[CS1961: Lecture 14] Spectral Graph Theory

1 Graph Adjacency Matrix and Its Spectrum

Given an undirected graph $G = (V, E)$ where $V = [n]$, let $A_G = \left(a_{ij}\right)_{i,j\in[n]}$ be the adjacent matrix of G. That is, A_G is a boolean matrix with $a_{ij} = 1$ iff $(i, j) \in E$. Clearly A_G is symmetric. Therefore the n eigenvalues of A_G, $\lambda_1, \lambda_2, \ldots, \lambda_n$, are all real numbers. W.l.o.g, we assume $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. This is called the spectrum of G. For example, when G is the complete graph K_n,

$$A_{K_n} = \begin{bmatrix} 0 & 1 & \cdots & & \\ 1 & 0 & & & \\ \vdots & & \ddots & 1 \\ & & 1 & 0 \end{bmatrix}.$$

The n eigenvalues of A_{K_n} is $\lambda_1 = n - 1$ and $\lambda_2 = \cdots = \lambda_n = -1$. The corresponding eigenvectors are

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} 1 \\ -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \cdots, \quad \mathbf{v}_n = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ -1 \end{bmatrix}.$$

When the graph G is given, its spectrum is also determined. However, the same spectrum may corresponds to different graphs. The properties of the spectrum usually reflect certain properties of the graph and have been extensively studied.

Proposition 1. *If the maximium degree of a graph G is Δ, then $\lambda_1 \leq \Delta$. In particular, if G is Δ-regular, then $\lambda_1 = \Delta$.*

Proof. Let $\delta = \max_{i\in[n]} \sum_{j=1}^{n} \left|a_{ij}\right|$ be the maximum absolute row sum of A. We claim that $\|A\|_\infty = \delta$.[1] Here A is not necessarily a binary matrix.

Choosing $\mathbf{x} = \mathbf{v}_1$, we have

$$|\lambda_1|\|\mathbf{v}_1\|_\infty = \|A_G\mathbf{v}_1\|_\infty \leq \|A_G\|_\infty\|\mathbf{v}_1\|_\infty$$

by definition. If the claim holds, we can further yield that $|\lambda_1| \leq \|A_G\|_\infty = \delta = \Delta$. When G is Δ-regular, it is easy to verify that $\mathbf{1}$ is an eigenvector corresponding to the eigenvalue Δ. Therefore, we have $\lambda_1 = \Delta$.

It remains to prove the claim. We write A as $A = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n]$. Then $A\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + \cdots + x_n\mathbf{a}_n$. W.l.o.g, assume that $\arg\max_i \sum_i \left|a_{ij}\right| = 1$, i.e., the first row of A has the maximum absolute row sum. Note that $\frac{\|A\mathbf{x}\|_\infty}{\|\mathbf{x}\|_\infty}$ reaches the peak when $\mathbf{x} \in \{-1, 1\}^n$ and each $x_i = \mathrm{sgn}(a_{1i})$. This naturally yields that $\|A\|_\infty = \delta$. ☐

[1] The p-norm of a vector $\mathbf{x}$ is defined as $\|\mathbf{x}\|_p = \left(\sum_i |x_i|^p\right)^{\frac{1}{p}}$. Specifically, when $p = \infty$, $\|\mathbf{x}\|_\infty = \max_i |x_i|$. The p-norm of a matrix A is defined as $\|A\|_p = \max_{\mathbf{x}\neq\mathbf{0}} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p}$, which measures the size of the operator A.

The result shows that λ_1 is related to the degree of the graph. We will see how the other eigenvalues reflect graph properties.

2 Rayleigh Quotient

Given $A \in \mathbb{R}^{n\times n}$ and $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, the Rayleigh quotient is defined as $R_A(\mathbf{x}) \triangleq \frac{\langle \mathbf{x}, A\mathbf{x}\rangle}{\langle \mathbf{x},\mathbf{x}\rangle}$. By the spectral decomposition theorem, A can be written as $\sum_{i=1}^n \lambda_i \mathbf{v}_i\mathbf{v}_i^T$ where $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ is a group of orthonormal eigenvectors of A corresponding to eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ respectively.

Unless otherwise stated, we assume A is symmetric.

We can write $\mathbf{x}$ as $\sum_{i=1}^n a_i\mathbf{v}_i$ for some constants $a_1, a_2 \ldots, a_n$. Then

$$\langle \mathbf{x}, \mathbf{x}\rangle = \langle \sum_{i=1}^n a_i\mathbf{v}_i, \sum_{j=1}^n a_j\mathbf{v}_j\rangle = \sum_{i,j\in[n]} a_i a_j \langle \mathbf{v}_i, \mathbf{v}_j\rangle = \sum_{i=1}^n a_i^2$$

and

$$A\mathbf{x} = \left(\sum_{i=1}^n \lambda_i \mathbf{v}_i\mathbf{v}_i^T\right)\left(\sum_{j=1}^n a_j\mathbf{v}_j\right) = \sum_{i,j\in[n]} \lambda_i a_j \mathbf{v}_i \langle \mathbf{v}_i, \mathbf{v}_j\rangle = \sum_{i=1}^n \lambda_i a_i \mathbf{v}_i.$$

Similarly,

$$\langle \mathbf{x}, A\mathbf{x}\rangle = \langle \sum_{j=1}^n a_j\mathbf{v}_j, \sum_{i=1}^n \lambda_i a_i\mathbf{v}_i\rangle = \sum_{i=1}^n \lambda_i a_i^2.$$

Therefore, $R_A(\mathbf{x}) = \frac{\langle \mathbf{x}, A\mathbf{x}\rangle}{\langle \mathbf{x},\mathbf{x}\rangle} = \frac{\sum_{i=1}^n \lambda_i a_i^2}{\sum_{i=1}^n a_i^2}$. With this form of Rayleigh quotient, we can introduce the Courant-Fischer theorem, which gives a variational characterization of the eigenvalues.

Claim 2. $\lambda_1 = \max_{\mathbf{x}\neq\mathbf{0}} R_A(\mathbf{x})$

Proof. Since $R_A(\mathbf{x}) = \frac{\sum_{i=1}^n \lambda_i a_i^2}{\sum_{i=1}^n a_i^2} = \sum_{i=1}^n \frac{a_i^2}{\sum_{j=1}^n a_j^2}\lambda_i$ achieves the maximum when the weight concentrates on λ_1, we have $\max_{\mathbf{x}\neq\mathbf{0}} R_A(\mathbf{x}) = R_A(\mathbf{v}_1) = \lambda_1$. □

With the same argument, we have $\lambda_2 = \max_{\mathbf{x}\neq\mathbf{0}, \mathbf{x}\perp\mathbf{v}_1} R_A(\mathbf{x})$. This can be generalized to the k-th largest eigenvalue:

$$\lambda_k = \max_{\substack{\mathbf{x}\neq\mathbf{0} \\ \mathbf{x}\perp\mathrm{span}(\mathbf{v}_1,\ldots,\mathbf{v}_{k-1})}} R_A(\mathbf{x}).$$

We also have

$$\lambda_k = \max_{\substack{V\subseteq\mathbb{R}^n \\ dim(V)=k}} \min_{\mathbf{x}\in V\setminus\{\mathbf{0}\}} R_A(\mathbf{x}). \tag{1}$$

Equation (1) can be interpreted as the competition between the max player and min player. The best choice of the max player is to set $V = \mathrm{span}(\mathbf{v}_1, \ldots, \mathbf{v}_k)$ and the min player will choose $\mathbf{x} = \mathbf{v}_k$ to minimize $R_A(\mathbf{x})$.

Proposition 3. *For a simple d-regular graph $G = (V, E)$, G is connected iff $\lambda_2 \neq d$.*

Proof. Recall that $\mathbf{v}_1 = \frac{1}{\sqrt{n}} \cdot \mathbf{1}$ for d-regular graphs. Then by the Courant-Fischer theorem, $\lambda_2 = \max_{\mathbf{x}\neq\mathbf{0}, \mathbf{x}\perp\mathbf{1}} R_{A_G}(\mathbf{x})$. Note that

$$R_{A_G}(\mathbf{x}) = \frac{\sum_{(i,j)\in E} 2x_ix_j}{\sum_{i=1}^n x_i^2} = d - \frac{d\sum_{i=1}^n x_i^2 - \sum_{(i,j)\in E} 2x_ix_j}{\sum_{i=1}^n x_i^2} = d - \frac{\sum_{(i,j)\in E}\left(x_i - x_j\right)^2}{\sum_{i=1}^n x_i^2}.$$

Therefore $\lambda_2 = d$ iff $\left(x_i - x_j\right)^2 = 0$ for all $(i,j) \in E$. Since $\mathbf{x} \perp \mathbf{1}$, $\sum_{(i,j)\in E}\left(x_i - x_j\right)^2 = 0$ indicates that G is not connected. □

Proposition 4. *Suppose $G = (V, E)$ is a simple d-regular graph which is connected. Then G is bipartite iff $\lambda_n = -d$.*

Proof. By the Courant-Fischer theorem,

$$\lambda_n = \min_{\mathbf{x} \neq \mathbf{0}} R_{A_G}(\mathbf{x}) = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{i,j \in [n]} a_{ij} x_i x_j}{\sum_{i=1}^n x_i^2}.$$

Note that

$$\frac{\sum_{i,j \in [n]} a_{ij} x_i x_j}{\sum_{i=1}^n x_i^2} = \frac{\sum_{(i,j) \in E} 2 x_i x_j}{\sum_{i=1}^n x_i^2} + d - d = \frac{\sum_{(i,j) \in E} \left(x_i + x_j\right)^2}{\sum_{i=1}^n x_i^2} - d.$$

Therefore $\lambda_n = -d$ iff $x_i = -x_j$ for all $(i, j) \in E$. This indicates that G is bipartite. □

Now we prove that λ_1 is least the average deree of G.

Theorem 5. $d_{\text{ave}} \leq \lambda_1$. [2]

[2] Here d_{ave} denotes the average degree $\frac{\sum_{v \in V} \deg(v)}{|V|}$.

Proof. Using Courant-Fischer, we have

$$\mu_1 = \max_{\mathbf{x} \neq 0} \frac{\mathbf{x}^\mathsf{T} A \mathbf{x}}{\mathbf{x}^\mathsf{T} \mathbf{x}} \geq \frac{\mathbf{1}^\mathsf{T} A \mathbf{1}}{\mathbf{1}^\mathsf{T} \mathbf{1}} = \frac{\sum_{i,j \in [n]} a_{ij}}{n} = \frac{\sum_i \deg(i)}{n} = d_{\text{ave}}.$$

□

3 Laplacian Matrix

When the graph is not necessarily regular, it is convenient to normalize its first eigenvalue.

3.1 The Spectrum of Laplacian Matrix

Let $A_G = \left(w_{ij}\right)_{i,j \in [n]}$ be the adjacent matrix of some graph G (probably weighted) and define $w_i = \sum_{j=1}^n w_{ij}$ for all $i \in [n]$. Let $D_G = \operatorname{diag}(w_1, w_2, \ldots, w_n)$. The *Laplacian matrix* of G is defined as $L_G = D_G - A_G$.

With the definition of Laplacian matrix, we can turn to consider the spectrum of L_G instead of A_G. For example, when G is d-regular, $L_G = d\mathbb{I} - A_G$. Let $\gamma_1 \leq \gamma_2 \leq \cdots \leq \gamma_n$ be the eigenvalues of L_G and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A_G. Then $\gamma_i = d - \lambda_i$ by definition and we have $\gamma_1 = 0$. We claim that this also applies to general graphs.

Lemma 6. $\mathbf{x}^\mathsf{T} L_G \mathbf{x} = \sum_{\{i,j\} \in E} w_{ij} \left(x_i - x_j\right)^2$.

For a weighted graph G, $E = \left\{\{i, j\} \mid w_{ij} \neq 0\right\}$.

Proof. This can be proved by a direct calculation:

$$\begin{aligned}
\sum_{\{i,j\}\in E} w_{ij}\left(x_i - x_j\right)^2 &= \sum_{\{i,j\}\in E} w_{ij}\left(x_i^2 - 2x_ix_j + x_j^2\right) \\
&= \sum_{\{i,j\}\in E} w_{ij}\left(x_i^2 + x_j^2\right) - 2\sum_{\{i,j\}\in E} w_{ij}x_ix_j \\
&= \sum_{i\in V} x_i^2 \sum_{j\sim i} w_{ij} + \sum_{i\in V} x_i^2 w_{ii} - 2\sum_{\{i,j\}\in E} w_{ij}x_ix_j \\
&= \sum_{i\in V} x_i^2 w_i + \sum_{i\in V} x_i^2 w_{ii} - \left(\sum_{i,j\in V} w_{ij}x_ix_j + \sum_{i\in V} w_{ii}x_i^2\right) \\
&= \sum_{i\in V} x_i^2 w_i - \sum_{i,j\in V} w_{ij}x_ix_j \\
&= \mathbf{x}^\mathsf{T} D_G \mathbf{x} - \mathbf{x}^\mathsf{T} A_G \mathbf{x} = \mathbf{x}^\mathsf{T} L_G \mathbf{x}.
\end{aligned}$$

□

Equipped with Lemma 6, we then prove our claim.

Claim 7. *For any graph G with $w_{ij} \geq 0$, $\gamma_1(L_G) = 0$.*

Proof. By the Courant-Fischer theorem,

$$\gamma_1(L_G) = \min_{\mathbf{x}\neq 0} \frac{\mathbf{x}^\mathsf{T} L_G \mathbf{x}}{\mathbf{x}^\mathsf{T}\mathbf{x}} = \min_{\mathbf{x}\neq 0} \frac{\sum_{\{i,j\}\in E} w_{ij}\left(x_i - x_j\right)^2}{\sum_{i=1}^n x_i^2} \geq 0$$

where the second equation follows from Lemma 6. Furthermore,

$$\gamma_1(L_G) \leq \frac{\mathbf{1}^\mathsf{T} L_G \mathbf{1}}{\mathbf{1}^\mathsf{T}\mathbf{1}} = 0.$$

Therefore, we have $\gamma_1(L_G) = 0$. □

Example 1 (Complete Graph)**.** *When G is a complete graph K_n,*

$$L_G = \begin{bmatrix} n-1 & 0 & \cdots & & \\ 0 & n-1 & & & \\ \vdots & & & \ddots & 0 \\ & & & 0 & n-1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & \cdots & & \\ 1 & 0 & & & \\ \vdots & & & \ddots & 1 \\ & & & 1 & 0 \end{bmatrix}.$$

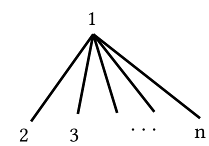
Pick $\mathbf{v} \perp \mathbf{1}$. That is, $\sum_{i=1}^n \mathbf{v}(i) = 0$, or equivently, $v(1) = -\sum_{i=2}^n \mathbf{v}(i)$. Then

$$L_G\mathbf{v}(1) = (n-1)\mathbf{v}(1) - \sum_{i=2}^n \mathbf{v}(i) = n\mathbf{v}(1).$$

Similarly we have $L_G\mathbf{v}(i) = n\mathbf{v}(i)$ for every other $i \in [n]$ and thus $L_G\mathbf{v} = n\mathbf{v}$ for all $\mathbf{v} \perp \mathbf{1}$. Therefore, the spectrum of L_{K_n} is $0, n, n, \ldots, n$, which respectively corresponds to the eigenvectors $\mathbf{1}$ and the $n-1$ independent vectors that are perpendicular to $\mathbf{1}$.

Example 2 (Star Graph). *When G is a star,*

$$L_G = \begin{bmatrix} n-1 & 0 & \cdots & \\ 0 & 1 & & \\ \vdots & & \ddots & 0 \\ & & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & & \\ \vdots & & \ddots & 0 \\ 1 & & 0 & 0 \end{bmatrix} = \begin{bmatrix} n-1 & -1 & \cdots & -1 \\ -1 & 1 & & \\ \vdots & & \ddots & 0 \\ -1 & & 0 & 1 \end{bmatrix}.$$



Let $\mathbf{e}_i = (0, 0, \ldots, 0, 1, 0, \ldots, 0)$ be a unit vector where only the i-th entry is 1*. Then for every $i, j \geq 2$ and $i \neq j$, $e_i - e_j$ is an eigenvector of L_G with eigenvalue* 1*. Since* $\dim\left(\mathrm{span}\left(\{e_i - e_j\}_{\substack{i \neq j \\ i,j \geq 2}}\right)\right) = n - 2$*, it only needs to determine the remaining one eigenvalue (we have already known that $\lambda_1 = 0$). Note that*

$$\mathtt{Tr}(L_G) = n - 1 + n - 1 = \sum_{i=1}^{n} \lambda_i = 0 + (n-2) + \lambda_n.$$

Therefore, we have $\gamma_n = n$. It is easy to verify that the eigenvector corresponds to γ_n is $[1-n \quad 1 \quad \cdots \quad 1]^\mathsf{T}$.