Notes 18 Sampling spanning trees by random walk

1. RANDOM SPANNING TREES

Fix a connected graph G = (V, E) on *n* vertices. A spanning tree in *G* is an acyclic subgraph of *G* containing n - 1 edges.

We want to sample a spanning tree of G, (nearly) uniformly at random, as follows.

Random walk on spanning trees

Let T_0 be an arbitrary spanning tree of G

For $t = 0, 1, 2, \ldots$

Remove an edge from T_t uniformly at random to obtain F_t

Among all spanning trees containing F_t , uniformly pick one as the new T_{t+1}

This is a random walk/Markov chain on an auxiliary weighted graph \mathcal{T}_G , whose nodes are spanning trees in G, and two nodes in \mathcal{T}_G are adjacent if they share exactly n-2 edges.

For decades, this random walk was conjectured to mix in polynomial time. It was recently proved by Anari, Liu, Oveis Gharan, and Vinzart.

Theorem 1.1. The above random walk has eigenvalue gap at least 1/(n-1).

Eigenvalue gap β is the difference $\lambda_1 - \lambda_2$ between the two largest eigenvalues. By results in Notes12, the lazy version of the random walk mixes in polynomial time. Recall that the lazy random walk mixes in time $O((\log |V(\mathcal{T}_G)|)/\beta)$. Since $|V(\mathcal{T}_G)| \leq {\binom{n}{2}}{n-1} \leq {\binom{n^2}{n-1}} \leq n^{2(n-1)} = \exp(O(n \log n))$, the lazy random walk mixes in time $O(n^2 \log n)$. (In fact the usual, non-lazy random walk also has the same mixing time bound.)

2. BIPARTITE INCLUSION GRAPHS

Since the ambient graph G is fixed, we identify a spanning tree T in G with the set of n-1 edges in T.

Denote by Y(n-1) the sets of edges of spanning trees in G. More generally, define

$$Y(k) = \left\{ F \in {E \choose k} \mid F \text{ is acyclic} \right\} \quad \text{for } 0 \leq k \leq n-1 .$$

Decompose the random walk over spanning trees into two transitions:

- (Down) Go from $T_t \in Y(n-1)$ to $F_t \in Y(n-2)$ by removing an edge uniformly at random
- (Up) Then from F_t to $T_{t+1} \in Y(n-1)$ by choosing T_{t+1} uniformly from among all $T_{t+1} \supset F_t$

Down transition corresponds to matrix D_{n-1} , which is Y(n-1)-by-Y(n-2) (recall that a row probability vector multiplies on the left to a transition matrix). Likewise up transition corresponds to matrix U_{n-1} , which is Y(n-2)-by-Y(n-1).

 $D_{n-1}U_{n-1}$ is the transition matrix for the random walk. We want to bound $\beta(D_{n-1}U_{n-1})$.

We think of up and down transitions as random walk transitions on the auxiliary graph Γ_{n-1} :

Definition 2.1 (Bipartite inclusion graph). For $0 \le k \le n-1$, Γ_k has vertex set $Y(k) \cup Y(k-1)$. $F \in Y(k)$ is adjacent to $F' \in Y(k-1)$ if $F \supset F'$.

We will look at Γ_k for $0 \leq k \leq n-1$ later on to apply induction.

In Γ_k , down transition means moving from $F \in Y(k)$ to a random neighbor $F' \in Y(k-1)$, uniformly from among all k neighbors of F.

We will define up transition matrix U_k shortly, to move from $F' \in Y(k-1)$ to a random neighbor $F \in Y(k)$ from some distribution.

Thanks to the following proposition, $D_{n-1}U_{n-1}$ and $U_{n-1}D_{n-1}$ have the same eigenvalue gap, whenever this gap is at most 1.

Proposition 2.2. Given any matrices A and B, AB and BA have the same non-zero eigenvalues with the same multiplicities.

This proposition can be proved by showing AB and BA have essentially the same characteristic polynomials. Look up "Characteristic polynomials" on Wikipedia if interested.

Kaufman and Oppenheim came up with a way to relate $\beta(U_{n-1}D_{n-1})$ to $\beta(D_{n-2}U_{n-2})$. Of course, $\beta(D_{n-2}U_{n-2}) = \beta(U_{n-2}D_{n-2})$. One can then inductively bound $\beta(U_kD_k) = \beta(D_kU_k)$.

Proposition 2.3 (Kaufman–Oppenheim). $\beta(D_k U_k) \ge 1/k$ for $1 \le k \le n-1$.

This main proposition implies the main theorem.

3. MATRICES OF CONDITIONAL PROBABILITIES AND THEIR EIGENVALUE GAPS

To bound $\beta(D_k U_k)$ in Proposition 2.3 for each fixed k, Kaufman and Oppenheim do another induction (as we will see later) and study, for every $F \in Y(0) \cup \cdots \cup Y(n-1)$, the matrix of conditional probabilities

$$A_F \stackrel{\text{def}}{=} \left(\mathbb{P}[e \in T \text{ and } f \in T \mid F \subseteq T] \mathbb{1}(e \neq f) \right)_{e, f \in E \setminus F}$$

To get some intuition about these matrices of conditional probabilities, take $F = \emptyset$. Then

$$A_{\emptyset} = \left(\mathbb{P}[e \in T \text{ and } f \in T] \mathbb{1}(e \neq f) \right)_{e, f \in E}$$

encodes the probability that every pair of edges both appear in a random spanning tree.

The adjacency matrix A_F has a normalized version \mathcal{A}_F , whose eigenvalue gap $\beta(\mathcal{A}_F)$ measures how random the edges are in a random spanning tree T, after conditioning on F appearing in T. The closer this gap is to 1, the closer for every edge in T to be uniform (from among those that can be added to F to form a spanning tree).

To help compute the above conditional probabilities, we will look at

$$\sigma(F) \stackrel{\text{def}}{=} \mathbb{P}[\text{random spanning tree } T \text{ in } G \text{ contains } F]$$
.

For example, given distinct edges e and f not in F, the entry $A_F(e, f)$ equals $\frac{\sigma(F \cup \{e, f\})}{\sigma(F)}$.

4. n-bipartite inclusion graph

We can visualize using the *n*-bipartite inclusion graph $\Gamma_{n-1} \cup \cdots \cup \Gamma_1$. Its vertex set is $\mathcal{F} = Y(0) \cup \cdots \cup Y(n-1)$. In this and subsequent sections, we denote vertices in this graph with lowercase letters such as t and b, as opposed to uppercase letters such as F in the previous section.

Let's focus on a particular layer Y(k). Sampling a random forest f from Y(k) with probability proportional to its probability mass $\sigma(f)$ gives us a distribution π_k on Y(k), so that $\pi_k(f) = \sigma(f) / \sum_{g \in Y(k)} \sigma(g)$. The distribution π_k coincides with the following:

(1) Pick a random spanning tree T from G, then randomly remove all but k edges from T.

The probability mass function π_k satisfies

(2)
$$\pi_k(f) = \frac{1}{k+1} \sum_{g \in Y(k+1), g \supset f} \pi_{k+1}(g)$$

because the random process in Eq. (1) is the same as the following:

- (i) Choose a random spanning tree T from G
- (ii) Randomly remove all but k+1 edges from T to obtain g
- (iii) Randomly remove one more edge from g to obtain f

Every $g \in Y(k+1)$ containing f has probability $\frac{1}{k+1}$ to give rise to f.

For some applications, one may want to sample from a nonuniform target distribution π over spanning trees in Y(n-1). For example, G may have edge weights w_G , and a natural distribution π on spanning trees T would be proportional to the product of edge weights in T, so that $\pi(T) \propto \prod_{e \in T} w_G(e)$.

Almost everything in our analysis still holds with an arbitrary distribution π of spanning trees over Y(n-1).

5. UP-WALK AND DOWN-WALK

In Γ_k , layer k of the n-partite inclusion graph, there are two natural two-step walks:

• Up-walk $P_{k-1}^{\wedge} = U_k D_k$ on a weighted graph on vertex set Y(k-1)

• Down-walk $P_k^{\vee} = D_k U_k$ on a weighted graph on vertex set Y(k)

Focusing on Γ_k , abbreviate

$$T = Y(k) \qquad B = Y(k-1)$$

The down transition D_k is given by

$$D_k(t,b) \stackrel{\text{def}}{=} \frac{1}{k} \mathbb{1}(b \subset t) \quad \text{for } t \in T, b \in B \;.$$

Using Eq. (2), the up transition is given by

$$U_k(b,t) \stackrel{\text{def}}{=} \frac{\pi_k(t)}{k\pi_{k-1}(b)} \mathbb{1}(b \subset t) \qquad \text{for } b \in B, t \in T$$

Then $\pi_{k-1}^{\top}U_k = \pi_k^{\top}$. This equality means the random process in Eq. (1) is equivalent to the following:

- (i) Pick a random spanning tree T from G
- (ii) Randomly remove all but k-1 edges from T to get b
- (iii) Randomly add an edge outside b to get a forest t with probability proportional to $\pi_k(t)$
- 5.1. Down-walk. $P_k^{\vee} = D_k U_k$ induces a random walk on a weighted graph on T. A step in P_k^{\vee} also corresponds to a length-2 walk in Γ_k , from T to B to T.
- 5.2. Up-walk. $P_{k-1}^{\wedge} = U_{k-1}D_{k-1}$ corresponds to the random walk on a weighted graph on B. A step in P_{k-1}^{\wedge} also corresponds to a length-2 walk in Γ_k , from B to T to B.

An up-walk from any vertex $b \in B$ has probability 1/k of staying there, so that $P_{k-1}^{\wedge}(b,b) = 1/k$, because no matter which intermediate vertex in T is visited by this length-2 walk, there is exactly probability 1/k of finally returning to b.

5.3. Non-lazy up-walk. \tilde{P}_{k-1}^{\wedge} is the non-lazy version of P_{k-1}^{\wedge} .

A step in \tilde{P}_{k-1}^{\wedge} also corresponds to a length-2 path in Γ_k , from B to T to a different vertex in B.

$$P_{k-1}^{\wedge} = \frac{1}{k}I + \frac{k-1}{k}\tilde{P}_{k-1}^{\wedge}$$

 π_{k-1} is stationary for both P_{k-1}^{\wedge} and \tilde{P}_{k-1}^{\wedge} , as a common left-eigenvector with eigenvalue 1.

6. Spectral comparison

We now upperbound the spectrum of \tilde{P}_k^{\wedge} by the spectrum of P_k^{\vee} . It is more convenient to first transform each of them into a symmetric matrix with the same spectrum.

 \tilde{P}_k^{\wedge} and P_k^{\vee} share a common stationary distribution π_k . These transitions are both of the form $P(b,b') = A_P(b,b')/\pi_k(b)$ for symmetric A_P , so $P = \Pi^{-1}A_P$, where $\Pi = \text{Diag}(\pi_k)$. They both represent a random walk with adjacency matrix $A_P = \Pi P$ and common degree matrix Π .

Definition 6.1. Given matrices P, Q, Π , if $\Pi P, \Pi Q$ are symmetric, we write

$$P \preccurlyeq_{\Pi} Q \quad \iff \quad \Pi P \preccurlyeq \Pi Q .$$

 $P \preccurlyeq_{\Pi} Q$ is equivalent to $\Pi^{1/2} P \Pi^{-1/2} \preccurlyeq \Pi^{1/2} Q \Pi^{-1/2}$, if Π is symmetric and $\Pi \succ 0$.

Since P is similar to the symmetric matrix $\mathcal{A}_P = \Pi^{1/2} P \Pi^{-1/2}$ (the normalized adjacency matrix), they have the same spectra.

In our application, P and Q often represent transitions with a common stationary distribution (the main diagonal of Π). \mathcal{A}_P and \mathcal{A}_Q will have the same top eigenspace (spanned by $\sqrt{\pi}$, with eigenvalue 1). Applying Courant–Fischer to the orthogonal subspace,

$$P \preccurlyeq_{\Pi} Q \quad \iff \quad \mathcal{A}_P \preccurlyeq \mathcal{A}_Q \quad \Longrightarrow \\ \lambda_2(\mathcal{A}_P) = \sup_{\substack{x \perp \sqrt{\pi} \\ \|x\| = 1}} x^\top \mathcal{A}_P x \leqslant \sup_{\substack{x \perp \sqrt{\pi} \\ \|x\| = 1}} x^\top \mathcal{A}_Q x = \lambda_2(\mathcal{A}_Q) ,$$

and hence $\lambda_2(P) = \lambda_2(\mathcal{A}_P) \leq \lambda_2(\mathcal{A}_Q) = \lambda_2(Q).$

Proposition 6.2. For $1 \leq k \leq n-2$, let $\Pi_k = \text{Diag}(\pi_k)$. Then $\tilde{P}_k^{\wedge} \preccurlyeq_{\Pi_k} P_k^{\vee}$.

This proposition is proved in the next section. We now show how it implies Proposition 2.3.

Proof of Proposition 2.3. $\lambda_1(P_k^{\vee}) = 1$. We prove by induction that $\lambda_2(P_k^{\vee}) \leq 1 - \frac{1}{k} = \frac{k-1}{k}$. When k = 1, $P_1^{\vee}(t, t') = \pi_1(t')$, so $P_k^{\vee} = \mathbb{1}\pi_1^{\top}$ has rank 1, and $\lambda_2(P_k^{\vee}) = 0 \leq \frac{k-1}{k}$. For k > 1, $\tilde{P}_{k-1}^{\wedge} \preccurlyeq_{\Pi_k} P_{k-1}^{\vee}$ by Proposition 6.2, so $\lambda_2(\tilde{P}_{k-1}^{\wedge}) \leq \lambda_2(P_{k-1}^{\vee}) \leq \frac{k-2}{k-1}$. Also $\lambda_2(P_{k-1}^{\wedge}) = \frac{1}{d} + \frac{k-1}{k}\lambda_2(\tilde{P}_{k-1}^{\wedge}) \leq \frac{k-1}{k}$. $P_{k-1}^{\wedge} = U_k D_k$ and $P_k^{\vee} = D_k U_k$ share the same non-zero eigenvalues, thus $\lambda_2(P_k^{\vee}) \leq \frac{k-1}{k}$.

7. GARLAND'S METHOD

We now discuss Proposition 6.2 that bounds \tilde{P}_k^{\wedge} by P_k^{\vee} . Focusing on adjacent layers $\Gamma_{k+1} \cup \Gamma_k$, abbreviate

T = Y(k+1) M = Y(k) B = Y(k-1) ("top" "middle" "bottom")

Garland method decomposes transitions of P_k^{\vee} and \tilde{P}_k^{\wedge} into unions of subgraphs.

7.1. **Down-walk.** A step in $P_k^{\vee} = D_k U_k$ represents a length-2 walk (m, b, m') from M to B to M. Decompose the set of all such walks (over all possible starting vertex $m \in M$) based on the bottom vertex b.

Walks with the same b corresponds to transitions on a weighted clique (with self-loops) over $S_b \subseteq M$, where

$$S_b = \{ m \in M \mid m \supset b \} .$$

7.2. Non-lazy up-walk. A step in \tilde{P}_k^{\wedge} represents a length-2 path (m, t, m') from M to T to a different vertex in M. Decompose the set of all such walks (over all possible starting vertex $m \in M$) based on the common intersection $b = m \cap m'$ of this path.

Walks with the same b corresponds to transitions on the weighted graph $H_b = (S_b, E_b)$ over S_b with edge set

$$E_b = \{(m, m') \in S_b \times S_b \mid m \cup m' \in T\}.$$

7.3. Spectra. The down-walk and non-lazy up-walk are now decomposed into subgraphs on S_b , over various $b \in B$.

Let π_b denotes the distribution of picking $t \sim S_b$ conditioned on $t \supset b$, and $\Pi_b = \text{Diag}(\pi_b)$.

For P_b^{\vee} , the subgraph (with adjacency matrix $\Pi_b P_b^{\vee}$) is a clique with self-loops.

For \tilde{P}_b^{\wedge} , the subgraph H_b (with adjacency matrix $\Pi_b \tilde{P}_b^{\wedge}$) has its edges determined by Y(k+1).

Kaufman and Oppenheim proved that Proposition 6.2 still holds "when restricted to these two subgraphs on S_b ".

Lemma 7.1. For $1 \leq k \leq n-2$ and $b \in Y(k-1)$, let $\Pi_b = \text{Diag}(\pi_b)$. Then $\tilde{P}_b^{\wedge} \preccurlyeq_{\Pi_b} P_b^{\vee}$.

This lemma is proved in the next lecture. Summing over $b \in Y(k-1)$ yields Proposition 6.2. For P_b^{\vee} : It has rank 1 since $\prod_b P_b^{\vee} = \mu_b \mu_b^{\top} / \pi_{k-1}(b)$ (μ_b is the vector of edge weights incident to b).

Therefore $\lambda_2(P_b^{\vee}) = \cdots = \lambda_n(P_b^{\vee}) = 0$, and $\Pi_b P_b^{\vee}$ is a clique that mixes perfectly in one step. For \tilde{P}_b^{\wedge} : Turns out \tilde{P}_b^{\wedge} and P_b^{\vee} share the same top eigenvector with the same eigenvalue. Therefore $\tilde{P}_b^{\wedge} \preccurlyeq_{\Pi_b} P_b^{\vee}$ is equivalent to $\lambda_2(\tilde{P}_b^{\wedge}) \leqslant 0$.

In particular \tilde{P}_b^{\wedge} must be a weighted expander.

8. VARIATIONS

Suppose you want apply the same random walk algorithm to a different setting, such as

- Uniformly sample a path of length d in a graph G; or
- Uniformly sample a clique of size d in a graph G.

Does the same random walk mix quickly in these settings?

All the constructions still make sense in those settings ((d + 1)-partite inclusion graph, up- and down-walks, Garland's decomposition). But Lemma 7.1 may or may not hold.

Turns out P_b^{\vee} from the previous section will still has rank 1 and represents a perfectly mixing weighted clique with $\lambda_2(P_b^{\vee}) = \cdots = \lambda_n(P_b^{\vee}) = 0$.

But now \tilde{P}_b^{\wedge} may not represent weighted expanders and may violate $\lambda_2(\tilde{P}_b^{\wedge}) \leq 0$, because the subgraphs H_b depend crucially on Y(k+1) (and also indirectly on distribution π at the top level).

9. Matroid

One general situation in which Lemma 7.1 holds (and hence fast mixing) is when the set system $Y(0) \cup \cdots \cup Y(d)$ is a matroid.

A matroid is a family \mathcal{I} of subsets over a ground set U that is:

- (1) Nonempty: $\mathcal{I} \neq \emptyset$
- (2) Downward closed: If $A \in \mathcal{I}$ and $B \subseteq A$, then $B \in \mathcal{I}$
- (3) Exchangable: If $A, B \in \mathcal{I}$ and |A| > |B|, then there is $e \in A \setminus B$ such that $B \cup \{e\} \in \mathcal{I}$

Turns out all maximal $A \in \mathcal{I}$ have the same size d (called the rank of the matroid).

The family of acyclic edges in a graph G is an example of a matroid. The ground set U is the set E of edges in G. A subset $F \subseteq U$ belongs to \mathcal{I} if F is acyclic. Maximal $F \in \mathcal{I}$ are spanning trees in G. This matroid has rank n-1, where n is the number of vertices in G. Fast mixing over spanning trees is thus a special case.