Advanced Algorithms

Spectral methods and algorithms

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Recap

Previous lecture:

Random walks on undirected graphs

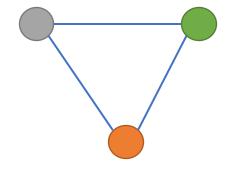
- Fundamental theorem of Markov chains
- Spectral analysis
- Mixing time
- Random sampling

What next?

Random walks on undirected graphs

- From sampling to counting and MCMC
- Expander graphs and random walks

Coupling for Graph Coloring



- Start with any k-coloring σ
- Pick a vertex v and a color c uniformly at random, recolor v with c if it is legal; otherwise do nothing

Say we have two arbitrary copies of the Markov chain, (X_t) and (Y_t) At each step, we let them choose the same vertex v and same color cLet d_t = number of vertices X_t disagree with Y_t Unlike the previous example, d_t can increase now We need to consider Good Moves that decrease d_t , and balance them with Bad Moves that increase d_t



Start with any k-coloring σ Pick a vertex v and a color c u.a.r., recolor v with c if legal

Coupling for Graph Coloring

Say we have two arbitrary copies of the Markov chain, (X_t) and (Y_t) At each step, we let them choose the same vertex v and same color cLet d_t = number of vertices X_t disagree with Y_t

Good Moves that decrease d_t :

If we chose a disagreeing vertex v, and color c does not appear in the neighborhood of v in X_t or Y_t , this is a good move

Because we can safely recolor a disagreeing vertex v with color c, and they agree from then on

Let g_t be the number of good moves (among all possible kn choices)

There are d_t vertices to choose from, and each disagreeing vertex has a neighborhood of at most Δ colors in either process, so each disagreeing vertex has $k - 2\Delta$ "safe colors"

$$g_t \ge d_t(k - 2\Delta)$$

Start with any k-coloring σ Pick a vertex v and a color c u.a.r., recolor v with c if legal

Coupling for Graph Coloring

Say we have two arbitrary copies of the Markov chain, (X_t) and (Y_t) At each step, we let them choose the same vertex v and same color cLet d_t = number of vertices X_t disagree with Y_t

Bad Moves that increase d_t : a legal move in one process but not the other This happens when (and only when) the chosen color c is already the color of some neighbor of v in one process but not the other

In other words, v must be a neighbor of some disagreeing vertex u, and c must be the color of u in either X_t or Y_t

Let b_t be the number of bad moves (among all possible kn choices) There are d_t choices of disagreeing vertex u, then Δ choices for v, then 2 for X_t or Y_t $b_t \leq 2\Delta d_t$

Coupling for Graph Coloring

Say we have two arbitrary copies of the Markov chain, (X_t) and (Y_t) At each step, we let them choose the same vertex v and same color cLet d_t = number of vertices X_t disagree with Y_t

Combined:
$$\mathbb{E}[d_{t+1}|d_t] = d_t + \frac{b_t - g_t}{kn} \le d_t + d_t \frac{4\Delta - k}{kn} \le d_t \left(1 - \frac{1}{kn}\right)$$

Since $d_0 \le n$, we have $\mathbb{E}[d_t|d_0] \le 1/e$ for $t = 2k n \ln n$. Thus,

 $d_{TV}(p_t, \pi) \leq \Pr_{(X_t, Y_t) \sim \mu} [X_t \neq Y_t] \leq \Pr[d_t > 0 | X_0, Y_0] = \Pr[d_t \geq 1 | X_0, Y_0] \leq \mathbb{E}[d_t | d_0] \leq 1/e$ This concludes that the ϵ -mixing time is $O\left(nk \log \frac{n}{\epsilon}\right)$

To improve this to $k \ge 2\Delta + 1$, one tries to pair bad moves in (X_t) but blocked in (Y_t) , with bad moves in (Y_t) but blocked in (X_t)

Start with any k-coloring σ Pick a vertex v and a color c u.a.r., recolor v with c if legal

Now that we have a Markov chain that outputs a k-coloring σ almost uniformly at random from all proper colorings after $O\left(nk\log\frac{n}{\epsilon}\right)$ steps

Can we estimate the total number of proper colorings?

This task is known as *approximate counting*

For many natural concrete problems *ApproxCount* ≡ *ApproxSample* ≡ *UniformSample* ⊂ *ExactCount*

Denote the number of proper colorings of a graph G by Z_G We start by finding an arbitrary proper coloring σ in G Then, we reveal the colors in σ one by one We count how many proper colorings are consistent with the revealed colors

Let Z_i be the number of proper colorings τ such that in the first i coordinates, τ agrees with σ

Notice that
$$Z_0 = Z_G$$
, $Z_n = 1$, and
 $Z_G = \frac{Z_0}{Z_1} \cdot \frac{Z_1}{Z_2} \cdots \frac{Z_{n-1}}{Z_n}$

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Suppose we estimate each ratio within $\left(1 \pm \frac{\epsilon}{2n}\right) \cdot \frac{Z_{i+1}}{Z_i}$ except with prob. $\frac{\delta}{n}$ Then multiplying them all together gives $(1 \pm \epsilon) \cdot Z_G$ except with prob. δ

Let Z_i be the number of proper colorings τ such that: in the first *i* coordinates, τ agrees with σ Let π_i be the uniform distribution of proper colorings τ such that: in the first *i* coordinates, τ agrees with σ

Recall that $Z_0 = Z_G$, $Z_n = 1$, and $Z_G = \frac{Z_0}{Z_1} \cdot \frac{Z_1}{Z_2} \cdots \frac{Z_{n-1}}{Z_n}$

How do we estimate each ratio $\frac{Z_{i+1}}{Z_i}$?

We run a Markov chain that samples from π_i , and use Monte Carlo method to estimate how many are counted in Z_{i+1}

<u>Markov chain</u>: in the first *i* coordinates, we fix the colorings as in σ , and only update the remaining n - i coordinates <u>Monte Carlo</u>: given a sample τ , we check if $\tau_{i+1} = \sigma_{i+1}$

Sampling from π_i is an unbiased estimator for the ratio:

$$E_{\tau \sim \pi_i} \left[[\tau_{i+1} = \sigma_{i+1}] \right] = \frac{Z_{i+1}}{Z_i}$$

Sampling from a rapidly mixing Markov chain p_t only introduces a small bias (recall the def. of TV distance): $|E_{\tau \sim p_t} [[\tau_{i+1} = \sigma_{i+1}]] - E_{\tau \sim \pi_i} [[\tau_{i+1} = \sigma_{i+1}]]| \le d_{TV}(p_t, \pi_i)$

 $d_{TV}(p_t, \pi) = \max_{S \subseteq [n]} |p_t(S) - \pi(S)|$

We run a Markov chain that samples from π_i , and use Monte Carlo method to estimate how many are counted in Z_{i+1}

<u>Markov chain</u>: in the first *i* coordinates, we fix the colorings as in σ , and only update the remaining <u>Monte Carlo</u>: given a sample τ , we check if $\tau_{i+1} = \sigma_{i+1}$

Sampling from π_i is an unbiased estimator for the ratio:

 $E_{\tau \sim \pi_i} \left[[\tau_{i+1} = \sigma_{i+1}] \right] = \frac{Z_{i+1}}{Z_i}$ Variance can also be bounded because $\frac{Z_{i+1}}{Z_i}$ is strictly between (0,1): $\frac{\Delta}{k(k-\Delta)} \leq \frac{Z_{i+1}}{Z_i} \leq \frac{1}{k-\Delta}$ It suffices to take the average over poly $\left(n, \frac{1}{\epsilon}, \frac{1}{\delta}\right)$ samples Then apply Chebyshev's inequality

See Chapter 14.4 of <u>LPW</u> book

Upperbound for the ratio follows from having many colors available lowerbound from bounding the prob. that any neighbors take the same color

Expander Graphs

- Combinatorial: graphs with good expansion
- Probabilistic: graphs in which random walks mix rapidly
- Algebraic: graphs with large spectral gap

Let G be a d-regular graph, and let $d = \alpha_1 \ge \alpha_2 \ge \cdots \ge \alpha_n \ge -d$ be the spectrum of its adjacency matrix.

We will be interested in the <u>spectral radius</u>, given by $\alpha \coloneqq \max\{\alpha_2, |\alpha_n|\}$

If α is much smaller than d, we have good <u>spectral expansion</u>.

There are many nice properties associated with expander graphs

Among others, say if we want more than one sample in MCMC, do we have to resample entirely?

Cauchy-Schwarz inequality: $\langle u, v \rangle \leq \sqrt{\langle u, u \rangle} \cdot \sqrt{\langle v, v \rangle}$

Expander Mixing lemma

Intuitively, an expander can be seen as an approximation to the complete graph, because edges are distributed evenly

Induced edges: $E(S,T) \coloneqq \{(u,v): u \in S, v \in T, uv \in E\}$

We also allow non-disjoint S, T, in which case an edge can be counted twice.

Expander Mixing lemma

Let *G* be a *d*-regular graph with *n* vertices. If the spectral radius of G is α , then for every $S \subseteq [n], T \subseteq [n]$, we have $\begin{vmatrix} E(S,T) - \frac{d|S||T|}{n} \end{vmatrix} \leq \alpha \sqrt{|S||T|}.$

Proof: Note that $E(S,T) = \chi_S^T A \chi_T$. Let $\chi_S = \sum_i a_i v_i$, $\chi_T = \sum_i b_i v_i$, where $\{v_i\}$ is an orthonormal basis for A, with eigenvalues $\{\alpha_i\}$.

$$E(S,T) = \frac{d|S||T|}{n} + \sum_{i\geq 2} \alpha_i a_i b_i$$

By Cauchy-Schwarz,

$$\left| E(S,T) - \frac{d|S||T|}{n} \right| \le \alpha ||a||_2 ||b||_2 = \alpha ||\chi_S||_2 ||\chi_T||_2 = \alpha \sqrt{|S||T|}$$

Expander Mixing lemma

Intuition: Expander mixing lemma tells us that a spectral expander looks like a random graph.

Exercise: Let G be a *d*-regular graph with spectral radius α . Show that the size of the maximum independent set of G is at most $\frac{\alpha n}{d}$. Use this result to conclude that the chromatic number is at least $\frac{d}{\alpha}$.

Converse to Expander Mixing lemma

(By Bilu and Linial)

Suppose that for every $S \subseteq [n], T \subseteq [n]$ with $S \cap T = \emptyset$, we have

$$\left| E(S,T) - \frac{d|S||T|}{n} \right| \le \alpha \sqrt{|S||T|}.$$

Then all but the largest eigenvalue of A in absolute value is at most

$$O\left(\alpha\left(1+\log\frac{d}{a}\right)\right)$$

- Proof is based on LP duality
- Would be nice to see an analog of Trevisan's Cheeger's rounding proof

Existence of expanders

- Complete graphs are obviously the best expanders in terms of "expansion" (in all three notions of "expansion")
- What's interesting is the existence of sparse expanders: e.g. d-regular expanders for constant d
- A random *d*-regular graph is a (combinatorial) expander with high probability
- However, deterministic and explicit construction of expanders seems to be much harder to come up with

Alon-Boppana Bound

- For *d*-regular graphs, how small can the spectral radius be?
- Ramanujan graphs: graphs whose spectral radius are at most $2\sqrt{d-1}$

Alon-Boppana Bound

Let G be a *d*-regular graph with n vertices, and α_2 be the second largest eigenvalue of its adjacency matrix. Then

$$\alpha_2 \ge 2\sqrt{d-1} - \frac{2\sqrt{d-1} - 1}{\left\lfloor \operatorname{diam}(G)/2 \right\rfloor}$$

Alon-Boppana Bound

An easy lower bound on spectral radius

Let G be a *d*-regular graph with n vertices, and α be its spectral radius. Then $\alpha \ge \sqrt{d} \cdot \sqrt{\frac{n-d}{n-1}}$.

Proof: Consider $Tr(A^2)$. Counting length-2 walks we have $Tr(A^2) \ge nd$

On the other hand, $\operatorname{Tr}(A^2) = \sum_i \alpha_i^2 \le d^2 + (n-1)\alpha^2$. Combined, we have $\alpha \ge \sqrt{d} \cdot \sqrt{\frac{n-d}{n-1}}$.

For the Alon-Boppana bound, one may consider $Tr(A^{2k})$.

Random walks in expanders

- We knew that it mixes rapidly, in time $O\left(\frac{\log n}{1-\epsilon}\right)$ for $\alpha = \epsilon d$.
- Perhaps surprisingly, not just the final vertex is close to the uniform distribution, but the entire sequence of walks looks like a sequence of independent samples for many applications.

 In fact, expander random walks can fool many test functions: *Expander random walks: a Fourier-analytic approach*, by Cohen, Peri and Ta-Shma

Probability amplification

Say you have a randomized algorithm that fails with probability β

To boost success probability, we can run it multiple times until it succeed

Run independently for t rounds, the failure probability becomes β^t

Q: Can we save randomness while still achieving the same probability amplification?

Imagine a random walk on the $N = 2^n$ random bits

There is a set *B* of size βN that we try to escape from (or avoid)

We want that the escape probability close to β^t

Q: Can we use a sparse expander instead of a complete graph for the random walk?

Hitting property of expander walks

Let G be a *d*-regular graph with n vertices, $\alpha = \epsilon d$ be its spectral radius and *B* be a set of size at most βn .

Then, starting from a uniformly random vertex, the probability that a t-step random walk has never escaped from *B*, denoted by P(B,t), is at most $(\beta + \epsilon)^t$.

 $Pr[X_0 \in B, X_1 \in B, X_2 \in B, \dots, X_t \in B]$

Remarks before a proof:

- Compare this to a sequence of independent samples.
- Expander mixing lemma is like t = 2: Note that $\varphi(S) = \Pr(X_2 \notin S \mid X_1 \sim \pi_S)$
- Bound can be strengthened → see Chapter 4 of *Pseudorandomness*, by Vadhan
- Applications to error reduction for randomized algorithms
 - Instead of using kt bits of randomness, only need $k + O(t \log d)$
 - for one-sided error, escaping the bad set of "random bits"
 - for two-sided error, a Chernoff type bound can also be shown → then take the majority of the answers

 $\Pi_B = \frac{B}{V \setminus B} \begin{bmatrix} I_B & 0\\ 0 & 0 \end{bmatrix}$

 $\Pi_B \Pi_B = \Pi_B$

Hitting property of expander walks

 $W = \frac{1}{d}A$ Proof. Observe that $P(B, t) = \|(\Pi_B W)^t \Pi_B u\|_1$ $u = \frac{1}{n}\vec{1}$ To see this, notice that $\Pr[X_0 \in B] = \|\Pi_B u\|_1$ $\Pr[X_0 \in B, X_1 \in B] = \|\Pi_B W \Pi_B u\|_1$

And so on and so forth.

Suppose that we can show $\forall f : f$ is a probability distribution, we have $\|\Pi_B W \Pi_B f\|_2 \le (\beta + \epsilon) \|f\|_2$

Then,

$$\begin{aligned} \|(\Pi_B W)^t \Pi_B u\|_1 &\leq \sqrt{n} \|(\Pi_B W)^t \Pi_B u\|_2 \\ &= \sqrt{n} \|(\Pi_B W \Pi_B)^t u\|_2 \\ &\leq \sqrt{n} (\beta + \epsilon)^t \|u\|_2 \\ &= (\beta + \epsilon)^t \end{aligned}$$

Cauchy-Schwarz inequality: $\langle u, v \rangle \leq \sqrt{\langle u, u \rangle} \cdot \sqrt{\langle v, v \rangle}$

Hitting property of expander walks

 $\Pi_B = \frac{B}{V \setminus B} \begin{bmatrix} I_B & 0\\ 0 & 0 \end{bmatrix}$

 $W = \frac{1}{d}A$ has $\lambda_2(W^{\mathsf{T}}W) = \epsilon^2$

Proof (cont'd): It remains to show $\forall f: f$ is a probability distribution, $\|\Pi_B W \Pi_B f\|_2 \le (\beta + \epsilon) \|f\|_2$

Without loss of generality, we can assume f is supported only on B. $\|\Pi_B W \Pi_B f\|_2 = \|\Pi_B W f\|_2 = \|\Pi_B W (u+v)\|_2 \le \|\Pi_B u\|_2 + \|\Pi_B W v\|_2$

$$u = \frac{1}{n} \vec{1}$$
, so $\frac{\langle f, u \rangle}{\langle u, u \rangle} u = u$, then $v \perp \vec{1}$

Next, $\|\Pi_B W v\|_2 \le \|Wv\|_2 \le \epsilon \|v\|_2 \le \epsilon \|f\|_2$. On the other hand, $\|\Pi_B u\|_2 = \sqrt{\frac{\beta}{n}} \le \beta \|f\|_2$, where last inequality follows from Cauchy-Schwarz: $1 = \|f\|_1 = \langle 1_B, f \rangle \le \sqrt{\beta n} \|f\|_2$

Cauchy-Schwarz inequality: $\langle u, v \rangle \leq \sqrt{\langle u, u \rangle} \cdot \sqrt{\langle v, v \rangle}$

Combined together, we have $\|\Pi_B W \Pi_B f\|_2 \le (\beta + \epsilon) \|f\|_2$ as desired.

Hitting property of expander $P(S,t) = \|\Pi_{Z_t} W \Pi_{Z_{t-1}} W \dots \Pi_{Z_1} u\|_1$ where $S = (Z_t, Z_{t-1}, \dots, Z_1)$ indicates whether $Z_i \in \{B, \overline{B}\}$

Proof. Observe that $P(B, t) = \|(\Pi_B W)^t \Pi_B u\|_1$

Suppose that we can show $\forall f: f$ is a probability distribution, we have $\|\Pi_B W \Pi_B f\|_2 \leq (\beta + \epsilon) \|f\|_2$. Then, $\|(\Pi_B W)^t \Pi_B u\|_1 \leq \sqrt{n} \|(\Pi_B W)^t \Pi_B u\|_2 = \sqrt{n} \|(\Pi_B W \Pi_B)^t u\|_2 \leq \sqrt{n} (\beta + \epsilon)^t \|u\|_2 = (\beta + \epsilon)^t$

It remains to show $\forall f: f$ is a probability distribution, $\|\Pi_B W \Pi_B f\|_2 \le (\beta + \epsilon) \|f\|_2$ Without loss of generality, we can assume f is supported only on B. $\|\Pi_B W \Pi_B f\|_2 = \|\Pi_B W f\|_2 = \|\Pi_B W (u + v)\|_2 \le \|\Pi_B u\|_2 + \|\Pi_B W v\|_2$

Next, $\|\Pi_B W v\|_2 \le \|Wv\|_2 \le \epsilon \|v\|_2 \le \epsilon \|f\|_2$. On the other hand, $\|\Pi_B u\|_2 = \sqrt{\frac{\beta}{n}} \le \beta \|f\|_2$,

The last inequality follows from Cauchy-Schwarz:

 $1 = \|f\|_1 = \langle 1_B, f \rangle \le \sqrt{\beta n} \|f\|_2$

Combined together, we have $\|\Pi_B W \Pi_B f\|_2 \le (\beta + \epsilon) \|f\|_2$ as desired.