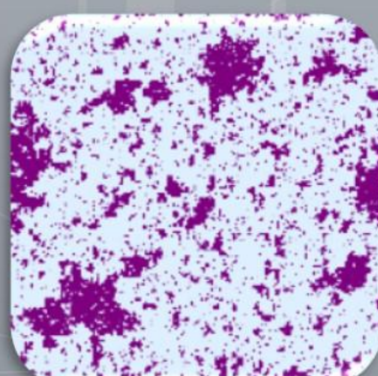
PIMS

Summer school in Probability



Markov Chain Minicourse

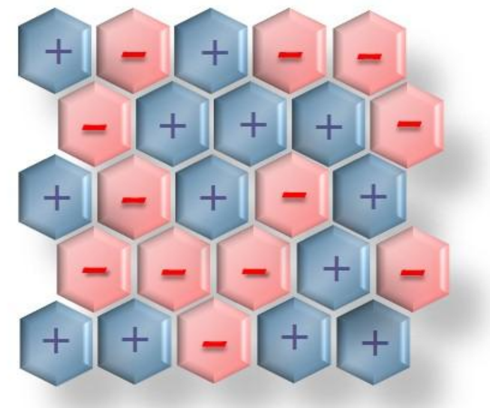
lecture 2

Eyal Lubetzky

Microsoft Research

The Ising model

- Underlying geometry: finite graph $G=(V,E)$.
- Set of possible configurations:



$$\Omega=\{\pm 1\}^V$$

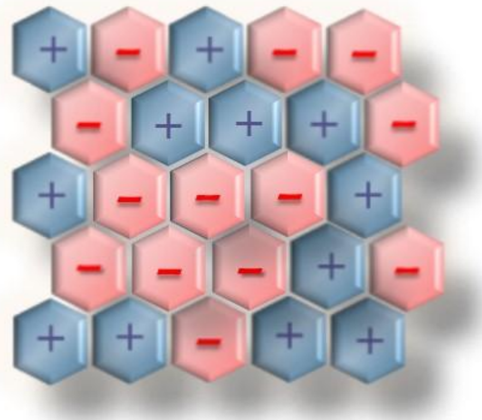
- Probability of a configuration $\sigma\in\Omega$ given by the *Gibbs distribution*

$$\mu(\sigma)=\frac{1}{Z(\beta)}\exp\left(\beta\sum_{xy\in E}\sigma(x)\sigma(y)\right)$$ [no external field]

- *Ferromagnetic* $\leftrightsquigarrow$ inverse-temperature $\beta\geq 0$.
- Goal: sample the Gibbs distribution efficiently. Main focus is on lattices at or near a certain critical β_c.

Glauber dynamics for Ising

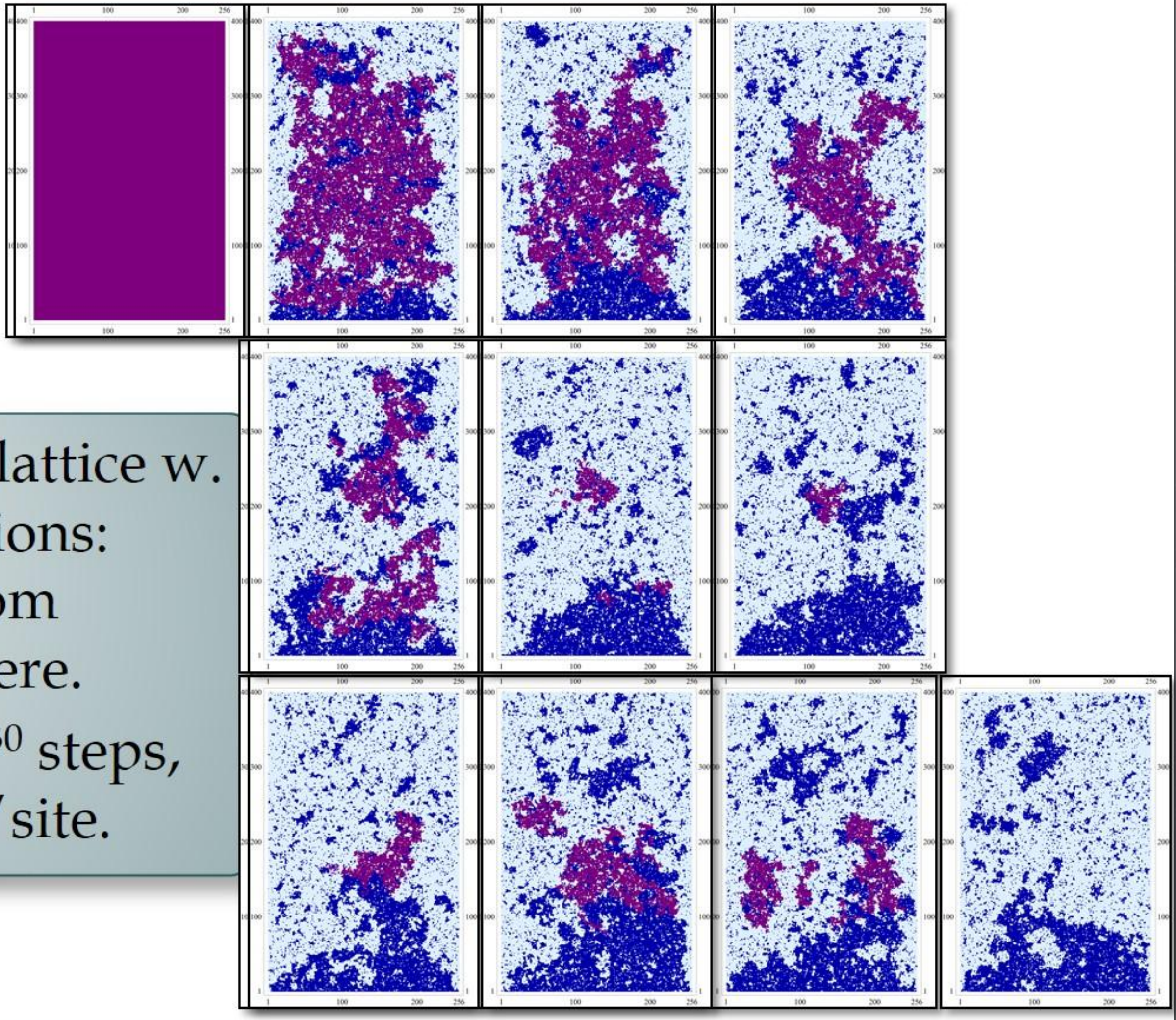
- One of the most commonly used MC samplers for the Gibbs distribution:
  - Update sites via *iid* Poisson(1) clocks
  - Each update replaces a spin at $u \in V$ by a new one $\sim \mu$ conditioned on $V \setminus \{u\}$ (heat-bath version).



- Ergodic reversible MC with stationary measure μ.
- Introduced by Glauber in 1963. Other versions of the dynamics include e.g. Metropolis.
- For $\beta \geq 0$ we can couple two chains such that one is always above the other (*monotone coupling*).

Glauber dynamics for critical Ising

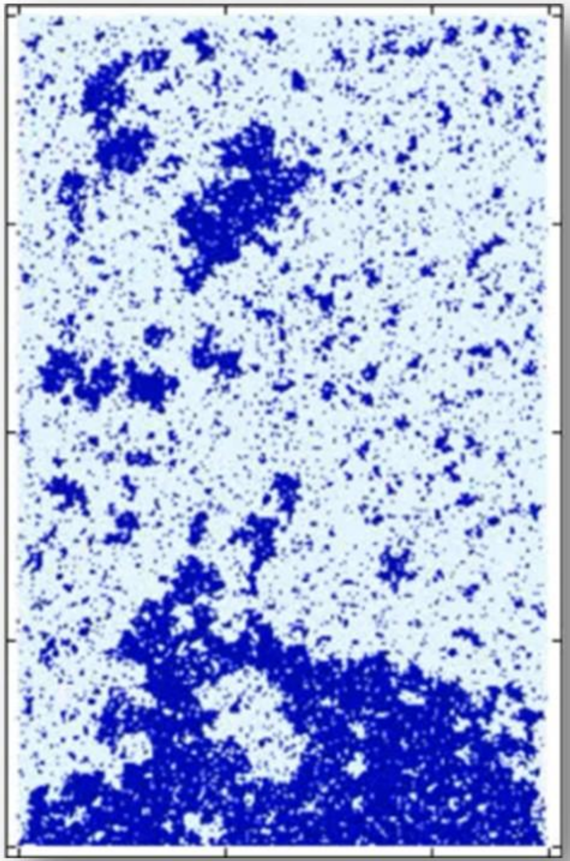
- *How fast does the dynamics converge?*



- 256 x 400 square lattice w. boundary conditions:
  (+) at bottom
  (−) elsewhere.
- Frame every $\sim 2^{30}$ steps, *i.e.* $\sim 2^{13}$ updates/site.

Example: Glauber dynamics for critical Ising on the square lattice

- 256 x 400 square lattice w. boundary conditions:
  - (+) at bottom
  - (−) elsewhere.
- Frame after 2^{20} steps, i.e. $\sim$10 updates per site.



Strong stationary times

- Recall: Let (X_t) be a Markov chain.
  - The *random mapping representation* of (X_n) is an i.i.d. sequence (Z_t) and a map f such that $X_t = f(X_{t-1}, Z_t)$.
  - We say that τ is a *randomized stopping time* for (X_t) if it is a stopping time for such a representation (Z_t) .
- Def.: A *strong stationary time* for a Markov chain (X_t) with stationary measure π is a randomized stopping time τ such that $X_\tau \sim \pi$ independent of τ, *i.e.*

$$\forall t : \mathbb{P}(\tau = t, X_\tau = y) = \mathbb{P}(\tau = t)\pi(y).$$

$$(\iff \forall t : \mathbb{P}(\tau \le t, X_\tau = y) = \mathbb{P}(\tau \le t)\pi(y).)$$

Bounding the mixing time

- **THEOREM:** ([Aldous-Diaconis '86,'87]

If τ is a strong stationary time for a Markov chain (X_t) with stationary distribution π then

$$\max_{x\in\Omega}\left\|\mathbb{P}_x(X_t\in\cdot)-\pi\right\|_{\mathrm{TV}}\leq\max_{x\in\Omega}\mathbb{P}_x(\tau>t).$$

- **COROLLARY:**

Let τ be a strong stationary time for a Markov chain (X_t) with stationary distribution π and let t_0 be an integer such that $\max_{x\in\Omega}\mathbb{P}_x(\tau>t_0)\leq\varepsilon$. Then $t_{\mathrm{mix}}(\varepsilon)\leq t_0$.

Example 1: strong stationary times

- Let (X_t) be a lazy simple RW on the hypercube $\{0,1\}^n$.
- Random mapping representation: $Z_t = (J_t, I_t)$ where $J_t \in [n]$ and $I_t \in \{0,1\}$ are both independent uniform.
- Strong stationary time:

$$\tau_{\text{refresh}} = \min\left\{t : \{J_1,\ldots,J_t\} = [n]\right\}.$$

- By the coupon collector paradigm:

$$\max_{x\in\Omega} \mathbb{P}_x\left(\tau_{\text{refresh}} > n\log n + cn\right) \le \mathrm{e}^{-c},$$

and so

$$t_{\text{mix}}(\varepsilon) \le n\log n + \log(\tfrac{1}{\varepsilon})n\,.$$

Example 2: strong stationary times

- Let (X_t) be the top-to-random card shuffle: Start with n cards, repeatedly insert top into a random position.
- Strong stationary time: 1 step after bottom reaches top:

$$\tau = \min\left\{t : X_t(1) = n\right\} + 1.$$

  - Proof: By induction, given that the cards below original bottom card (card # n) are $\{x_1,\ldots,x_k\}$ their ordering is uniform over S_k.
- Similarly to the coupon collector: $\tau = \tau_1 + \tau_2 + \ldots + \tau_{n-1} + 1$ for $\tau_i \sim \mathrm{Geom}(k/n)$ ind.
- COROLLARY:

$$t_{\mathrm{mix}}(\varepsilon) \le n \log n + \log(\tfrac{1}{\varepsilon})n\,.$$

Proof (strong stationary times bound)

- Use *separation distance*: $$\mathrm{sep}(t) \triangleq \max_{x,y\in\Omega}\left[1 - \frac{\mathbb{P}_x(X_t = y)}{\pi(y)}\right].$$
- Proof will follow from showing that:
  - Strong stationary times bound separation distance:

$$\mathrm{sep}(t) \le \max_{x\in\Omega} \mathbb{P}_x(\tau > t).$$

  - Separation distance bounds total variation distance:

$$\max_{x\in\Omega}\left\|\mathbb{P}_x(X_t \in \cdot) - \pi\right\|_{\mathrm{TV}} \le \mathrm{sep}(t).$$

- Strong stationary times bound separation distance:

If τ is a strong stationary time then for any $x, y \in \Omega$,

$$1 - \frac{\mathbb{P}_x(X_t = y)}{\pi(y)} \le 1 - \frac{\mathbb{P}_x(X_t = y,\ \tau \le t)}{\pi(y)} = \mathbb{P}_x(\tau > t)$$

and therefore $\mathrm{sep}(t) \le \max_{x\in\Omega} \mathbb{P}_x(\tau > t)$.

- Separation distance bounds total variation distance:

$$\begin{aligned}\left\|\mathbb{P}_x(X_t \in \cdot) - \pi\right\|_{\mathrm{TV}} &= \sum_{\substack{y\in\Omega \\ \pi(y)>\mathbb{P}_x(X_t=y)}} \left[\pi(y) - \mathbb{P}_x(X_t = y)\right] \\ &= \sum_{\substack{y\in\Omega \\ \pi(y)>\mathbb{P}_x(X_t=y)}} \pi(y)\left[1 - \tfrac{\mathbb{P}_x(X_t=y)}{\pi(y)}\right]\end{aligned}$$

and hence $\max_{x\in\Omega} \left\|\mathbb{P}_x(X_t \in \cdot) - \pi\right\|_{\mathrm{TV}} \le \mathrm{sep}(t)$. ∎

Lower bounds on mixing

- We have seen that the top-to-random shuffle has
$$t_{\mathrm{mix}}(\varepsilon) \le n \log n + \log(\tfrac{1}{\varepsilon})n\,.$$
Is this tight? How do we provide lower bounds?
- Direct approach: by definition of TV distance.
- <u>PROPOSITION</u>: [Aldous-Diaconis '86]

Let (X_t) be the top-to-random shuffle on n cards. Then for any $\varepsilon > 0$ there exists some $C > 0$ such that
$$d_{\mathrm{TV}}(n \log n - Cn) > 1 - \varepsilon\,.$$
In particular, $t_{\mathrm{mix}}(1-\varepsilon) > n \log n - Cn\,.$

Top-to-random lower bound

- Start from the inverse identity $X_0=(n,\ldots,1)$.
- Def: $A_j \triangleq \{\text{items } j, j-1,\ldots,1 \text{ have original relative order}\}$
  Observe:
  - As long as card j (*i.e.* j-th from bottom) did not reach the top (even +1 step) the event A_j necessarily holds!
  - Stationary (uniform) probability: $\pi(A_j) = 1/j!$
- Def: $\tau_j = \min\{t : X_t(1) = j\}$. (j[th]-bottom $\rightsquigarrow$ top)
- Proof will follow from showing that for some $C(j)>0$,

  $$\mathbb{P}(\tau_j \geq t_n) \geq 1 - \frac{1}{j-1}, \text{ where } t_n \triangleq n\log n - Cn,$$

  by choosing a large enough constant j.

Top-to-random lower bound (*ctd.*)

- Remains to analyze τ_j , the time it takes the j[th] from bottom card to hit the top of the deck. As before, τ_j is a sum of independent geometrics:

$$\tau_j = \sum_{i=j}^{n-1} \tau_{j,i} \quad , \quad \tau_{j,i} \sim \mathrm{Geom}(i / n)$$

$$\mathbb{E}[\tau_{j,i}] = n/i \qquad \mathrm{Var}(\tau_{j,i}) < n^2/i^2$$

- It follows that $\mathbb{E}[\tau_j] \geq n \log n - n(1 + \log(j))$,
$\mathrm{Var}(\tau_j) \leq n^2/(j-1)$,

and Chebyshev's inequality implies that

$$\mathbb{P}(\tau_j < n \log n - Cn) \leq \frac{1}{j-1}$$

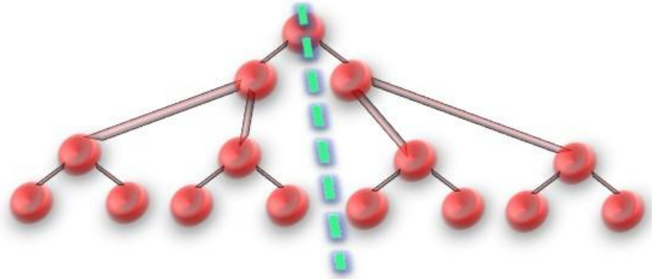
for a choice of $C = 2 + \log(j)$. ∎

Lower bounds via conductance

- Systematic approach: Relate mixing to conductance ([Lawler-Sokal '88, Jerrum-Sinclair '89]) :
  - For a chain with transition kernel P and stationary distribution π define:
$$Q(x,y) \triangleq \pi(x)P(x,y) \;\; ; \;\; Q(A,B) \triangleq \sum_{x\in A,\, y\in B} Q(x,y).$$
  - The *conductance* (or *bottleneck ratio*) of a set S is
$$\Phi(S) \triangleq \frac{Q(S,S^c)}{\pi(S)}$$
and the *conductance* (*Cheeger constant*) of the chain is
$$\Phi \triangleq \min_{S:\pi(S)\leq \frac{1}{2}} \Phi(S).$$
- Intuitively: the chain is trapped inside S and this represents a bottleneck for the mixing.

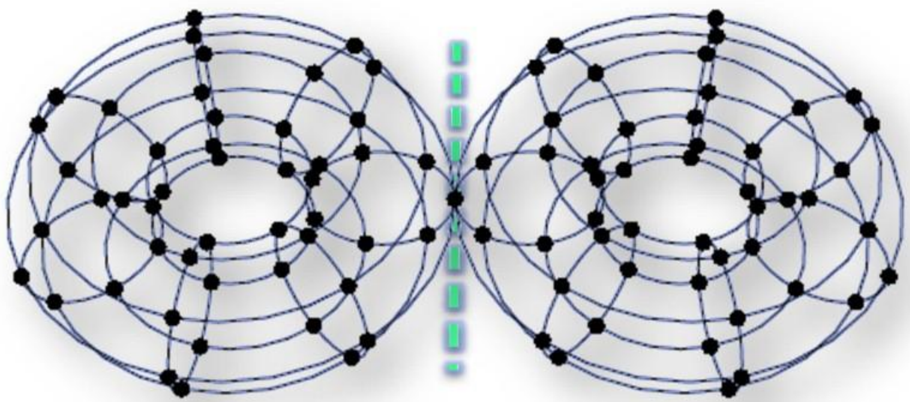
Examples of bottlenecks

- Binary tree on $n = 2^k - 1$ vertices:



$$\Phi \asymp 1/n$$
$$t_{\text{mix}} \asymp n$$

- Two glued 2-dimensional tori on n^2 vertices each:



$$\Phi \asymp 1/n^2$$
$$t_{\text{mix}} \gtrsim n^2$$

Lower bound on mixing

- THEOREM:

Every Markov chain satisfies $t_{\text{mix}}(\frac{1}{4}) \geq \dfrac{1}{4\Phi}$.

- PROOF:

Let μ_S be the stationary dist. conditioned on being in S :

$$\mu_S(x) \triangleq \pi(x)\mathbf{1}_{\{x\in S\}} / \pi(S).$$

By the triangle inequality

$$\underbrace{\left\|\mu_S - \pi\right\|_{\text{TV}}}_{\geq \frac{1}{2} \text{ due to } S^c} \leq \underbrace{\left\|\mu_S - \mu_S P^t\right\|_{\text{TV}}}_{\text{CLAIM: This is } \leq t\,\Phi(S)} + \underbrace{\left\|\mu_S P^t - \pi\right\|_{\text{TV}}}_{\leq \frac{1}{4} \text{ for } t = t_{\text{mix}}(\frac{1}{4})}.$$

Lower bound on mixing (ctd.)

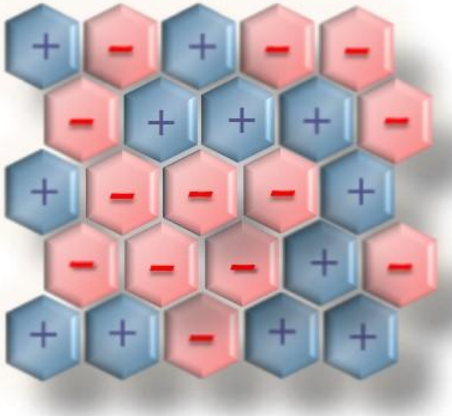
- It remains to show $\left\| \mu_S - \mu_S P^t \right\|_{\mathrm{TV}} \le t\,\Phi(S)$.
- Key inequality: $\left\| \mu_S - \mu_S P \right\|_{\mathrm{TV}} = \Phi(S)$ by definition.
- Using the fact $\left\| \varphi P - \psi P \right\|_{\mathrm{TV}} \le \left\| \varphi - \psi \right\|_{\mathrm{TV}}$ (coupling) and the triangle inequality:

$$\left\| \mu_S P^t - \mu_S \right\|_{\mathrm{TV}} \le \left\| \mu_S P^t - \mu_S P^{t-1} \right\|_{\mathrm{TV}} + \ldots + \left\| \mu_S P - \mu_S \right\|_{\mathrm{TV}}$$
$$\le t\,\Phi(S).$$

- It now follows that $t_{\mathrm{mix}}(¼)\ \Phi(S) \ge ¼$. ■

Bottlenecks in Glauber for Ising

- Recall the definition of the dynamics:
  - Update sites via *iid* Poisson(1) clocks
  - Each update replaces a spin at $u \in V$ by a new one $\sim \mu$ conditioned on $V \setminus \{u\}$ (heat-bath version).

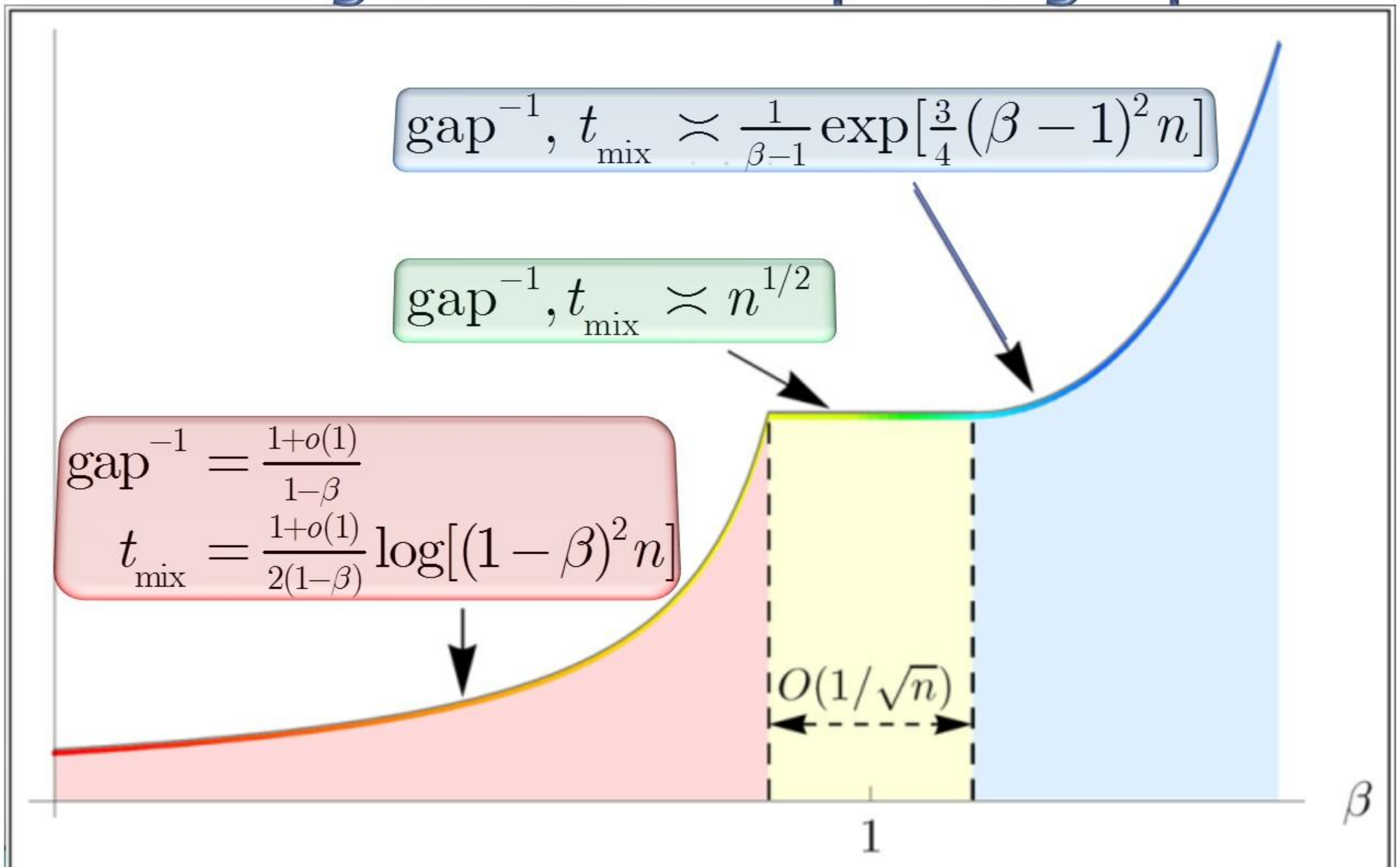


- *How fast does it converge to equilibrium?*
  - Can be exponentially slow in the size of the system: At low temp. (large β) there may be a bottleneck between "plus" and "minus" states (see tutorial).

General (believed) picture for the Glauber dynamics

- Setting: Ising model on the lattice $(\mathbb{Z}/n\mathbb{Z})^d$.
  Belief: For some critical inverse-temperature β_c :
- Low temperature: $(\beta > \beta_c)$
  gap^{-1} and t_{mix} are ***exponential*** in the surface area.
- Critical temperature: $(\beta = \beta_c)$
  gap^{-1} and t_{mix} are ***polynomial*** in the surface area.
- High temperature: $(\beta < \beta_c)$
  - ***Rapid*** mixing: $\mathrm{gap}^{-1} = \mathrm{O}(1)$ and $t_{\mathrm{mix}} \asymp \log\ n$
  - Mixing occurs abruptly, *i.e.* there is ***cutoff***.

Gap/mixing-time evolution for Ising on the complete graph



(Scaling window established in [Ding, L., Peres '09])