Ising

Metropolis

Glauber

dynamics

\[
\text{G} = (v, E)
\]

\[
V = E, t, x, t - \text{spin configuration}
\]

binary alphabet \[X = \{t, \bar{t}\}\]

"degrees of freedom" on "spins"
a) Ising Model  

b) Metropolis algo.

c) Glauber algo or dynamics.  

(Heat bath dynamics.)

\[ G = (\mathcal{V}, \mathcal{E}) , \quad \mathcal{V} = \{1, 2, 3, \ldots, N\} \]

binary alphabet \( \chi = \{-1, 1\} \) and

"degrees of freedom" or "spins" \( \sigma \in \chi \).  

\( \sigma_1 \in \{+1\} \)

\( \sigma_2 \in \{-1\} \)

\( \sigma_3 \in \{+1\} \)

\( \sigma_4 \in \{-1\} \)

\( \sigma_5 \in \{+1\} \)

Complete graph for example:

\[ \prod(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z} \]

Hamiltonian:

\[ H(\sigma) = -\sum_{(n,m) \in \mathcal{E}} J_{nm} \sigma_n \sigma_m - \sum_{n \in \mathcal{V}} h_n \sigma_n \]

assignment or "spin configuration"

\[ \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N) \]

\[ Z = \sum_{\sigma \in \chi^N} e^{-\beta H(\sigma)} \]

"Partition function"
Another important example: square grid $\mathbb{Z}^d$.

Some intuition: (from physics)

- The “spins” represent magnetic moments, which are carried by atoms in a crystal. Say:

- Up spin $\sigma = +1$
- Down spin $\sigma = -1$

- Gross simplification with only two directions for the magnetic moments.

- There “spins” interact.

Energy of a configuration of two spins

- Favorable:
  - $J_{sw} > 0$
  - $J_{sw} < 0$

- Unfavorable:
  - $J_{sw} > 0$
  - $J_{sw} < 0$
The ferromagnetic model: all $J_{\omega\omega} > 0$.

Consider the special case $h_\omega = 0$:

$$H(\sigma) = -\sum_{(\omega\omega) \in \mathcal{E}} J_{\omega\omega} \sigma_\omega \sigma_\omega$$

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

- The anti-ferromagnetic: all $J_{\omega\omega} < 0$.

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

is a minimum, second min.

Stepened configuration

Frustration: difficulty will come for large graphs because you cannot win all terms simultaneously in $H(\sigma)$. 
The study of optimization of $H(S)$ and of sampling $W(S) = \frac{e^{-\beta H(S)}}{Z}$ is a difficult problem especially for "frustrated" systems with all possible signs for $\sum_i m_i > 0$ and $\sum_i m_i < 0$.

- Interpretation of $\beta$: inverse of the temperature of the system $\beta = \frac{1}{kT}$
  - $\beta$ small: corresponds to a nearly high temperature uniform Measure on state space $\mathcal{X}^N$.
  - Typical spin configurations will be more a less uniform at random from $\mathcal{X}^N$.

\[ \begin{array}{c}
\begin{array}{ccccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\end{array} \]

$-\beta H(S)$ is peaked around the Minima of $H(S)$ ($\beta \rightarrow +\infty$).

$\beta$ large: $e^{-\beta H(S)}$ is peaked around the Minima of $H(S)$ ($\beta \rightarrow +\infty$).

Typical spin configuration fluctuations around Minima.
Formal definitions:

- **Magnetization:**

  \[
  m(\beta) = \frac{1}{N} \sum_{\sigma} \langle \sigma \rangle
  \]

  where notation \( \langle \sigma \rangle = \frac{E}{\Omega} (\sigma) = \sum \sigma \times \Omega(\sigma) \) is the bracket notation.

  \[\text{average}\]

  \( \rightarrow \) Intuitively this is the total magnetic moment.

  \( \rightarrow \) If \( m(\beta) \approx 0 \) the system is not magnetized.

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

  Model displays transition between these two behaviors typically as \( \beta \) varies from high temp to low high temp.

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

  Remark (exercise):

  \[
  \langle \sigma \rangle = \frac{1}{\beta} \frac{\partial}{\partial \beta} \ln Z
  \]

  \[
  Z = \sum_{\sigma \in \chi} \exp \left\{ \beta \sum_{\omega \in \omega} \sigma_{\omega} + \beta \sum_{\omega \in \omega} \omega \sigma_{\omega} \right\}
  \]

  But computing \( Z \) is difficult and in general impossible.
Instead we go back to:

\[ m(\beta) = \langle \frac{1}{N} \sum_{\mathbf{\sigma} \in \mathcal{V}} \sigma \rangle = \frac{1}{N} \sum_{\mathbf{\sigma} \in \mathcal{V}} \sigma \]

and consider an estimator based on an MCMC algo.

\[ \hat{m}(\beta) = \lim_{t \to \infty} \left\{ \frac{1}{N} \sum_{\mathbf{\sigma} \in \mathcal{V}} \sigma(t) \right\} \]

where \( \sigma_0, \sigma_1, \ldots, \sigma(t), \ldots \) is an MCMC chain with stationary \( \bar{\sigma} \).

We can also compute any sort of average:

\[ \left\langle A(\sigma) \right\rangle \quad \text{e.g.} \quad \frac{1}{N} \left\langle H(\sigma) \right\rangle \]

\( \frac{1}{N} \) internal energy per vertex per site.

again:

\[ \lim_{t \to \infty} \left\{ \frac{1}{N} \sum_{\mathbf{\sigma} \in \mathcal{V}} H(\sigma(t)) \right\} \]
A bit of background on the phase transition phenomena (scratch the surface of the subject).

\[ G = (V, E) \] is a complete graph.

\[ S_{vw} = \frac{S}{N} > 0 \quad \text{for all } (v, w) \in E \]

\[ h_v = h \in \mathbb{R} \quad \text{for all } v \in V. \]

Ferromagnetic Ising Model on a complete graph.

\[ H(\sigma) = -\frac{S}{2N} \sum_{v \neq w} \sigma_v \sigma_w - h \sum_{v \in \text{complete graph}} \sigma_v \]

acts like a bias in \( \exp(-\beta H(\sigma)) \).

\[ \frac{1}{2} \left( \sum_{v \in \text{complete graph}} \sigma_v \right)^2 - N \cdot \exp(-\beta H(\sigma)). \]

It possible to in fact compute \( Z \) and also average \( \sigma \); and in particular

\[ m(\beta) = \frac{1}{N} \sum_{v \in \text{complete graph}} \sigma_v. \]
Finding is eventually:

\[ m(\beta, h) = \left\langle \frac{1}{N} \sum_{\sigma} \sigma \right\rangle. \]

\[ \text{for} \quad \beta > 0 \quad \text{for the complete ferro-magnetic model} \]

\[ \text{you can plot} \quad m(\beta) = \lim_{h \to 0^+} m(\beta, h). \]

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

\[ m(\beta) \]

\[ +1 \rightarrow +1 \]

\[ -1 \rightarrow -1 \]

\[ T = T_c = 5^{-1} \]

\[ \text{sharp phase transition "sudden" at} \]

\[ T = \beta^{-1}. \]

\[ \text{high temperature behavior.} \]

\[ \text{Average spin magnetization is zero.} \]

\[ \text{Typical spin conf is "disordered".} \]

\[ \text{Lowtemp behavior} \]

\[ \text{Average spin Mag} \neq 0. \]

\[ \text{Typical spin conf are fluctuations of (all+1)} \]

\[ \text{and (all-1).} \]
d) **Metropolis algorithm (Trial)**

c) **Glauber dynamics**

- Heat bath dynamics in general

d) **Simulation results**

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**Metropolis algorithm**

Hamiltonian (energy a cost).

$$ H(\sigma) = - \sum_{\text{edges} \in E} J_{\sigma_w \sigma_v} - \sum_{v \in V} h_v \sigma_v. $$

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

$$ G = (V, E). $$

**Also:**

- Select a vertex $v \in V$ uniformly at random (with prob $\frac{1}{N}$).
- Propose the move $\sigma \rightarrow \sigma'$: $\sigma'_w = \sigma_w$ \quad $w \neq v$
  $\sigma'_v = -\sigma_v$ \quad $v \in E$.

- Compute the cost difference: $\Delta E(\sigma \rightarrow \sigma') = H(\sigma') - H(\sigma)$.

- Accept the move with probability $A(\sigma \rightarrow \sigma') = \min(1, e^{-\beta \Delta E})$. 
\[ H(\sigma) = -\sum_{\omega\in \omega} J_{\omega \omega} \sigma_{\omega} \sigma_{\omega} - \sum_{\nu} h_{\nu} \sigma_{\nu}. \]

\[ \Delta E(\sigma \rightarrow \sigma') = H(\sigma') - H(\sigma). \]

New energy - old energy.

\[ A(\sigma \rightarrow \sigma') = \min \left(1, e^{-\beta \Delta E(\sigma \rightarrow \sigma')} \right) \]

\[ = \begin{cases} 1 & \text{if } \Delta E(\sigma \rightarrow \sigma') < 0 \quad \text{New Energy} \prec \text{Old Energy} \\ e^{-\beta \Delta E} & \text{if } \Delta E \geq 0 \quad \text{New Energy} \succ \text{Old Energy} \end{cases} \]

Remark

\[ e^{-\beta \Delta E} = \frac{e^{-\beta H(\sigma')}}{e^{-\beta H(\sigma)}} = \frac{\pi(\sigma')}{\pi(\sigma)}. \]

- chain is irreducible, aperiodic (self loops), detailed balance is satisfied and \( \pi \) is invariant.

\[ \begin{cases} \text{chain is ergodic and} \\ \text{it is a limiting distribution} \end{cases} \]

- This is certainly true for \( N \) finite and time (\# of steps)
. Final important point,

\[ \Delta E(\sigma \to \sigma') = H(\sigma') - H(\sigma), \]

\[ = \left\{ - \sum_{(k, \ell) \in E} k\ell \sigma_k \sigma'_{\ell} - \sum_{k \in V} h_k \sigma_k \right\} \]

\[ - \left\{ - \sum_{w, \ell \in E} w\ell \sigma_w \sigma'_{\ell} - \sum_{k \in V} h_k \sigma_k \right\}. \]

We have selected vertex \( \sigma \) and \( \sigma'_w = \sigma_w \) if \( w \in \sigma \)

If \((k, \ell) \notin \sigma\) and \( k \notin \sigma\) then terms simplify.

and it remains only:

\[ \sigma'_w = \sigma_w \]

\[ = \left( \sum_{w} \sum_{\sigma'_w} w \sigma_w \sigma'_w - h_w \sigma'_w \right) - \left( \sum_{w} \sum_{\sigma'_w} w \sigma_w \sigma'_w - h_w \sigma'_w \right) \]

\[ = 2 \left( \sigma'_w \sum_{w} \sigma_w + h_w \right) \]

For interaction you get only neighbors of \( w \) that share an edge count. For the bias, only the vertex \( v \) enter.
Glauber dynamics, or algo.

- Select a vertex $i$ at random with uniform
  $V = \{1, \ldots, N\}$

- Propose the move $\sigma \rightarrow \sigma'$ s.t.
  $\sigma'_w = \sigma_w, \quad w \neq i$
  $\sigma'_i = -\sigma_i \quad \text{flip of } i \text{ spin.}$

- Accept the move with acceptance probability
  \[ A(\sigma \rightarrow \sigma') = \frac{1}{2} \left\{ 1 + \tanh \left( \frac{\Delta E(\sigma \rightarrow \sigma')}{2} \right) \right\} \]

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

\[ \Delta E(\sigma' \rightarrow \sigma) = H(\sigma') - H(\sigma) \]
\[ = 2 \left( \sum_w J_{ww} \sigma_w + h_w \sigma_w \right) \quad (\text{as before}). \]
Again this chain is irreducible and aperiodic.

Exercise: detailed balance is satisfied again.

⇒ There is a flat dish which is flat.

... ⇒ chain is irreducible, periodic, for an i.e. cycodic and it is a limiting dish.

Remark:

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

\[ \Delta E = 2 \sigma_\alpha \sum_w \Delta_{\sigma w} \sigma_w + 2 h_\alpha \sigma_\alpha \]

⇒ \[ A(\sigma \to \sigma') = \frac{1}{2} \left( 1 - \tanh \frac{\beta}{2} \left( \sum_w \Delta_{\sigma w} \sigma_w + h_\alpha \right) \right) \]

\[ \tanh(-x) = -\tanh x \]

\[ \tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}} \]

\[ A(\sigma \to \sigma') = \frac{1}{2} \left( 1 - \sigma_\alpha \tanh \beta h_{\text{loc}} \right) \]

\[ h_{\text{loc}} = \sum_w \Delta_{\sigma w} \sigma_w + h_\alpha \]

Total effective bias on spin.

"Total local magnetic field"
\[
A(c \rightarrow c') = \frac{1}{2} \left( 1 - \sigma_c \tanh \beta h^\text{loc}_c \right) \cdot \text{accept move.}
\]

Reject move with prob
\[
1 - A(c \rightarrow c') = \frac{1}{2} \left( 1 + \sigma_c \tanh \beta h^\text{loc}_c \right) \equiv R(c \rightarrow c').
\]

Case:

- \( \sigma_c = +1 \) initially, and \( h^\text{loc}_c = \sum \sum \sigma_w h_w + h_c > 0 \).

\( R(c \rightarrow c') > A(c \rightarrow c') \) i.e. tendency is not to flip.

- \( \sigma_c = -1 \) initially, and \( h^\text{loc}_c > 0 \).

\( R(c \rightarrow c') < A(c \rightarrow c') \) i.e. tendency is to flip.

In Glauber dynamics at the end what controls the move on the spin flip at a vertex is the "local bias or mean field." The spin has the tendency to flip so as to align with \( h^\text{loc}_c \).