $\mathcal{X} = \{-1, +1\}$ and

"degrees of freedom" or "spins" $\sigma_v \in \mathcal{X}$.

$v \in V$.

Complete graph for example:




assignment or "spin configuration"

$\underline{\sigma} = (\sigma_1, \sigma_2, \dots, \sigma_N)$.

$$\pi(\underline{\sigma}) = \frac{e^{-\beta H(\underline{\sigma})}}{Z}$$

interaction

Magnetic field

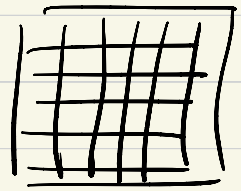
Hamiltonian:

$$H(\underline{\sigma}) = -\sum_{(v,w)\in E} J_{vw}\,\sigma_v\sigma_w - \sum_{v\in V} h_v\,\sigma_v$$

$$Z = \sum_{\underline{\sigma}\in\mathcal{X}^N} e^{-\beta H(\underline{\sigma})}$$

"Partition function".

Another important example: square grid $\subset \mathbb{Z}^d$.



Some intuition: (from physics)

- The "spins" represent magnetic moments, which are carried by atoms in a crystal say.

| up | down |
|---|---|
| $\uparrow$ | $\downarrow$ |
| $\sigma=+1$ | $\sigma=-1.$ |

gross simplification with only two direction for the magn moments.

- These "spins" interact.

anti-ferromagnetic interaction

$J_{vw}>0$

$J_{vw}<0$

Energy of a configuration of two spins

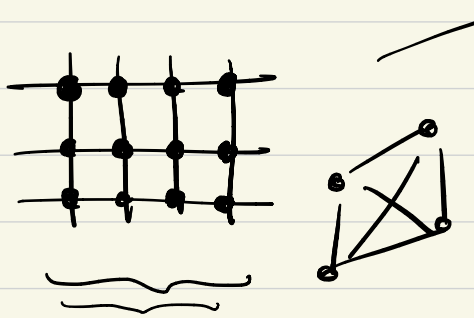
| $v$ | $w$ | | $J_{vw}>0$ | $J_{vw}<0$ |
|---|---|---|---|---|
| $\uparrow$ | $\uparrow$ | $-J_{vw}\overbrace{\sigma_v\sigma_w}^{+1} = -J_{vw}$ | favorable | unfavorable |
| $\uparrow$ | $\downarrow$ | $-J_{vw}\overbrace{\sigma_v\sigma_w}^{-1} = +J_{vw}$ | unfavorable | favorable |
| $\downarrow$ | $\uparrow$ | $-J_{vw}\overbrace{\sigma_v\sigma_w}^{-1} = +J_{vw}$ | unfavorable. | favorable |
| $\downarrow$ | $\downarrow$ | $-J_{vw}\overbrace{\sigma_v\sigma_w}^{+1} = -J_{vw}$ | favorable | unfavorable |

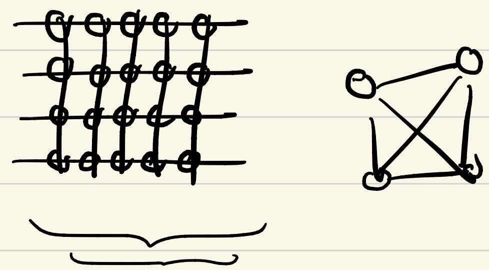
- **The ferromagnetic model**: all $J_{vw} > 0$.

Consider the special case $h_v = 0$:

$$H(\underline{\sigma}) = -\sum_{(vw)\in E} J_{vw}\,\sigma_v\sigma_w$$

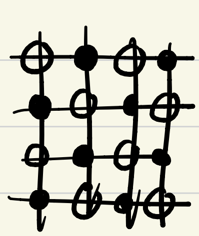
has two minima (all $\sigma_v = +1$) or (all $\sigma_v = -1$).





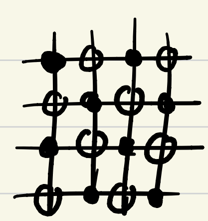
- **The anti-ferromagnetic**: all $J_{vw} < 0$.

Situation more complicated and will depend on the graph. E.g



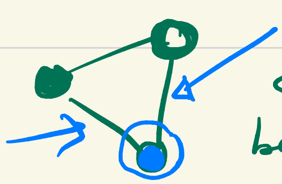
is a minimum

staggered configuration



second min.

Frustration:



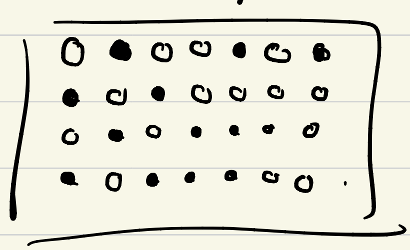
← difficulty will come for large graphs because you cannot min all terms simultaneously in $H(\underline{\sigma})$.

- The study of optimization of $H(\underline{\sigma})$ and of sampling $\pi(\underline{\sigma}) = \frac{e^{-\beta H(\underline{\sigma})}}{Z}$ is a difficult problem specially for "frustrated" systems with all possible signs for $J_{vw} > 0$ and $J_{vw} < 0$.

- <u>Interpretation of $\beta$</u> : inverse of the temperature of the system $\beta = \frac{1}{KT}$

<u>$\beta$ small</u> : corresponds to a nearly uniform measure on state space $\chi^N$.
<u>high temperature</u>

Typical spin configurations will be more or less <u>unif at random</u> from $\chi^N = \{-1, +1\}^N$.



<u>$\beta$ large</u> : $\frac{e^{-\beta H(\underline{\sigma})}}{Z}$ is peaked around the <u>Minima of $H(\underline{\sigma})$</u> $(\beta \to +\infty)$.
<u>low temperature</u>

Typical spin conf will fluctuations around <u>Minima</u>.

## Formal definitions:

- **Magnetization:**

$$\boxed{m(\beta) = \frac{1}{N}\sum_{v=1}^{N} \langle \sigma_v \rangle} \checkmark$$

where Notation $\underbrace{\langle \sigma_v \rangle}_{\text{bracket notation.}} = \mathbb{E}_\pi(\sigma_v) := \sum_{\underline{\sigma} \in \chi^N} \sigma_v \pi(\underline{\sigma})$

→ Intuitively this is the total $\overbrace{\text{magnetic moment}}^{\text{average}}$.

→ If $m(\beta) \approx 0$ the system is Not magnetized.

→ If $m(\beta) \neq 0$ the system is magnetized.

Model displays transition between these two situations typically as $\beta$ varies from high temp to low high temp.

- How would you calculate $m(\beta)$?

Remark (exercise): $\langle \sigma_v \rangle = \frac{1}{\beta}\frac{\partial}{\partial h_v}(\ln Z)$

$$Z = \sum_{\underline{\sigma} \in \chi^N} \exp\Big\{\beta \sum_{vw \in E} J_{vw}\sigma_v\sigma_w + \beta \sum_{v \in V} h_v \sigma_v\Big\}$$

But computing $Z$ is difficult and in general impossible.

Instead we go back to:

$$m(\beta) = \left\langle \frac{1}{N} \sum_{v \in V} \sigma_v \right\rangle = \mathbb{E}_{\sigma}\left( \frac{1}{N} \sum_{v \in V} \sigma_v \right).$$

and consider an estimator based on an MCMC algo.

$$\hat{m}(\beta) = \lim_{t \to +\infty} \left\{ \frac{1}{N} \sum_{v \in V} \sigma_v(t) \right\}.$$

where $\sigma_v(0), \sigma_v(1), \ldots, \sigma_v(t), \ldots$ is an MCMC chain with stat distr $\pi(\underline{\sigma})$.

We can also compute any sort of average:

$$\langle A(\underline{\sigma}) \rangle \quad \text{e.g} \quad \underbrace{\frac{1}{N} \langle H(\underline{\sigma}) \rangle}_{\substack{\text{internal energy per vertex} \\ \text{per site.}}}$$

again: $$\lim_{t \to +\infty} \left\{ \frac{1}{N} \sum_{v \in V} H(\underline{\sigma}(t)) \right\}.$$

# A bit of background on the phase transition phenomena

(scratch the surface of the subject.).

$$\begin{cases} G = (V, E) \text{ is a } \underline{\text{complete graph}}. \\ J_{vw} = \dfrac{J}{N} > 0 \quad \text{for all } (v,w) \in E. \\ h_v = h \in \mathbb{R} \quad \text{for all } v \in V. \end{cases}$$

Ferromagnetic Ising Model on a complete graph.

$$H(\sigma) = -\frac{J}{2N} \underbrace{\underbrace{\sum_{v,w \in V^2}}_{\text{complete graph.}} \sigma_v \sigma_w}_{\frac{1}{2}\left(\sum_{v \in V} \sigma_v\right)^2 - N} \; - h \underbrace{\sum_{v \in V} \sigma_v}_{\text{acts like a bias in } e^{-\beta H(\sigma)}}.$$

→ It possible to in fact compute $Z$ and also averages and in particular

$$m(\beta) = \left\langle \frac{1}{N} \sum_{v \in V} \sigma_v \right\rangle.$$

⟶

show the result.

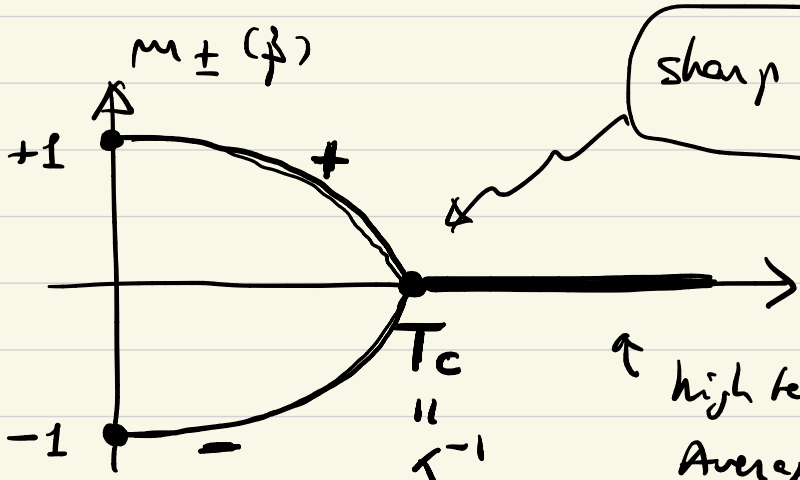
Finding is eventually:

$$\underline{m(\beta, h)} = \left\langle \frac{1}{N} \sum_{v \in V} \sigma_v \right\rangle$$

for $\langle - \rangle$ for the complete $^{\text{graph}}$ ferro-magnetic model

you can plot $\quad m_{\pm}(\beta) = \lim_{h \to 0\pm} m(\beta, h)$.

The spontaneous magnetization or zero bias magn or zero-magnetic field magnetization.




sharp phase transition "sudden" at $T = T_c = J^{-1}$

$T = \beta^{-1}$.

high temperature behavior.
Average spin-magnetization is zero.
Typical spin conf is "disordered".

Low temp behavior
Average spin Magn $\neq 0$.
Typical spin conf are fluctuations of (all $+1$) and (all $-1$).

b) <u>Metropolis algorithm</u> (Ising) ✓

c) <u>Glauber dynamics</u>

<u>c bis</u>. Heat bath dynamics in general.

d) <u>Simulation results.</u>

#.

## Metropolis algo.

Hamiltonian (energy or cost).

$$H(\underline{\sigma}) = -\sum_{(v,w)\in E} J_{vw}\,\sigma_v \sigma_w - \sum_{v\in V} h_v \sigma_v .$$

$\underline{\sigma} = (\sigma_1 \ldots \sigma_N) \in \{-1,+1\}^N$.

$G = (V, E)$.

Algo:

- Select a vertex $v \in V$ unif at random (with prob $1/N$).
- Propose the move $\underline{\sigma} \to \underline{\sigma}'$ : $\sigma'_w = \sigma_w \quad w \neq v$
  $\sigma'_v = -\sigma_v$ <u>flip at $v \in V$.</u>
- Compute the cost difference: $\Delta E(\underline{\sigma}\to\underline{\sigma}') = H(\underline{\sigma}') - H(\underline{\sigma})$.
- Accept the move with probability $A(\underline{\sigma}\to\underline{\sigma}') = \min(1, e^{-\beta \Delta E})$.

$$H(\underline{\sigma}) = -\sum_{(v,w)\in E} J_{vw}\,\sigma_v \sigma_w - \sum_{v\in V} h_v \sigma_v .$$

$$\Delta E(\underline{\sigma}\to\underline{\sigma}') = \underbrace{H(\underline{\sigma}')}_{\text{New energy}} - \underbrace{H(\underline{\sigma})}_{\text{old energy}} .$$

$$A(\underline{\sigma}\to\underline{\sigma}') = \min\left(1, e^{-\beta \Delta E(\underline{\sigma}\to\underline{\sigma}')}\right)$$

$$= \begin{cases} 1 & \text{if } \Delta E(\underline{\sigma}\to\underline{\sigma}') < 0 \quad \text{New Energy} < \text{Old Energy} \\ e^{-\beta \Delta E} & \text{if } \Delta E > 0 \quad \text{New Energy} \geq \text{Old Energy.} \end{cases}$$

**Remark**

- $$e^{-\beta \Delta E} = \frac{e^{-\beta H(\underline{\sigma}')}}{e^{-\beta H(\underline{\sigma})}} = \frac{\pi(\underline{\sigma}')}{\pi(\underline{\sigma})} .$$ <u>Metropolis rule.</u>

- chain is irred., aperiodic (self loops), detailed balance is satisfied and $\pi$ is stat distr.
  ↳ exist
  ↳ pos recurrent chain

$\boxed{\text{chain is ergodic and } \pi \text{ is a limiting distribution}}$

- This is certainly true for $N$ finite and time (# of steps)

- Final important point:

$$\Delta E(\underline{\sigma} \to \underline{\sigma}') = H(\underline{\sigma}') - H(\underline{\sigma}).$$

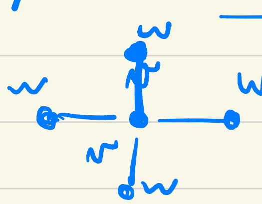
$$= \Big\{ - \sum_{(k,l)\in E} J_{kl}\, \sigma'_k \sigma'_l - \sum_{k\in V} h_k \sigma'_k \Big\}$$

$$- \Big\{ - \sum_{(k,l)\in E} J_{kl}\, \sigma_k \sigma_l - \sum_{k\in V} h_k \sigma'_k \Big\}.$$

We have selected vertex $v$ and $\sigma'_w = \sigma_w$ if $w \neq v$, $\sigma'_v = -\sigma_v$.

if $(k,l) \not\ni v$ and $k \neq v$ then terms simplify.

and it remains only:




$$= \Big( - \sum_w J_{vw}\, \sigma_w \underbrace{\sigma'_v}_{-\sigma_v} - h_v \underbrace{\sigma'_v}_{-\sigma_v} \Big) - \Big( - \sum_w J_{vw}\, \sigma_w \sigma_v - h_v \sigma_v \Big)$$

$$= 2\Big( \sigma_v \underbrace{\sum_w J_{vw}\, \sigma_w}_{} + h_v \Big).$$

For interaction you get only neighbours of $v$ that share an edge count // For the bias only the vertex $v$ enters.

# Glauber dynamics or algo.

- Select a vertex $v$ at random unif among $V = \{1, \dots, N\}$
- Propose the move $\underline{\sigma} \to \underline{\sigma}'$ s.t

$$\sigma_w' = \sigma_w \, , \quad w \neq v$$

$\sigma_v' = -\sigma_v$ flip of the spin.

- Accept the move with acceptance probability

$$A(\underline{\sigma} \to \underline{\sigma}') = \frac{1}{2} \left\{ 1 - \tanh\left( \frac{\beta \, \overbrace{\Delta E(\underline{\sigma}' \to \underline{\sigma})}}{2} \right) \right\}$$

✓✓✓

[ Reject the move with prob $1 - A(\underline{\sigma} \to \underline{\sigma}')$
$= \frac{1}{2} \left\{ 1 + \tanh \frac{\beta \Delta E}{2} \right\}$. ]

$$\Delta E(\underline{\sigma}' \to \underline{\sigma}) = H(\underline{\sigma}') - H(\underline{\sigma})$$

$$= 2\left( \sigma_v \sum_w J_{vw} \sigma_w + h_v \sigma_v \right)$$ (as before).

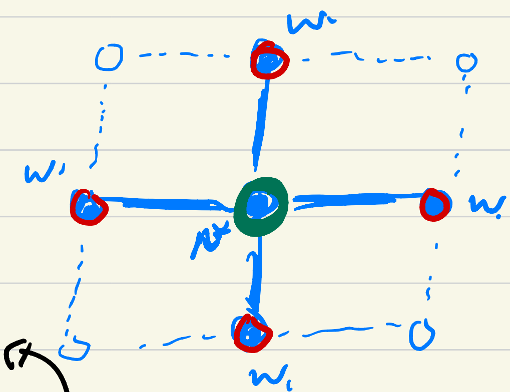
Again this chain is irred. & aperiodic.

Exercise: detailed balance is satisfied again.

$\Rightarrow \exists$ stat distr which is $\pi$

.... $\Rightarrow$ chain is irred, aperiodic, pos rec i.e ergodic and $\pi$ is a limiting distr.

Remark:




$$A(\underline{\sigma} \to \underline{\sigma}') = \frac{1}{2}\left(1 - \tanh \frac{\beta \Delta E}{2}\right)$$

$$\Delta E = 2\sigma_v \sum_w J_{vw}\sigma_w + 2h_v\sigma_v.$$

$$\Rightarrow A(\underline{\sigma} \to \underline{\sigma}') = \frac{1}{2}\left(1 - \tanh \beta \sigma_v \left\{ \sum_w J_{vw}\sigma_w + h_v \right\}\right)$$

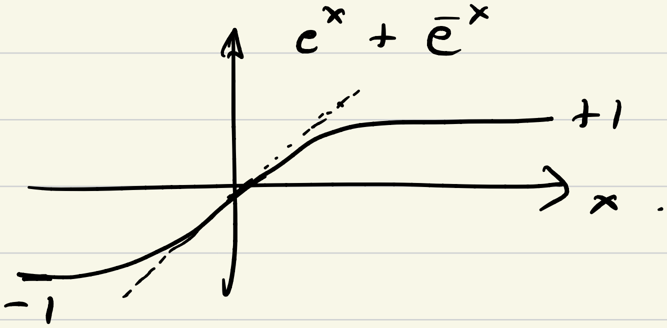
$$\tanh(-x) = -\tanh x. \qquad \tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\boxed{A(\underline{\sigma} \to \underline{\sigma}') = \frac{1}{2}\left(1 - \sigma_v \tanh \beta h_v^{loc}\right)}$$

$$h_v^{loc} = \sum_w J_{vw}\sigma_w + h_v.$$

Total effective bias on spin.

"Total local magnetic field".



$$A(\underline{\sigma} \to \underline{\sigma}') = \frac{1}{2}\left(1 - \sigma_v \tanh \beta h_v^{loc}\right)$$ . accept prob

Reject move with prob

$$1 - A(\sigma \to \underline{\sigma}') = \frac{1}{2}\left(1 + \sigma_v \tan \beta h_v^{loc}\right) \equiv R(\underline{\sigma} \to \underline{\sigma}').$$

Cases :

- $\sigma_v = +1$ initially and $\underline{h_v^{loc}} = \sum_w J_{vw}\sigma_w + h_v > 0$.

  $R(\underline{\sigma} \to \underline{\sigma}') > A(\underline{\sigma} \to \underline{\sigma}')$ . i.e tendency is not to flip.

- $\sigma_v = -1$ initially and $\underline{h_v^{loc}} > 0$.

  $R(\underline{\sigma} \to \underline{\sigma}') < A(\underline{\sigma} \to \underline{\sigma}')$ i.e tendency is to flip.

In Glauber dynamics at the end <u>what controls the move or the spin flip at a vertex</u> is the <u>"local bias or magn field"</u>.

|| The spin has the tendency to flip so as to align with $h_v^{loc}$.

## Heat bath dynamics or Gibbs sampling.

- can be viewed as a generalization of Glauber to general measures and general alphabets.
- really useful when $\pi$ is of "Gibbs type" or Markov Random Field.

Algo:
- Select an initial assignment $\underline{x} = (x_1 \dots x_N)$.
- Select a vertex $v \in V \in \{1 \dots N\}$ unif at random
- Compute the conditional probability of $\underline{y}$ conditioned on $(y_w = x_w \text{ for } w \neq v)$.

  and make the move $\underline{x} \to \underline{y}$ with this conditional probability:

$$\mathbb{P}(\underline{y} \mid \{y_w = x_w, w \neq v\}) = \frac{\pi(x_1 \dots x_{v-1}, y_v, x_{v+1} \dots x_N)}{\sum_{y_v \in \mathcal{X}} \pi(x_1 \dots x_{v-1}, y_v, x_{v+1} \dots x_N)}.$$

$$\mathbb{P}(A \mid B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}.$$

Exercise: Detailed Balance in General & Reduction to Glauber for Ising.