Modern Spectral Graph Theory

Lecture 1: Random Walks

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Disclaimer: These notes have not been subjected to the usual scrutiny reserved for formal publications.

In this note we study random walks and mixing time in weighted undirected non-regular graphs G. The notation that we define here will be used later to study high dimensional random walks on simplicial complexes.

Given an undirected (weighted) graph G = (V, E) with weight function $w : E \to \mathbb{R}_{\geq 0}$, let $A \in \mathbb{R}_{\geq 0}^{V \times V}$ be the adjacency matrix of G.

Consider a natural probability distribution on edges of G where for any edge $\{u, v\}$

$$\pi_1(\{u,v\}) = \frac{w(\{u,v\})}{\sum_e w(e)}.$$

This distribution naturally induces a distribution on vertices; given a random edge e, we randomly drop one of the endpoints of e:

$$\pi_0(v) = \sum_e \mathbb{P}_{\pi_1}[e] \mathbb{P}[v|e] = \sum_{e:v \in e} \frac{1}{2} \pi_1(e) = \frac{\sum_{u \sim v} \frac{1}{2} w(\{u, v\})}{\sum_e w(e)} = \frac{d_w(v)}{\sum_u d_w(u)}$$

Conversely, suppose we want to sample an edge $e = \{u, v\} \sim \pi_1$. One way is to first sample a vertex $v \sim \pi_0$ and then sample an edge e|v, i.e., among all edge incident to v choose one proportional to its weight.

$$\mathbb{P}[\{u,v\}|u\}] := \frac{\pi_1\{u,v\}}{\sum_{x \sim u} \pi_1\{u,x\}}$$

We claim this process chooses e with probability $\pi_1(e)$, because,

$$\begin{split} \mathbb{P}\left[e\right] &= \mathbb{P}_{\pi_{0}}\left[v\right] \mathbb{P}\left[e|v\right] + \mathbb{P}_{\pi_{0}}\left[u\right] \mathbb{P}\left[e|u\right] \\ &= \pi_{0}(v) \frac{\pi_{1}(e)}{\sum_{f \sim v} \pi_{1}(f)} + \pi_{0}(u) \frac{\pi_{1}(e)}{\sum_{f \sim u} \pi_{1}(f)} \\ &= \pi_{0}(v) \frac{w(e)}{\sum_{f \sim v} w(f)} + \pi_{0}(u) \frac{w(e)}{\sum_{f \sim u} w(f)} \\ &= \pi_{0}(v) \frac{w(e)}{d_{w}(v)} + \pi_{0}(u) \frac{w(e)}{d_{w}(u)} = \frac{\pi(e)}{2} + \frac{\pi(e)}{2} = \pi(e). \end{split}$$

Fact 1.1. Summarizing the above observations,

- To choose $v \sim \pi_0$, we can first choose $e \sim \pi_1$ and then drop one endpoint.
- To choose $e \sim \pi_1$, we can first choose $v \sim \pi_0$ and then choose e|v.

Winter 2022

01/04/22

1.1 Random Walk Operator

We can look at the simple random walk operator on G that says if I am at vertex u, I choose an edge incident to u with probability proportional to its weight. Let

$$\mathbb{P}\left[u \to v\right] = \mathbb{P}\left[\{u, v\} | u\}\right].$$

For a function $f: V \to \mathbb{R}$, we have

$$Pf(v) := \mathbb{E}_{\{u,v\}|v} \left[f(u) \right] = \sum_{u} \mathbb{P} \left[v \to u \right] f(u).$$

The following reversibility property will also be used crucially.

$$P(u,v)\pi_0(u) = \pi_0(u)\mathbb{P}\left[\{u,v\}|u\} = \pi_1(\{u,v\})\mathbb{P}\left[u|\{u,v\}\right] = \pi_1(\{u,v\})\mathbb{P}\left[v|\{u,v\}\right] = P(v,u)\pi_0(v)$$
(1.1)

We equip the linear space \mathbb{R}^V with the following inner product: For two vectors $f, g: V \to \mathbb{R}$,

$$\langle f,g \rangle = \mathbb{E}_{v \sim \pi_0} f(v)g(v) = \sum_v \pi_0(v)f(v)g(v).$$

This naturally defines a norm, where for any such function f, $||f|| = \sqrt{\langle f, f \rangle}$.

Using the above fact, it follows that P is self-adjoint with respect to the above inner product, i.e., for any two $f, g: V \to \mathbb{R}$,

$$\langle f, Pg \rangle = \mathbb{E}_{v \sim \pi_0} \left[f(v) Pg(v) \right]$$

= $\mathbb{E}_{v \sim \pi_0} \left[f(v) \mathbb{E}_{\{u,v\}|v} \left[g(u) \right] \right]$
= $\mathbb{E}_{\{u,v\} \sim \pi_1} \mathbb{E}_{v|\{u,v\}} f(v) g(u) = \mathbb{E}_{\{u,v\} \sim \pi_1} \mathbb{E}_{v|\{u,v\}} f(u) g(v)$

Similarly, we can show that $\langle Pf, g \rangle$ is also equal to the RHS.

Fact 1.2. $\lambda_1 = 1$ and $\lambda_n \geq -1$.

Proof. First, observe that the all-ones function 1 is an eigenfunction,

 $P\mathbf{1} = \mathbf{1}.$

Second, we show $\lambda_i \leq 1$ for all *i*. For any eigenfunction $f: V \to \mathbb{R}$, with eigenvalue λ , i.e., $Pf = \lambda f$, we claim that $\lambda \leq 1$. Say $u = \operatorname{argmax}_v |f(v)|$. Then,

$$\lambda f(u) = Pf(u) = \mathbb{E}_{\{u,v\}|u} f(v) \le \mathbb{E}_{\{u,v\}|u} |f(v)| \le \mathbb{E}_{\{u,v\}|u} |f(u)| = |f(u)|.$$

In the second inequality we used $|f(v)| \leq |f(u)|$ for all $v \in V$. So, we have $\lambda \leq 1$ as desired. Also, observe from the same inequality that $|\lambda| \leq 1$ as desired. \Box

Fact 1.3. The matrix P has n-real eigenvalues with n-orthonormal eigefunctions.

Proof. The proof is fairly general and holds for any self-adjoint matrix with respect to an inner-product. First, Suppose $Pf = \lambda f$ for $f \in \mathbb{C}^n$ and $\lambda \in C$. And, recall for any function f, $\langle f, f \rangle = \mathbb{E}_u f(u) \overline{f(u)} \in \mathbb{R}$. Then,

$$\left\|Pf\right\|^{2} = \langle Pf, Pf \rangle = \langle P^{2}f, f \rangle = \lambda^{2} \left\|f\right\|^{2}$$

So, $\lambda^2 \in \mathbb{R}$.

On the other hand, suppose P has two eigenfunctions $f, g \in \mathbb{R}^n$ with eigenvalues $\lambda_f \leq \lambda_g$; then,

$$\langle \lambda_f f, g \rangle = \langle Pf, g \rangle = \langle f, Pg \rangle = \langle f, \lambda_g g \rangle.$$

Therefore, since $\lambda_f \neq \lambda_g$ we must have $\langle f, g \rangle = 0$.

It follows by the spectral theorem that P has n = |V| eigenvalues $\lambda_1 \ge \cdots \ge \lambda_n$ with corresponding orthonormal eigenfunctions f_1, \ldots, f_n such that for any $1 \le i < j \le n$,

 $\langle f_i, f_j \rangle = 0,$

and for any i, $||f_i|| = 1$.

1.2 Mixing

Theorem 1.4. For a weighted graph with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, if $\max\{|\lambda_2|, |\lambda_n|\} < 1$, then for any vertex u,

$$\lim_{t \to \infty} P^t f(u) = \mathbb{E}f.$$

Letting $f(v) = \mathbf{1}_v$, we have $\mathbb{E}f = \pi_0(v)$. So, the above theorem shows that as $t \to \infty$, the distribution of the walk converges to π_0 . In other words, π_0 is the *stationary distribution* of the simple random walk on G.

The mixing time of a random walk is defined as

$$\tau_{\max} = \min\left\{t : \|P^t(u, .) - \pi_0\|_{\mathrm{TV}} = \frac{1}{2} \sum_{v} |P^t \mathbf{1}_v(u) - \pi_0(v)| \le \frac{1}{4}, \forall u \in V\right\}$$
(1.2)

where τ_{mix} is the first time that the total variation distance of the distribution of the walk started at u, from the stationary distribution is at most a constant.

For a function $f: V \to \mathbb{R}$ define

$$\|f\|_p = (\mathbb{E}_{\pi} f^p)^{1/p}$$

More generally, we define the L_p mixing time of the walk as

$$\tau_{\min,p} := \min\left\{t: \left\|\frac{P^t(u, .)}{\pi} - \mathbf{1}\right\|_p \le \frac{1}{4}, \forall u \in V\right\}$$

Note that by Cauchy-Schwarz inequality

$$\sum_{v} |P^{t}(u,v) - \pi(v)| = \mathbb{E}_{\pi} |P^{t}(u,.)/\pi - \mathbf{1}| \le \sqrt{\mathbb{E}_{\pi} |P^{t}(u,.)/\pi - \mathbf{1}|^{2}} = \left\| \frac{P^{t}(u,.)}{\pi} - \mathbf{1} \right\|_{2}$$

So, the L_2 -mixing of a chain implies L_1 mixing (but not vice versa). And similarly, for any p > 1, L_p mixing implies L_1 mixing.

Theorem 1.5. Let G be a weighted graph with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$, such that $\lambda^* := \max\{|\lambda_2|, |\lambda_n|\} < 1$. For any $\epsilon > 0$, any function $f \in V \to \mathbb{R}$ and $t \geq \frac{\log \epsilon}{1 - \lambda^*}$

$$\left\|P^{t}f - \mathbb{E}f\right\| \leq \epsilon \left\|f\right\|.$$

Proof. Let f_1, \ldots, f_n be the orthonormal eigenfunctions of P with corresponding eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Recall $\lambda_1 = 1$ and $f_1 = \mathbf{1}$. Also note that P^t have exactly the same eigenfunctions with eigenvalues $\lambda_1^t, \ldots, \lambda_n^t$. Therefore, we can write $f = \sum_i \langle f, f_i \rangle f_i$. First, by (??),

$$P^{t}f - \mathbb{E}f = P^{t}\left(\sum_{i=1}^{n} \langle f, f_{i} \rangle f_{i}\right) - \langle f, \mathbf{1} \rangle \mathbf{1}$$
$$= \sum_{i=1}^{n} \lambda_{i}^{t} f_{i} \langle f, f_{i} \rangle - \langle f, \mathbf{1} \rangle \mathbf{1} = \sum_{i=2}^{n} \lambda_{i}^{t} \langle f, f_{i} \rangle f_{i}$$

Therefore, using the orthonormality of f_i 's,

$$\left\|P^{t}f - \mathbb{E}f\right\|^{2} = \left\langle \sum_{i} \lambda_{i}^{t} \langle f, f_{i} \rangle, \sum_{j} \lambda_{i}^{t} \langle f, f_{j} \rangle \right\rangle$$
$$= \sum_{i=2}^{n} \lambda_{i}^{2t} \langle f, f_{i} \rangle^{2}$$
$$\leq \lambda^{*2t} \left\|f\right\|^{2}$$

where in the last inequality we used $|\lambda_i| \leq \lambda^*$ for all i > 1. By the above inequality, for $t \geq \frac{\log \epsilon}{1-\lambda^*}$ we have

$$\left\|P^{t}f(u) - \mathbb{E}f\right\| \le \lambda^{*t} \left\|f\right\| = (1 - (1 - \lambda^{*}))^{t} \left\|f\right\| \le e^{-(1 - \lambda^{*})t} \left\|f\right\| = \epsilon \left\|f\right\|$$

where in the second inequality we used $1 - x \leq e^{-x}$.

Corollary 1.6. Suppose for any function $f: V \to \mathbb{R}$, $\epsilon > 0$ and $t \ge \frac{\log \epsilon^{-1}}{1-\lambda^*} \|P^t f - \mathbb{E}f\| \le \epsilon \|f\|$ then,

$$\tau_{mix,1} \le \tau_{mix,2} \le \max_{u} \frac{\log \epsilon^{-1} \pi(u)^{-1}}{1 - \lambda^*}$$

Note that in particular, if we want to bound the mixing time starting at a given vertex u, we don't need the max on the right hand side.

Proof. Fix a vertex $u \in V$ and let $f := \mathbf{1}_u / \pi_0(u)$. Then, $\mathbb{E}f = 1$.

$$||P^{t}f - \mathbb{E}f||^{2} = ||P^{t}f - (\mathbb{E}f)\mathbf{1}|| = ||P^{t}f||^{2} - 1.$$

On the other hand,

$$\begin{aligned} \left| P^{t} f \right\|^{2} &= \left\langle P^{t} f, P^{t} f \right\rangle = \mathbb{E}_{v} P^{t} f(v) \cdot P^{t} f(v) \\ &= \\ f(w) \neq 0, \forall w \neq u} \mathbb{E}_{v \sim \pi_{0}} \frac{P^{t}(v, u)}{\pi(u)} \cdot \frac{P^{t}(v, u)}{\pi(u)} \\ &= \\ \mathbb{E}_{v \sim \pi_{0}} \left(\frac{P^{t}(u, v)}{\pi(v)} \right)^{2} \end{aligned}$$

Putting these together, $\|P^t f - \mathbb{E}f\|^2 = \left\|\frac{P^t(u, \cdot)}{\pi(\cdot)} - 1\right\|^2$. Finally, since $\|f\|^2 = \frac{1}{\pi(u)}$, letting ϵ of Theorem 1.5 $\epsilon \pi(u)$ proves the claim.

Theorem 1.5 allows us to estimate the probability of any event. Say $A \subseteq V$ and we want to estimate $\pi_0(A)$. For $f = \mathbf{1}_A$ we have $\mathbb{E}f = \pi_0(A)$ and $\langle f, f \rangle \leq \pi_0(A) < 1$. So, we can use $P^t f(u)$, for a vertex $u \in V$, as an estimate of $\mathbb{E}f$. By Cauchy-Scwharz inequality,

$$\mathbb{E}_{v}|P^{t}f(v) - \mathbb{E}f| \leq \sqrt{\mathbb{E}_{u}|P^{t}f(u) - \mathbb{E}f|^{2}} = \left\|P^{t}f - \mathbb{E}f\right\|.$$

So, for $t = \frac{\log \epsilon^{-1} \log \pi(u)^{-1}}{1 - \lambda^*}$

$$|P^t f(u) - F| \le \frac{1}{\pi_0(u)} \mathbb{E}_v |P^t(v) - F| \le \epsilon \|f\|$$

Having this, we can simply estimate $\pi_0(A)$ within an additive error of ϵ (with probability $1-\delta$) by averaging k independent $f(X_t)$, where X_t is the *t*-th state that the simple random walk started at u lands on. Here, $k = O(\frac{1}{\epsilon^2} \log \delta)$ and t is as defined above.