Phase transitions:

Statistical Physics:

Goal: understand physical phase transitions, where small change in a parameter such as temperature controlling local interactions causes dramatic change in global (macroscopic) properties.

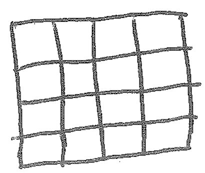
Example: boiling point: water (liquid) $\Leftrightarrow$ steam (gas).

Ising model: most well studied (& simplest) model.

Model of ferromagnetism (metal becomes magnetized)

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

Common example: 2-dimensional integer lattice $\mathbb{Z}^2$ of volume $n=|V|$, so box of side length $\sqrt{n} \times \sqrt{n}$:



5×5 box of $\mathbb{Z}^2$

Ising model configurations: $\Omega = \{+1,-1\}^V$

Let $\beta = \dfrac{1}{\text{Temperature}} > 0$ be inverse temperature.

For $\sigma \in \Omega$, energy $H(\sigma)$ for the Ising model:

Hamiltonian: $$H(\sigma) = -\sum_{(v,w)\in E} \sigma(v)\sigma(w) = -\big(M(\sigma) - D(\sigma)\big)$$

where $M(\sigma) = \#$ of monochromatic edges $= \left|\{(v,w)\in E : \sigma(v) = \sigma(w)\}\right|$

$D(\sigma) = \#$ of non-mono. edges $= \left|\{(v,w)\in E : \sigma(v) \neq \sigma(w)\}\right|$

Gibbs Distribution:

$$\mu(\sigma) = \frac{\exp(-\beta H(\sigma))}{Z}$$

where $Z = \sum_{\tau\in\Omega} \exp(-\beta H(\tau))$ = Partion function.

Note, $$\mu(\sigma) = \frac{e^{\beta(M(\sigma)-D(\sigma))}}{Z} = \frac{e^{2\beta M(\sigma)}}{e^{\beta|E|}\,Z} \propto e^{2\beta M(\sigma)}$$

proportional to

$e^{\beta|E|}$: constant for graph G.

Since $M(\sigma) + D(\sigma) = |E|$

Configurations with highest weight: all + & all −
(called ground states)

but only 2 such low energy configurations
whereas many configurations with half + & half −
(namely, $\binom{n}{n/2}$ such configurations)

Which dominates? energy or entropy.

$\beta = 0$ (infinite temperature) then vertices are indpt. of each other (all configurations equally likely).
So typical configuration is half +/half −.

$\beta = \infty$ (zero temperature) only all + & all − have positive prob.

What happens for $0 < \beta < \infty$?

For $\sqrt{n} \times \sqrt{n}$ box, ∂V are vertices on (internal) boundary of V.

Boundary condition is assignment $\tau : \partial V \to \{+1, -1\}$

Given τ, look at μ_τ is conditional Gibbs dist.:

$$\text{Let } \Omega_\tau = \{\sigma \in \Omega : \tau(\partial V) = \sigma(\partial V)\}$$

$$\text{then } \mu_\tau(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\tau} \text{ for } \sigma \in \Omega_\tau$$

$$\& \ Z_\tau = \sum_{\sigma \in \Omega_\tau} e^{-\beta H(\sigma)}$$

Let O = origin of $(2l+1) \times (2l+1)$ box, $l = \Theta(\sqrt{n})$.

$$\text{Let } P_\tau^l = \Pr_{\mu_\tau}(\sigma(O) = +) = \Pr\left(\begin{array}{c}\text{origin is } + \\ \text{for b.c. } \tau\end{array}\right)$$

Note, P^l_τ is maximized for τ=all+

$\rightarrow$ denote as P^l_+

& minimized for τ'=all−

$\rightarrow$ denote as P^l_-

Is $P^l_+ \stackrel{?}{=} P^l_-$

No since l is finite they are different.

What about as $l \to \infty$?

Is $\underbrace{\lim_{l\to\infty} P^l_+}_{= P_+} \stackrel{?}{=} \underbrace{\lim_{l\to\infty} P^l_-}_{= P_-}$

$\exists \beta_c$,

$\forall \beta \leq \beta_c \quad P_+ = P_-$ (disordered phase)

$\forall \beta > \beta_c \quad P_+ \neq P_-$ (ordered phase)

What is β_c?

$$\beta_c(q) = \ln(1+\sqrt{q}) \qquad \left(\text{for } q=2,\ \beta_c \approx .8814\right)$$

$q=2$ is the Ising model, 2 possible spins $\{+,-\}$ [Onsager '44]

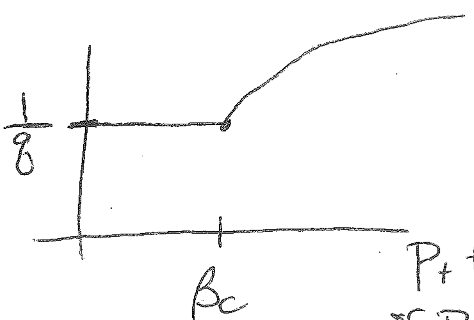
$q\geq 3$ is the Potts model, q possible spins $\{1,\dots,q\}$

energy same as $H(\sigma) = $ (# of mono. edges)

$\Rightarrow$ phase transition at β_c

In fact, [Duminil-Copin et al. '16] showed that

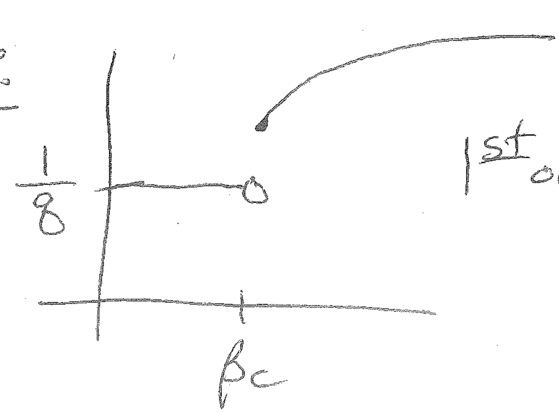
for $q\leq 4$:



2^{nd} order phase transition

P_+ for Ising or P_1 for Potts

for $q\geq 5$:



1^{st} order

MC to sample from the Gibbs distribution:

<u>Glauber dynamics</u>:

From $X_t \in \Omega$, (think of no boundary condition τ for simplicity)

1. Choose $v \in V$ u.a.r.
2. For all $w \neq v$, set $X_{t+1}(w) = X_t(w)$.
3. Choose $X_{t+1}(v) = \mu\left(\sigma(v) \mid \sigma(w) = X_{t+1}(w) \text{ for all } w \neq v\right)$

In other words,

$$X_{t+1}(v) = \begin{cases} + & \text{w.prob. } \dfrac{e^{2\beta p}}{e^{2\beta n} + e^{2\beta p}} \\ - & \text{w.p. } \dfrac{e^{2\beta n}}{e^{2\beta n} + e^{2\beta p}} \end{cases}$$

where $p = \#$ of $+$ neighbors of v in X_t

$n = \#$ of $-$ neighbors of v in X_t

The mixing time for free (or periodic) boundary: 8

$\forall \beta < \beta_c$, $T_{mix} = O(n \log n)$

$\forall \beta > \beta_c$, $T_{mix} = e^{\Omega(\sqrt{n})}$

[Lubetzky-Sly '12] $\to$ For $q=2$, at $\beta=\beta_c$, $T_{mix} = \text{Poly}(n)$.

[Gheissari-Lubetzky '18]
& $q=3$
for $q=4$, at $\beta=\beta_c$, $T_{mix} = n^{O(\log n)}$ (should be ?)
& $q \geq 5$, at $\beta=\beta_c$, $T_{mix} = \exp(\Theta(n))$

Why slow for low-temperatures?

$q=2$ Ising:

to go mostly + to mostly − have to pass balanced at some time but these are unlikely.

for $\beta > \beta_c$, for $\sigma \sim \mu$, $\Pr\Big(\underbrace{\frac{1}{n}\Big|\sum_{v \in V} \sigma(v)\Big| \gg 0}_{\text{mostly + or mostly −}}\Big) \geq 1 - \exp(\Omega(n))$

How to overcome bottleneck for $\beta > \beta_c$?

1) Simulated annealing:

Goal: Sample from μ_{β^*} for given β^*

define sequence: $\beta_0 < \beta_1 < \cdots < \beta_\ell$

where $\beta_0 \simeq 0$, $\beta_\ell = \beta^*$

& $Z_{\beta_i} \approx Z_{\beta_{i-1}}$ so $\mu_{\beta_i} \approx \mu_{\beta_{i-1}}$

how to do that:

set $\beta_{i-1} = \beta_i \left(1 - \frac{1}{m}\right)$

Note, for $\sigma \in \{+1,-1\}^V$,

Then $w_{\beta}(\sigma) = e^{\beta M(\sigma)}$

So $\frac{w_{\beta_{i-1}}}{w_{\beta_i}} \geq \left(1 - \frac{1}{m}\right)^m \geq e^{-1/2}$

thus, $Z_{\beta_i} \geq Z_{\beta_{i-1}} \geq Z_{\beta_i}/e^{1/2}$.

How to set $\beta_0 \simeq 0$?

$$\beta_0 = \frac{1}{n!} \simeq \left(1-\frac{1}{m}\right)^{\ell} \simeq e^{-\ell/m} = \frac{1}{n^n}$$

for $\ell = mn\ln n$

But we know rapid mixing for β small

So maybe suffices to choose such a β as β_0?

Simulated annealing alg.:

~~For $i=0 \rightarrow$~~

Let X_0 be arbitrary. Let $t=0$.

For $i=0 \rightarrow \ell$:

From the last state X_t run the Glauber Dynamics at inverse temp. β_i for t_i steps.

Idea: use sample from ~~μ_{β_i}~~ $\mu_{\beta_{i-1}}$ as initial state for Glauber dynamics at μ_{β_i}

Metropolis coupled MCMC:

have l chains run simultaneously

$$X_t = (X_t^0, X_t^1, \ldots, X_t^l)$$

i^{th} chain: X_t^i is run at β_i

Within temp. step: choose random i & perform Glauber step on X_t^i

Between temp. step: choose random $i < l$ & ~~attempt to~~ swap X_t^i & X_t^{i+1} with prob.

$$\min\left\{1, \frac{\omega_{\beta_i}(X_t^{i+1})}{\omega_{\beta_i}(X_t^i)} \times \frac{\omega_{\beta_{i+1}}(X_t^i)}{\omega_{\beta_{i+1}}(X_t^{i+1})}\right\}$$

& o/w stay the same.