COL866: Foundations of Data Science

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Spectral Graph Theory:
Eigenvalues and graph properties

- We shall work with d-regular undirected graphs.
- It will be convenient to work with the matrix $L = I - \frac{1}{d}A$ instead of the adjacency matrix A.
- The matrix L defined above is called the Normalized Laplacian Matrix of the graph.
- We prove the following basic results of spectral graph theory.

Theorem

Let G be a d-regular undirected graph, and $L = I - \frac{1}{d}A$ be its normalized Laplacian matrix. Let $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$ be the real eigenvalues of L with multiplicities. Then

1. $\lambda_1 = 0$ *and* $\lambda_n \leq 2$.
2. $\lambda_k = 0$ *if and only if* G *has at least* k *connected components.*
3. $\lambda_n = 2$ *if and only if at least one of the connected components of* G *is bipartite.*

- Given a d-regular undirected graph with normalised graph laplacian $L = I - \frac{1}{d}A$ having eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n \leq 2$.
- We know that the second eigenvalue $\lambda_2 = 0$ if and only if G has at least two connected components.
- In other words, the second eigenvalue $\lambda_2 = 0$ if and only if $\phi(G) = 0$.
- We will prove an *approximate* version of this result that says that λ_2 is small if and only if $\phi(G)$ is small.

Theorem (Cheeger's Inequality)

$\frac{\lambda_2}{2} \leq \phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

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- First we will prove the following direction.

Lemma

$\lambda_2 \leq \sigma(G) \leq 2\phi(G)$.

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Proof sketch

- We can write:

$$\begin{aligned}\sigma(G) &= \min_{\mathbf{x}\in\{0,1\}^n - \{\mathbf{0},\mathbf{1}\}} \frac{\sum_{\{u,v\}\in E} |\mathbf{x}_u - \mathbf{x}_v|}{\frac{d}{n}\sum_{\{u,v\}} |\mathbf{x}_u - \mathbf{x}_v|} \\ &= \min_{\mathbf{x}\in\{0,1\}^n - \{\mathbf{0},\mathbf{1}\}} \frac{\sum_{\{u,v\}\in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{\frac{d}{n}\sum_{\{u,v\}} (\mathbf{x}_u - \mathbf{x}_v)^2}\end{aligned}$$

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$$\sigma(G) = \min_{x \in \{0,1\}^n - \{\mathbf{0},\mathbf{1}\}} \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{\frac{d}{n} \sum_{\{u,v\}} (\mathbf{x}_u - \mathbf{x}_v)^2}$$

- Also, we have

$$\lambda_2 = \min_{x \in \mathbb{R}^n - \{\mathbf{0}\}, \mathbf{x} \perp \mathbf{1}} \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{d \cdot \sum_v \mathbf{x}_v^2}$$

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$$\stackrel{?}{=} \min_{x \in \mathbb{R}^n - \{\mathbf{0}\}, \mathbf{x} \perp \mathbf{1}} \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{\frac{d}{n} \cdot \sum_{\{u,v\}} (\mathbf{x}_u - \mathbf{x}_v)^2}$$

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&= \min_{x \in \mathbb{R}^n - \{\mathbf{0}\}, \mathbf{x} \perp \mathbf{1}} \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{\frac{d}{n} \cdot \sum_{\{u,v\}} (\mathbf{x}_u - \mathbf{x}_v)^2} \\
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\end{aligned}$$

- So, $\lambda_2 \leq \sigma(G)$. □

Theorem (Cheeger's Inequality)

$\frac{\lambda_2}{2} \leq \phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

- First we will prove the following direction.

Lemma

$\lambda_2 \leq \sigma(G) \leq 2\phi(G)$.

- Now, we will prove the other direction.

Lemma

$\phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

- We prove the above statement using a constructive argument. That is, we will give an algorithm that outputs a cut S in the given graph G such that $\phi(S) \leq \sqrt{2 \cdot \lambda_2}$.

Lemma

$\phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

Spectral Partitioning Algorithm

SpectralPartitioning$(G, \mathbf{x})$

- Sort the vertices of G in non-increasing order of value of the vector $\mathbf{x}$. That is, $\mathbf{x}_{v_1} \leq \mathbf{x}_{v_2} \leq ... \leq \mathbf{x}_{v_n}$.
- Let $i \in \{1, ..., n-1\}$ that minimises $\max\{\phi(\{v_1, ..., v_i\}), \phi(\{v_{i+1,...,v_n}\})\}$
- Output $S = \{v_1, ..., v_i\}$

- What is the running time of the above algorithm?

Lemma

$\phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

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- What is the running time of the above algorithm?
  $O(|V| \log |V| + |E|)$

Lemma

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Lemma

Let $G = (V, E)$ be a d-regular graph, $\mathbf{x} \in \mathbb{R}^{|V|}$ be a vector such that $\mathbf{x} \perp \mathbf{1}$. Let

$$R(\mathbf{x}) \overset{def.}{=} \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{d \cdot \sum_v \mathbf{x}_v^2}$$

and let S be the output of `SpectralPartitioning`$(G, \mathbf{x})$*. Then* $\phi(S) \leq \sqrt{2 \cdot R(\mathbf{x})}$.

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$\phi(G) \leq \sqrt{2 \cdot \lambda_2}$.

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and let S be the output of SpectralPartitioning$(G, \mathbf{x})$. *Then* $\phi(S) \leq \sqrt{2 \cdot R(\mathbf{x})}$.

- Claim: Let $\mathbf{x}$ be an eigenvector of λ_2. Then $R(\mathbf{x}) = \lambda_2$.
- This implies that $\phi(S) \leq \sqrt{2 \cdot \lambda_2}$.

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and let S be the output of SpectralPartitioning$(G, \mathbf{x})$*. Then $\phi(S) \leq \sqrt{2 \cdot R(\mathbf{x})}$.*

- Claim: Let $\mathbf{x}$ be an eigenvector of λ_2. Then $R(\mathbf{x}) = \lambda_2$.
- This implies that $\phi(S) \leq \sqrt{2 \cdot \lambda_2}$.
- Note that the partitioning algorithm can be thought of as an approximation algorithm for finding the cut with smallest edge expansion.

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- We would prove that there exists an $i \in \{1, ..., n-1\}$ s.t. $\phi(\{1, ..., i\}) \leq \sqrt{2R(\mathbf{x})}$ and $\phi(\{i+1, ..., n-1\}) \leq \sqrt{2R(\mathbf{x})}$.

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- <u>Claim 1</u>: For the remaining proof, it will be safe to assume the following:
  1. $\mathbf{x}_{\lceil n/2 \rceil} = 0$
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- Claim 1: For the remaining proof, it will be safe to assume the following: (1) $\mathbf{x}_{\lceil n/2 \rceil} = 0$ and (2) $\mathbf{x}_1^2 + \mathbf{x}_n^2 = 1$.
- The distribution D over sets S of the form $\{1, ...i\}$ de defined by the following randomized process:

Random process

- Pick a real value t in the range $[\mathbf{x}_1, \mathbf{x}_n]$ with probability density function $f(t) = 2|t|$.
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- Claim 3: $\mathbf{Pr}[(i, j) \text{ is cut by } (S, V - S)] \leq |\mathbf{x}_i - \mathbf{x}_j| \cdot (|\mathbf{x}_i| + |\mathbf{x}_j|)$.

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- Claim 4: The following holds:

$$\mathbf{E}_S[|E(S, V - S)|] \leq \sqrt{\sum_{\{u,v\} \in E} (\mathbf{x}_i - \mathbf{x}_j)^2} \cdot \sqrt{\sum_{\{u,v\} \in E} (|\mathbf{x}_i| + |\mathbf{x}_j|)^2}$$

$$\leq \sqrt{\sum_{\{u,v\} \in E} (\mathbf{x}_i - \mathbf{x}_j)^2 \cdot (2d \sum_i \mathbf{x}_i^2)}$$

- The results that we discussed were for d-regular graphs.
- Question: Can we get similar results for irregular graphs?
- Given an undirected graph $G = (V, E)$, let d_v denote the degree of the vertex v.
- We can define the Rayleigh quotient of a vector $\mathbf{x} \in \mathbb{R}^{|V|}$ as:

$$R_G(\mathbf{x}) = \frac{\sum_{\{u,v\} \in E} (\mathbf{x}_u - \mathbf{x}_v)^2}{\sum_v d_v \mathbf{x}_v^2}.$$

- Let D be the diagonal matrix where $D_{u,v} = 0$ if $u \neq v$ and $D_{v,v} = d_v$.
- The Laplacian of G can be defined as $L_G = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$.
- Given this, we have

$$\lambda_k = \min_{k-dim\ S} \left\{ \max_{\mathbf{x} \in S} \frac{\mathbf{x}^T L_G \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \right\}$$

- Setting $\mathbf{y} = D^{-\frac{1}{2}} \mathbf{x}$, we have:

$$\lambda_k = \min_{k-dim\ S'} \left\{ \max_{\mathbf{x} \in S'} \frac{\mathbf{y}^T D^{\frac{1}{2}} L_G D^{\frac{1}{2}} \mathbf{y}}{\mathbf{y}^T D \mathbf{y}} \right\}$$

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- Note that $\mathbf{y}^T D^{\frac{1}{2}} L_G D^{\frac{1}{2}} \mathbf{y} = \mathbf{y}^T (D - A) \mathbf{y} = \sum_{\{u,v\}} (\mathbf{y}_u - \mathbf{y}_v)^2$.
- So, $\lambda_k = \min_{k-dim\ S} \{\max_{\mathbf{y} \in S} R_G(\mathbf{y})\}$.

- The results that we discussed were for d-regular graphs.
- Question: Can we get similar results for irregular graphs?
- Given an undirected graph $G = (V, E)$, let d_v denote the degree of the vertex v.
  - The point of showing some of the quantities for irregular graphs was to convince you that the arguments that worked for the Cheeger's inequality for d-regular graphs also work for the irregular graphs and we have:

$$\frac{\lambda_2}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}.$$

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- Question: Are there higher order versions of the Cheeger's inequality?
  - What this could mean is that the graph can be partitioned into at least k clusters iff λ_k is small.

- The results that we discussed were for d-regular graphs.
- Question: Can we get similar results for irregular graphs?
- Given an undirected graph $G = (V, E)$, let d_v denote the degree of the vertex v. Yes
- Question: Are there higher order versions of the Cheeger's inequality? Yes
- The proof of Cheeger's inequality gave us an algorithm to output a good cut in the given graph given a second eigenvector of the Laplacian.
- Question: How do we compute a second eigenvector? Can we estimate the second eigenvector? How well does an approximate version of the second eigenvector work with respect to giving a good cut?

- The proof of Cheeger's inequality gave us an algorithm to output a good cut in the given graph given a second eigenvector of the Laplacian.
- Question: How do we compute a second eigenvector? Can we estimate the second eigenvector? How well does an approximate version of the second eigenvector work with respect to giving a good cut?
  - Theorem: Let $\mathbf{x}$ be a vector such that $\mathbf{x}^T L\mathbf{x} \leq (\lambda_2 + \varepsilon)\mathbf{x}^T\mathbf{x}$, then the spectral partitioning algorithm finds a cut $(S, V - S)$ such that $\phi(S) \leq \sqrt{4\phi(G) + 2\varepsilon}$.
  - Such an approximate eigenvector can be obtained using the power method.

End