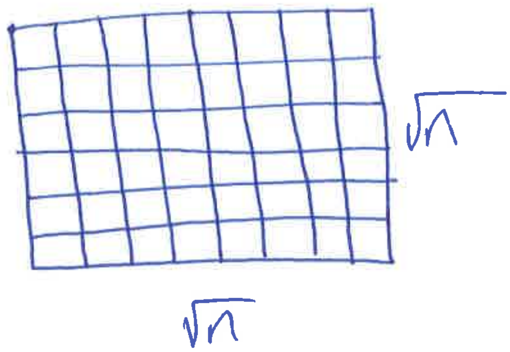
$\sqrt{n} \times \sqrt{n}$ box of 2-dimensional grid $\mathbb{Z}^2$.

$G =$ 

Configuration: $\sigma : V \to \{+1, -1\}$ & $\Omega = \{+1, -1\}^V$

Hamiltonian: $H(\sigma) = -\sum_{(i,j)\in E} \sigma_i \sigma_j$

inverse temperature $\beta \geq 0$:

Boltzmann or Gibbs Distribution:

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

where $Z = \sum_{\sigma} e^{-\beta H(\sigma)}$ is the partition function.

This is the ferromagnetic Ising model.
Antiferromagnetic model has $\beta < 0$.

$-H(\sigma) =$ # of monochromatic edges $-$ # of antiparallel edges

So most likely configurations are all $+$ & all $-$.

But there are a lot more configurations with $\frac{1}{2}+$ & $\frac{1}{2}-$, so which dominates? Energy or Entropy? Depends on β.

If $\beta = 0$ (this is infinite temperature)

Then every configuration is equally likely so μ is dominated by balanced configurations (half $+$/half $-$)

If $\beta = \infty$ (zero temperature)

then all $+$ & all $-$ are the only two configurations with positive probability.

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

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

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

Then,
$$\Omega_\tau = \{\sigma \in \Omega : \tau(\partial V) = \sigma(\partial V)\}$$

= configurations on V which are consistent with τ on ∂V.

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

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

Let O = origin be the center of $(2\ell+1) \times (2\ell+1)$ box.

$\ell = \Theta(\sqrt{n})$.

& $\cancel{\mu(\sigma(0)) =}$

let $p_\tau^\ell = \Pr(\mu_\tau(\sigma(0) = +)) = \Pr\left(\begin{array}{c}\text{Origin is } + \\ \text{for b.c. } \tau\end{array}\right)$

P^ℓ_τ is maximized for τ = all + $\to$ denote as P^ℓ_+
& minimized for τ = all − $\to$ P^ℓ_-

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

No, since ℓ is finite they are clearly different.

What about for $\ell \to \infty$?

Is $\lim\limits_{\ell\to\infty} P^\ell_+ \stackrel{?}{=} \lim\limits_{\ell\to\infty} P^\ell_-$

$$\underset{P_+}{\shortparallel} \qquad\qquad \underset{P_-}{\shortparallel}$$

$\exists\, \beta_c,$

$\forall \beta \le \beta_c$ $\quad$ $\cancel{\lim\limits_{\ell\to\infty}}$ $P_+ = P_-$ (disordered)

$\forall \beta > \beta_c$ $\quad$ $P_+ \neq P_-$ (long-range order)

What is β_c?

$$\beta_c(q) = \frac{q-1}{q}\log(1+\sqrt{q})$$

[Beffara, Duminil-Copin '12]

$q=2$ is the Ising model.

$q>2$ is $\Omega = \{1,2,\dots,q\}^V$ is the Potts model.

This is a phase transition,

$\lim_{l\to\infty} \mu_+^l$ gives a measure on $\mathbb{Z}^2$.

And for $\beta \le \beta_c$ there's a unique measure on $\mathbb{Z}^2$.

for $\beta > \beta_c$ multiple.

Glauber Dynamics / Gibbs sampler:

MC to sample from μ.

From $X_t \in \Omega$, (No b.c.)

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,

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

where $n = \#$ of $-$ neighbors of v
$p = \#$ of $+$ " "

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

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

For $q=2$: at $\beta = \beta_c$, $T_{mix} = poly(n)$.

How might we get around "torpid" <u>mixing</u> for $\beta > \beta_c$?

<u>Two popular approaches:</u>

Simulated annealing & Metropolis-coupled MCMC.

Markov Chain Monte Carlo.

Next class: Swendsen–Wang algorithm.

Simulated annealing:

Idea: physical annealing = heat a material above recrystallization & then slowly cooling

Sequence of inverse temperatures: $\beta_0 = 0 < \beta_1 < \cdots < \beta_N = \beta$

for our desired β.

For $i = 0 \to N$,

Run Glauber Dynamics for a large # of steps T at β_i.

Let X_T^i be the final step.

Let $X_0^{i+1} = X_T^i$ be the initial step for β_{i+1}.

Repeat

Cooling schedule: $\beta_0 = 0 \lneq \beta_1 < \cdots < \beta_N = \beta$

Naive cooling schedule: $\beta_{i+1} = \beta_i\left(1 + \frac{1}{n}\right)$

MC^3: N chains.

i^{th} chain run at β_i

At step t, configuration is $(X_t^0, X_t^1, \ldots, X_t^N)$

- With prob. $\frac{1}{2}$,

(or update all $N+1$ chains) Choose $i \in \{0, 1, \ldots, N\}$ u.a.r.

& do a Glauber step for X_t^i

others stay the same

- With prob. $\frac{1}{2}$,

Choose $i \in \{0, 1, \ldots, N-1\}$ u.a.r.

Set $X' = (X_t^0, \ldots, X_t^{i-1}, X_t^{i+1}, X_t^i, X_t^{i+2}, \ldots, X_t^N)$

So swap states i & $i+1$

Set $X_{t+1} = X'$ with prob.

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