

## Announcements

- start recording
- scribe: work w/other scribe to produce one set of notes
- My OH: Mon 12:30-1:30, Thu 9-10
- TF hybrid setting/OH: Mon 2-3, Wed 2-3, Wed 5-6, Thu 5:30-6:30
- PS 1 due Fri : note collaboration + late day policies
- If Zoom gets down, check Piazza
- sync whiteboard
- gather after class
- register to vote
- screenshare + jamboard?

## Agenda

- random walks on directed graphs
- Pagerank
- Markov Chain Monte Carlo

# Perron-Frobenius Thm for Symmetric Matrices

Let  $M =$  symmetric, nonnegative real matrix (e.g. adjacency or rw normalized adj. mx of undirected  $G$  or directed)  
 w/corresponding graph  $G$  (i.e.  $E = \{(a,b) : M(a,b) > 0\}$ ).

Complex Eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_n$  multiplicities = # occurrences as a root of  $\det(xI - M)$

Then 1)  $\exists$  nonnegative <sup>right</sup> e-vector  $v_1$  w/ <sup>real</sup> e-value  $\lambda_1$

2)  $\lambda_1 \geq |\lambda_j|$  for  $j > 1$

2)  $\lambda_1 \geq \lambda_2$  with strict inequality if  $G$  connected + strict positivity of  $v_1$

3)  $\lambda_1 \geq -\lambda_n$  with strict inequality if  $G$  connected + unibipartite

Moreover, if  $G$  bipartite then  $\lambda_{n-i} = -\lambda_i$  for  $i = 0, \dots, n-1$

$\rightarrow$  3) if  $G$  is strongly connected, <sup>can take</sup>  $v_1$  to be strictly positive

4) If  $G$  is strongly connected + aperiodic (gcd of all cycle lengths = 1)

then  $\lambda_1 > |\lambda_j|$  for  $j = 2, \dots, n$

5) If  $G$  has period  $k$ , then the set of e-values is closed under mult. by  $e^{2\pi i/k}$

# Random Walks on Undirected Graphs

$$M(a,b) = \underline{w(b,a)}$$

$n = \# \text{ vertices}$

$G$  undirected, weighted.  $W = MD^{-1}$   
out

$P_0 =$  initial probability distribution on vertices  $\in \mathbb{R}^n$

$P_t =$  prob dist. after  $t$  steps of r.w.

$$= W^t P_0$$

Let  $v_i =$  normed  $e^-$  vector  $i$  from P-F

How to analyze?

$$\pi = \frac{v_i}{\|v_i\|_2} \text{ prob dist.}$$

$\rightarrow \mu_i = 1$

Claim:  ~~$W$  has a basis of  $e$ -vectors  $\phi_1, \dots, \phi_n$~~

$$W\pi = \pi$$

~~w/ eigenvalues  $\omega_1 \geq \omega_2 \geq \omega_3 \geq \dots \geq \omega_n$~~   
 ~~$\leftarrow$  need not be orthogonal~~

$W = S L S^{-1}$  for an upper-triangular matrix  
whose diagonal is  $\mu_1, \mu_2, \dots, \mu_n$   
 $\pi = S e_1$  (by Jordan Normal Form)



Assume  $G$  strongly connected + aperiodic ("ergodic")

$$W^t = \underline{S} \underline{L^t} \underline{S^{-1}} \quad L^t \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega_2^t & 0 \\ 0 & 0 & \omega_3^t \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} 1 & & & \\ c_1 \pi & & & \\ & c_2 \pi & & \\ & & \dots & \\ & & & c_n \pi \\ & & & & 1 \end{pmatrix}$$

$$c_1 = c_2 = \dots = c_n = 1$$

We also don't know  $\pi$

well-defined even for directed  $G$

Thm:  $\max_{j \geq 1} |\omega_j| = \max_{\text{prob. dist } P} \frac{\|W_P - \pi\|_{\pi^{-1}}}{\|P - \pi\|_{\pi^{-1}}} \stackrel{\text{def}}{=} \omega_1$

where  $\|x\|_{\pi^{-1}} \stackrel{\text{def}}{=} \sqrt{\sum_{a=1}^n \frac{x(a)^2}{\pi(a)}}$

Proof:  $\max_{j \geq 1} |\omega_j| \stackrel{ps1}{=} \max_{x \perp \psi_1} \frac{\|Ax\|}{\|x\|}$

$= \max_{y: D^{1/2} y \perp \psi_1} \frac{\|D^{1/2} W y\|}{\|D^{1/2} y\|}$  ( $A = D^{1/2} W D^{1/2}$ )

$= \max_{y: \sum_a y_a = 0} \frac{\|W y\|_{\vec{d}^{-1}}}{\|y\|_{\vec{d}^{-1}}}$  ( $x = D^{-1/2} y$ )

$= \max_{\text{prob dist } P} \frac{\|W(P - \pi)\|_{\vec{d}^{-1}}}{\|P - \pi\|_{\vec{d}^{-1}}}$  ( $P = \pi + cy$ )

$= \max_{\text{prob dist } P} \frac{\|W_P - \pi\|_{\pi^{-1}}}{\|P - \pi\|_{\pi^{-1}}}$

By def:  $\|W^t P_0 - \pi\|_{\pi^{-1}} \leq \omega_{\pi}^t \cdot \|P_0 - \pi\|_{\pi^{-1}}$

- initial distance  $\|P_0 - \pi\|_{\pi^{-1}} \leq \|P_0\|_{\pi^{-1}} \leq \sqrt{\frac{1}{\pi_{\min}}}$

- final  $\ell_1$  distance (= 2 \* total variation distance)

$\|W^t P_0 - \pi\|_1 = \sum_a \frac{|W^t P_0(a) - \pi(a)|}{\pi(a)^{1/2}} \cdot \pi(a)^{1/2}$

$\leq \left( \sum_a \frac{(W^t P_0(a) - \pi(a))^2}{\pi(a)} \right)^{1/2} \cdot 1$

Cauchy-Schwarz  $= \|W^t P_0 - \pi\|_{\pi^{-1}}$

Thm: for every start distribution  $P_0$

$\|W^t P_0 - \pi\|_1 \leq \omega_{\pi}^t \cdot \|P_0\|_{\pi^{-1}} \leq \omega_{\pi}^t \cdot \frac{1}{\sqrt{\pi_{\min}}}$

where  $\pi_{\min} = \min_a \pi(a) \in \left[ \frac{d_{\min}}{d_{\max} n}, \frac{1}{n} \right]$

$\pi_{\min}$  can be exponentially small even in digraphs of bounded degree

Coc: "Mixing time" to get to within  $\ell_1$  dist.  $\epsilon$

is  $t = O\left(\frac{\log\left(\frac{nd_{\max}}{\epsilon d_{\min}} \cdot \frac{1}{\pi_{\min}}\right)}{1 - \omega_{\pi}}\right)$

PS2:  $\omega_{\pi}$  can be 1 even in ergodic G

Q: how to ensure  $\omega_{\pi} < 1$ ?

A:  $\omega_{\pi} = \max\{\omega_2, -\omega_n\}$

$\omega_2 < 1$  iff G connected

$\omega_n > -1$  iff G nonbipartite

Lazy Random Walk :  $\tilde{W} = \frac{1}{2}W + \frac{1}{2}I$

$\tilde{w}_i = \frac{1+w_i}{2} = 1$ , so  $\tilde{w}_\pi = \tilde{w}_2 = \frac{1+w_2}{2}$

if  $G$  is strongly connected and  $1 - \tilde{w}_\pi = \frac{1-w_2}{2} = \frac{\lambda_2}{2}$

then  $\tilde{w}_\pi < 1$  (PS2?)  $\lambda_2 = 2^{\text{nd}}$  smallest e-value of  $N = I - A$  normalized laplacian

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Converse (maybe ps 2):  $\forall$  undirected  $G \exists$  start vertex  $s$   
 such that for  $p_0 = \delta_s$ :

False for  $\omega_\pi$   $t = \Omega\left(\frac{\omega_\pi}{1-\omega_\pi} \cdot \log\left(\frac{1}{\epsilon}\right)\right)$

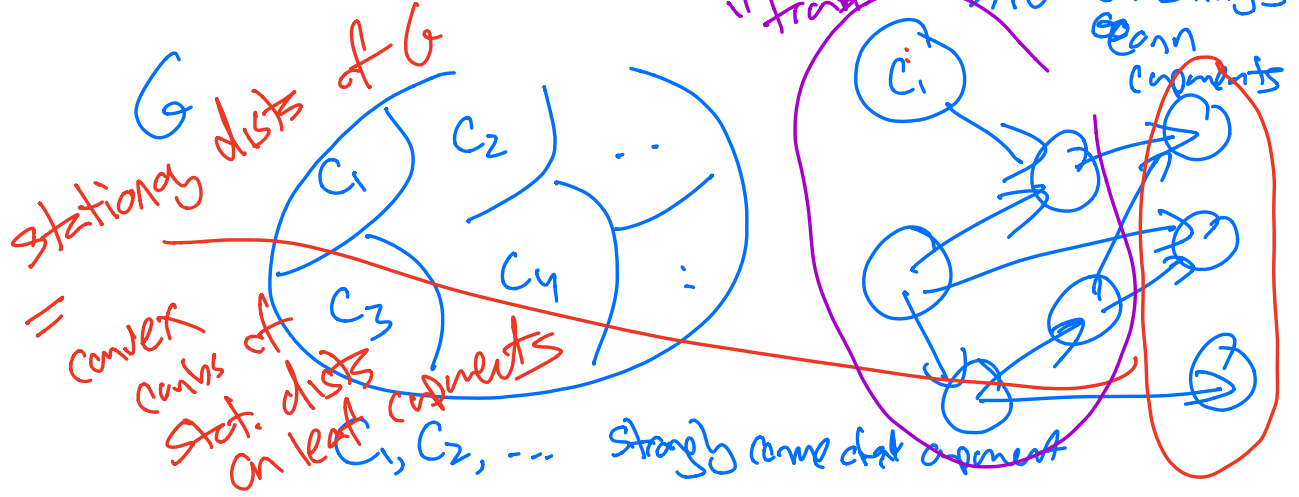
Not sure for  $\tilde{\omega}_\pi$  steps are needed to get to within  $\epsilon$  distance of  $\pi$ .

Also: for every undirected, connected, nonbipartite  $G$ ,  
 $\omega_\pi \leq 1 - 1/\text{poly}(n \cdot d_{\max})$  (cf. ps 1)  
 so mixing time  $\leq \text{poly}(n \cdot d_{\max})$ .

False for ergodic directed  $G$ .

Mixing time can be  $2^{\Omega(n)}$  even for bounded-degree digraphs.

Q: What happens in digraphs that are not strongly connected?



# PageRank

$M$  adjacency matrix of web graph

$M(a,b) = \#$  links from page  $b$  to page  $a$

$$W = M D_{out}^{-1}$$

$$\tilde{W} = (1-\alpha)W + \underbrace{\alpha J}_{\text{every entry } \frac{1}{n}}$$

PageRank vector = (unique) stationary distribution  $\pi$  of  $\tilde{W}$

→ Mixing time  $t_{mix} = O\left(\frac{\log(n/\epsilon)}{\alpha}\right)$

→ so can calculate  $\vec{u} = \frac{\vec{1}}{n}$

$$W\pi = \pi$$

$$(I-W)\pi = 0$$

$$\pi \approx \sum_{j=0}^t \alpha \cdot (1-\alpha)^j W^j \vec{u}$$

"Personalized" PageRank = other restart vectors

$$\pi \approx \sum_{j=0}^t \alpha \cdot (1-\alpha)^j W^j \vec{u}$$

$$\tilde{W}\pi = (1-\alpha)W\pi + \alpha \vec{u}$$

$$\left( \begin{aligned} \tilde{W}\pi = \pi &\Rightarrow \alpha \vec{u} = (I - (1-\alpha)W)\pi \\ &\Rightarrow \pi = \alpha (I - (1-\alpha)W)^{-1} \vec{u} \end{aligned} \right)$$

↑ cf. row laplacian  $I-W$

# Markov Chain Monte Carlo

goal: <sup>efficiently</sup> sample from a desired probability distribution on a high-dimensional space

Why?

- TCS: approximate counting
- Stats+ML: Bayesian inference (posterior sampling)
- Statistical physics: estimate physical properties

Example: given an undirected graph  $G$ ,  
count the # ~~spanning~~ forests of  $G$   
"  
(acyclic subgraphs)

- NP-hard to compute exactly  
(even "#P-complete")
- We'll see poly time alg for # spanning trees  
(forests)  
of size  $n-1$

Fact:

**MCMC**  
can sample a near-uniform spanning forest in  
time  $\text{poly}(n, 1/\epsilon)$

can approximately count spanning forests  
to within factor  $(1 \pm \epsilon)$   
in time  $\text{poly}(n, 1/\epsilon)$

(idea for  $\Downarrow$ ): 1) pick an edge  $e$

2) by repeated sampling, estimate

$$\hat{P}_e \approx \Pr[\text{random spanning forest contains } e]$$

Rapidly  
Mixing Markov  
Chains

3a) if  $\hat{P}_e < \frac{1}{2}$ , recursively estimate

$$\hat{Z}_{G - e} \approx \# \text{spanning forests in } G - \{e\}$$

# spanning forests

in  $G$

that don't  
contain  $e$

output

$$\frac{\hat{Z}_{G - e}}{1 - \hat{P}_e} = \hat{Z}_G$$

3b) else, merge endpoints of

# spanning forests  
in  $G$   
that contain  $e$

$e$  to get  $G'$ , recursively  
estimate  $\hat{Z}_{G'}$ , output  
 $\frac{\hat{Z}_{G'}}{\hat{P}_e}$

Q: how to sample a near-uniform spanning forest?

## Metropolis-Hastings Markov Chain

- State space = spanning forests of  $G=(V, E)$   
 $N = \# \text{ states} = \text{as large as } n^n$
- Transitions: from forest  $F \subseteq E$ 
  - pick a uniformly random edge  $e \in E$
  - let  $F' = \begin{cases} F \Delta \{e\} & \text{if this is acyclic} \\ F & \text{otherwise} \end{cases}$   
call this  $F \neq e$
- This is an  $|E|$ -regular graph on  $N$  vertices
- Goal: mixing time  $\text{poly}(n) = \text{poly}(\log N)$   
i.e.  $\omega_2 \leq 1 - 1/\text{poly}(n)$   
Proven last year! using spectral  
theory of high-dimensional expanders  
↳ [Anari-Liu-Chen Ghahramani, STOC 2019]

## Generalizations

- Weighted spanning forests

$$P[F] = \frac{w(F)}{Z}$$

$$\text{where } w(F) = \prod_{e \in F} w_e$$

$$Z = \sum_{\text{spanning forests}} w(F) \quad \text{"partition function"}$$

Statistical  
— physics

"random cluster model"

"Gibbs distribution"

- Exercise: modify Metropolis-Hastings

so that stationary distribution is above

assume all edge weights are in  $[w_{\min}, w_{\max}]$

- (Weighted) Perfect Matchings in Bipartite graphs "Dimer model"
- (Weighted) Matchings "Monomer-Dimer model"
- (Weighted) Independent Sets "Hardcore Gas Model"
- (Weighted) Colorings "Antiferromagnetic Potts Model"