MCAA lecture 7

Summary of the last two lectures

Let $(X_n, n \geq 0)$ be an ergodic Markov chain with finite state space S $(|S| = N)$ and limiting & stationary distribution π satisfying detailed balance.

Then $$\|P_i^n - \pi\|_{TV} \leq \frac{1}{2\sqrt{\pi_i}} \cdot \lambda_*^n \quad \forall i \in S, \forall n \geq 1$$

where $$\lambda_* = \max_{1 \leq k \leq N-1} |\lambda_k| = \max\{-\lambda_{N-1}, \lambda_1\} < 1$$

Is it the end of the story? In general, no!

The quest for a matching lower bound

Theorem

Under all the assumptions of the previous page and the additional assumption that

$$|\phi_0^{(k)}| = 1 \quad \text{and} \quad |\phi_j^{(k)}| \leq 1 \quad \forall j \in S \quad \forall_{0 \leq k \leq N-1}$$

it holds that $\|P_{\underset{\substack{\uparrow \\ i=0}}{0}}^n - \pi\|_{TV} \geq \frac{\lambda_*^n}{2}$

Reminder: $\|\mu - \nu\|_{TV} = \frac{1}{2} \cdot \sum_{i \in S} |\mu_i - \nu_i|$

$$= \sup_{A \in S} |\mu(A) - \nu(A)| \qquad \mu(A) = \sum_{i \in A} \mu_i$$

$$= \frac{1}{2} \cdot \sup_{\phi : S \to [-1,+1]} |\mu(\phi) - \nu(\phi)| \qquad \mu(\phi) = \sum_{i \in S} \mu_i \phi_i$$

Proof

$$\| P_0^n - \pi \|_{TV} = \frac{1}{2} \cdot \sup_{\phi : S \to [-1,+1]} | P_0^n(\phi) - \pi(\phi) |$$

$$\geq \frac{1}{2} \cdot \sup_{1 \leq k \leq N-1} | \underline{P_0^n(\phi^{(k)})} - \underline{\pi(\phi^{(k)})} | \qquad \left(\begin{array}{l} |\phi_j^{(k)}| \leq 1 \\ \forall k, \forall j \in S \end{array} \right)$$

$$P_0^n(\phi^{(k)}) = \sum_{j \in S} P_{0j}(n) \, \phi_j^{(k)} = (P^n \phi^{(k)})_0 = \underline{\lambda_k^n \cdot \phi_0^{(k)}}$$

$$\pi(\phi^{(k)}) = \sum_{j \in S} \pi_j \, \phi_j^{(k)} = \sum_{j \in S} \pi_j \, \phi_j^{(k)} \cdot \underbrace{\phi_j^{(0)}}_{\equiv 1} = \sum_{j \in S} u_j^{(k)} u_j^{(0)}$$

$$= (u^{(k)})^T \cdot u^{(0)} = 0 \qquad k \neq 0$$

So $\| P_0^n - \pi \|_{TV} = \frac{1}{2} \cdot \sup_{1 \leq k \leq N-1} | \lambda_k^n | \cdot \underbrace{| \phi_0^{(k)} |}_{=1} = \frac{1}{2} \cdot \lambda_*^n$ #

Recap: Under all the assumptions made, we have:

$$\frac{\lambda_*^n}{2} \leq \| P_0^n - \pi \|_{TV} \leq \boxed{\frac{1}{\sqrt{\pi_0}}} \cdot \frac{\lambda_*^n}{2}$$

Example 1

Cyclic RW on $S = \{0, 1, \ldots, N-1\}$ N odd

with $p_{ij} = \frac{1}{2}$ if $j = i+1$ or $i-1 \pmod N$

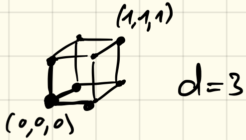
$\lambda_* = \cos\left(\frac{\pi}{N}\right) \simeq 1 - \frac{\pi^2}{2N^2}$ So $\lambda_*^n \simeq \left(1 - \frac{\pi^2}{2N^2}\right)^n \simeq \exp\left(-\frac{n\pi^2}{2N^2}\right)$

$$\underbrace{\frac{1}{2}\exp\left(-\frac{n\pi^2}{2N^2}\right)}_{\text{small when } n >> N^2} \leq \| P_0^n - \pi \|_{TV} \leq \underbrace{\frac{\sqrt{N}}{2} \cdot \exp\left(-\frac{n\pi^2}{2N^2}\right)}_{\text{small when } n >> N^2 \log N}$$

So mixing time $T_\varepsilon \in \left[\Theta(N^2), \Theta(N^2 \log N)\right]$

Example 2

RW on the hypercube $S=\{0,1\}^d$



States in S are denoted as $x \in \{0,1\}^d$

(= vector of 0's & 1's)

Transition matrix:

$$P_{xy} = \begin{cases} \frac{1}{d+1} & \text{if } y=x \text{ or } y = x \underset{\substack{\uparrow \\ \text{add} \\ \text{mod 2}}}{\oplus} \underset{\substack{\| \\ (0,0,\dots 0,\underset{\substack{\uparrow \\ \text{position } t}}{1},0\dots 0)}}{e_t} \text{ for some } 1\le t\le d \\ 0 & \text{otherwise} \end{cases}$$

Equivalently, the RW does the following:

at each time step, draw $t\in\{0,1,\dots d\}$ unif. at random

$$\begin{cases} \text{if } t=0: \text{ do not move} \\ \text{if } t\geq 1: \text{ flip the } t\text{-th component of the vector } x \end{cases}$$

finite state, irreducible, aperiodic $\Rightarrow$ ergodic

$\Rightarrow$ unique limiting & stationary distribution π, detailed balance

P = doubly stochastic matrix $\Rightarrow$ $\pi_x \equiv \frac{1}{2^d}$ $\forall x \in \{0,1\}^d$

What about $\| P_0^n - \pi \|_{TV}$ for a given n?
(all-0 state) $\hookleftarrow$

<u>Theorems</u>: $\frac{1}{2} \lambda_*^n \leq \| P_0^n - \pi \|_{TV} \leq \frac{1}{2\sqrt{\pi_0}} \lambda_*^n$ $\forall n \geq 1$

We need to compute λ_* ...

Lemma

The eigenvalues and eigenvectors of P are given by:

$$\rightarrow \begin{cases} \lambda_z = 1 - \frac{2|z|}{d+1} & z \in S = \{0,1\}^d \quad \text{where } |z| = \# \text{ non-zero components of } z \\ \phi_x^{(z)} = (-1)^{z \cdot x} & \text{where } z \cdot x = \sum_{i=1}^{d} z_i x_i \qquad x, z \in S \end{cases}$$

Proof: To be proven: $P \phi^{(z)} = \lambda_z \phi^{(z)} \quad \forall z \in S$

$$\left(P\phi^{(z)}\right)_x = \sum_{y \in S} p_{xy} \phi_y^{(z)} = \frac{1}{d+1} \left(\phi_x^{(z)} + \sum_{t=1}^{d} \phi_{x \oplus e_t}^{(z)} \right)$$

$$= \frac{1}{d+1} \left((-1)^{z \cdot x} + \sum_{t=1}^{d} (-1)^{z \cdot (x \oplus e_t)} \right) = \frac{1}{d+1} (-1)^{z \cdot x} \underbrace{\left(1 + \sum_{t=1}^{d} (-1)^{\overbrace{z \cdot e_t}^{= z_t}} \right)}_{= 1 + d - 2|z|}$$

$$= \frac{d+1-2|z|}{d+1} (-1)^{z \cdot x} = \underbrace{\left(1 - \frac{2|z|}{d+1}\right)}_{\lambda_z} \cdot \phi_x^{(z)} \quad \#$$

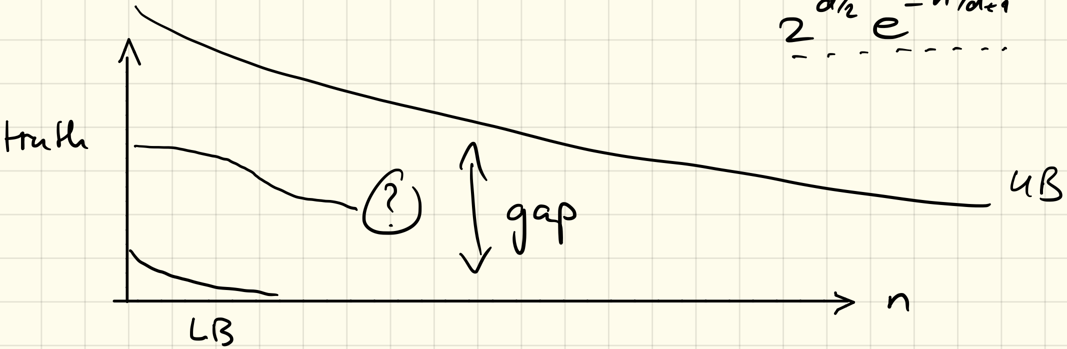
$\lambda_* = 1 - \frac{2}{d+1}$ (obtained by taking either $|z|=1$ or $|z|=d$)

So $\underline{\frac{1}{2}\left(1-\frac{2}{d+1}\right)^n} \le \| P_0^n - \pi \|_{TV} \le \frac{1}{2\sqrt{\pi_0}}\left(1-\frac{2}{d+1}\right)^n$

But $\pi_0 = \frac{1}{2^d}$, so : $= \frac{\boxed{2^{d/2}}}{2} \cdot \underline{\left(1-\frac{1}{d+1}\right)^n}$

So LB is small when $n \gg d$ $\simeq e^{-n/d+1}$

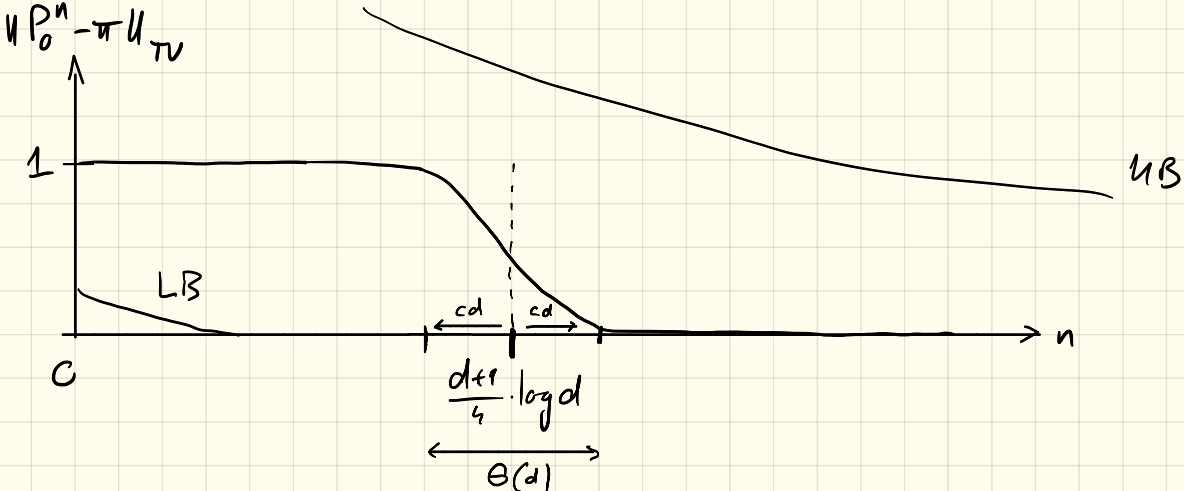
but UB is small when n is much larger than that : $\underline{2^{d/2} e^{-n/d+1}}$ i.e. $\underline{n \gg d^2}$



Cut-off phenomenon (Diaconis)

Let c be a large positive "constant". Then

- if $n = \frac{d+1}{4} \cdot (\log d + c)$, then $\| P_0^n - \pi \|_{TV} \longrightarrow 0$ as c increases
- if $n = \frac{d+1}{4} \cdot (\log d - c)$, then $\| P_0^n - \pi \|_{TV} \longrightarrow 1$ as c increases



Proof ideas

$$X_0 = (\overbrace{0,0,0,0,0,0}^{d \text{ bits}})$$

$$\downarrow \text{flip}$$

$$X_1 = (0,0,0,1,0,0)$$

$$\downarrow \text{flip}$$

$$X_2 = (1,0,0,1,0,0)$$

$$\downarrow \text{flip}$$

$$X_3 = (1,0,0,0,0,0)$$

...

X = "typical" sequence :

(distributed according to π)

$$\begin{cases} \text{each bit} = \begin{cases} 0 \\ 1 \end{cases} \text{wp } \frac{1}{2} \\ \text{all bits are independent} \end{cases}$$

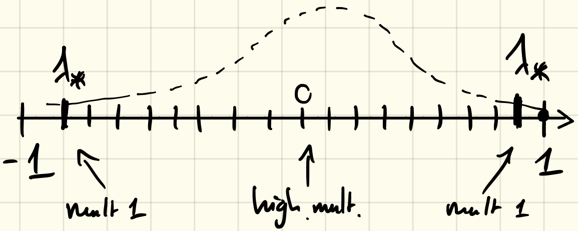
$$\mathbb{E}(|X|) = \frac{d}{2}$$

$$\text{Var}(|X|) = d$$

$$\underbrace{|X|}_{\#\ 1\text{'s in the sequence } X} \in \left[\frac{d}{2} - \sqrt{d}, \frac{d}{2} + \sqrt{d} \right]$$

UB: $\|P_0^n - \pi\|_{TV} \le \frac{1}{2}\sqrt{\sum_{z\in S\setminus\{0\}} \lambda_z^{2n} \underbrace{\left(\phi_0^{(z)}\right)^2}_{=1}}$

$\lambda_z = 1 - \frac{2|z|}{d+1}$: $\boxed{\cdots} = \frac{1}{\sqrt{2}} e^{-c/2}$ if $n = \frac{d+1}{4}(\log d + c)$



LB: $\|P_0^n - \pi\|_{TV} = \sup_{A\subset S} |P_0^n(A) - \pi(A)| \ge |P_0^n(A) - \pi(A)|$ $\forall A \in S$

choose A s.t. $P_0^n(A) \simeq 0$ and $\pi(A) \simeq 1$

"#"

$A = \left\{x\in S : \left||x| - \frac{d}{2}\right| \le \frac{\beta}{2}\sqrt{d}\right\}$: $\begin{cases} \pi(A) \simeq 1 \\ P_0^n(A) \simeq 0 \quad \text{if } n = \frac{d+1}{4}(\log d - c) \end{cases}$