COL866: Foundations of Data Science

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Spectral Graph Theory: Eigenvalues and graph properties

Spectral Graph Theory

- Graphs are used to model pairwise relationship between objects. The objects are denoted by vertices and pairwise relationships are denoted by edges.
- Classical techniques have had a lot of success in solving various problems on graphs such as shortest path, minimum spanning tree etc.
- More recently, algebraic techniques have been successful for certain graph problems. Such techniques involve analysing the adjacency matrix of the graph.
- The relationship between the structural properties of a given graph and the algebraic properties of the underlying (appropriate variant of) adjacency matrix is key in such analysis.

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- More recently, algebraic techniques have been successful for certain graph problems. Such techniques involve analysing the adjacency matrix of the graph.
- The relationship between the structural properties of a given graph and the algebraic properties of the underlying (appropriate variant of) adjacency matrix is key in such analysis.
- Spectral Graph Theory studies how eigenvalues of the adjacency matrix of a graph (an algebraic quantity) relates to combinatorial properties of the graph.

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- What does it mean to have good connectivity?
- An intuitive notion is that removing a small fraction of edges of the graph should not disconnect large portions of the graph.
- Sparsity and edge expansion discussed next, are useful in formalizing the notion of connectivity.

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Definition (Sparsity)

The sparsity of a cut (S, V - S), denoted by $\sigma(S)$, is defined as $\sigma(S) = \frac{|V|^2}{|E|} \cdot \frac{|E(S,V-S)|}{|S| \cdot |V-S|}$.

• In other words, the sparsity of the cut (S, V - S) is the fraction of edges across the cut divided by the fraction of vertex pairs across the partition (i.e., the fraction of edges in the ideal case of a complete graph).

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- Note that if the graph is *d*-regular, then $\sigma(S) = \frac{|E(S,V-S)|}{\frac{d}{|V|} \cdot |S| \cdot |V-S|}$
- The edge expansion of a set of vertices S ⊆ V, denoted by φ(S), of a d-regular graph is given by:

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- Constant degree graphs with constant expansion are sparse graphs with good connectivity property.

Theorem

Let G = (V, E) be a regular graph of expansion ϕ . Then, after an $\varepsilon < \phi$ fraction of edges are adversarially removed, the graph has a connected component that spans at least $(1 - \frac{\varepsilon}{2\phi})$ fraction of vertices.

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- In a *d*-regular expander (i.e., constant expansion), the removal of k edges can cause O(k/d) vertices to be disconnected from the remaining giant component.
- It is always possible to disconnect k/d vertices after removing k edges. So, the reliability of an expander is the best possible.

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Linear Algebra Recap: Eigenvalues

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- The *conjugate* of a complex number x = a + ib is denoted by \bar{x} and has value $\bar{x} = a ib$.
- For a complex matrix M ∈ C^{m×n}, the conjugate transpose of M, denoted by M^{*} ∈ C^{n×m} such that (M^{*})_{i,i} = M̄_{i,i}.
- The inner product of two vectors ${\bf x}$ and ${\bf y}$ is defined as $\langle {\bf x}, {\bf y} \rangle = {\bf x}^{\star} {\bf y}.$

Definition (Eigenvalue and eigenvector)

For a square matrix $M \in \mathbb{C}^{n \times n}$, $\lambda \in \mathbb{C}$ is a scalar, $\mathbf{x} \in \mathbb{C}^n - {\mathbf{0}}$ is a non-zero vector and

$$M\mathbf{x} = \lambda \mathbf{x}$$

then we say that λ is an eigenvalue of M and **x** is an eigenvector of M corresponding to eigenvalue λ .

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- The equation $M\mathbf{x} = \lambda \mathbf{x}$ can alternatively be written as $(M \lambda I)\mathbf{x} = \mathbf{0}$.
- This is equivalent to $det(M \lambda I) = 0$.
- The LHS of the equation is a polynomial of degree n in λ and so has n solutions (counting multiplicities).
- We will be studying the eigenvalues of adjacency matrices of undirected graphs which are real and symmetric. Next, we look at some properties of such matrices.

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- We will be studying the eigenvalues of adjacency matrices of undirected graphs which are real and symmetric. Next, we look at some properties of such matrices.
- A square matrix $M \in \mathbb{C}^{n \times n}$ is called Hermitian iff $M = M^{\star}$.

Lemma

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• We need another characterisation of eigenvalues and eigenvectors that help us relate these quantities with combinatorial properties of graphs such as connectivity.

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Theorem

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix and $\lambda_1 \leq ... \leq \lambda_n$ be its real eigenvalues (counted with multiplicities) sorted in non-decreasing order. Let $\mathbf{x}_1, ..., \mathbf{x}_k$, k < n, be orthonormal vectors such that $M\mathbf{x}_i = \lambda_i \mathbf{x}_i$ for i = 1, ..., k. Then

$$\lambda_{k+1} = \min_{\mathbf{x} \in \mathbb{R}^n - \{\mathbf{0}\}: \mathbf{x} \perp \mathbf{x}_1 \dots, \mathbf{x}_k} \frac{\mathbf{x}^T M \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

and any minimizer is an eigenvector of λ_{k+1} .

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• We need the following lemma.

Lemma

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix, and let $\mathbf{x}_1, ..., \mathbf{x}_k, k < n$ be orthogonal eigenvectors of M. Then there is an eigenvector \mathbf{x}_{k+1} of M that is orthogonal to $\mathbf{x}_1, ..., \mathbf{x}_k$.

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• The above lemma has the following interesting corollary.

Corollary (Spectral theorem)

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix, and $\lambda_1, ..., \lambda_n$ be its real eigenvalues, with multiplicities; then there are orthonormal vectors $\mathbf{x}_1, ..., \mathbf{x}_n, \mathbf{x}_i \in \mathbb{R}^n$ such that \mathbf{x}_i is an eigenvector of λ_i .

(4) (Eq. (4))

Theorem

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix and $\lambda_1 \leq ... \leq \lambda_n$ be its real eigenvalues (counted with multiplicities) sorted in non-decreasing order. Let $\mathbf{x}_1, ..., \mathbf{x}_k$, k < n, be orthonormal vectors such that $M\mathbf{x}_i = \lambda_i \mathbf{x}_i$ for i = 1, ..., k. Then

$$\lambda_{k+1} = \min_{\mathbf{x} \in \mathbb{R}^n - \{\mathbf{0}\}: \mathbf{x} \perp \mathbf{x}_1 \dots, \mathbf{x}_k} \frac{\mathbf{x}^T M \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

and any minimizer is an eigenvector of λ_{k+1} .

Proof sketch

- Applying the lemma repeatedly, we can obtain n k orthogonal vectors x_{k+1},..., x_n, where x_i is an eigenvector of λ_i.
- Claim 1: x_{k+1} is a feasible solution for the minimisation problem and has cost λ_{k+1}. So, the minimum us at most λ_{k+1}.
- <u>Claim 2</u>: For any arbitrary feasible solution **x**, we can write $\mathbf{x} = \sum_{i=1k+1}^{n} a_i \mathbf{x}_i$ and this has cost $\frac{\sum_{i=k+1}^{n} \lambda_i a_i^2}{\sum_{i=k+1}^{n} a_i^2} \ge \lambda_{k+1}$.
- Claim 3: Any minimiser **x** is a linear combination of eigenvectors of λ_{k+1} and hence is an eigenvector of λ_{k+1} .

Theorem

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix and $\lambda_1 \leq ... \leq \lambda_n$ be its real eigenvalues (counted with multiplicities) sorted in non-decreasing order. Let $\mathbf{x}_1, ..., \mathbf{x}_k$, k < n, be orthonormal vectors such that $M\mathbf{x}_i = \lambda_i \mathbf{x}_i$ for i = 1, ..., k. Then

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and any minimizer is an eigenvector of λ_{k+1} .

• The above theorem may also be written in the following manner:

Corollary

Let $M \in \mathbb{R}^{n \times n}$ be a real symmetric matrix, and $\lambda_1 \leq ... \leq \lambda_n$ its eigenvalues, counted with multiplicities and sorted in non-decreasing order. Then

$$_{k} = \min_{k-dimensional \ subspace \ V \ of \ \mathbb{R}^{n}} \left\{ \max_{\mathbf{x} \in V - \{\mathbf{0}\}} \frac{\mathbf{x}^{T} M \mathbf{x}}{\mathbf{x}^{T} \mathbf{x}} \right\}$$

The basics of spectral graph theory

Spectral Graph Theory Basic results

- 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

$$1 \lambda_1 = 0 \text{ and } \lambda_n \leq 2.$$

- **2** $\lambda_k = 0$ if and only if G has at least k connected components.
- λ_n = 2 if and only if at least one of the connected components of G is bipartite.

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