

## 1 Spectral Graph Theory

A beautiful and surprising area of computer science is studying the relationship between the eigenvalues of the adjacency matrix of a graph (or, more often, a very similar object called its *Laplacian*) and properties of the graph itself.

### 1.1 The Laplacian

The Laplacian of a graph  $G = (V, E)$  is a matrix  $L$  in  $\mathbb{R}^{n \times n}$  (for  $|V| = n$ ) so that  $L = D - A$ , where  $D$  is the diagonal matrix of degrees so that  $D_{ii}$  is the degree of the  $i$ th vertex and all off-diagonal entries are 0. For example:



$$L = D - A = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

**Fact 1.1.** For any graph  $G$ , its Laplacian  $L$  is positive semi-definite. Furthermore, we have

$$x^T L x = \sum_{\{v_i, v_j\} \in E} (x_i - x_j)^2$$

*Proof.* Let  $L_e$  be the Laplacian of the edge  $e$  between vertices  $v_i$  and  $v_j$ , i.e., the Laplacian of the graph  $G' = (V, \{e\})$ . This is going to be a matrix of the form  $\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$  (with some extra 0s at locations without an index  $i$  or  $j$ ). But this matrix is equal to  $b_e b_e^T$ , where  $b_e$  is the vector with a 1 at position  $i$  and a  $-1$  at position  $j$ . So,  $L_e$  is PSD. Now, notice that  $L = \sum_{e \in E} L_e$ . So,

$$x^T L x = x^T \left( \sum_{e \in E} L_e \right) x = \sum_{e \in E} x^T L_e x \geq 0$$

since each  $L_e$  is PSD, showing that  $L$  itself is PSD. Even better, for an edge  $e = \{v_i, v_j\}$  we can compute

$$x^T L_e x = x_i^2 - 2x_i x_j + x_j^2 = (x_i - x_j)^2$$

so that  $x^T L x = \sum_{\{v_i, v_j\} \in E} (x_i - x_j)^2$  as desired.  $\square$

From this we know that all the eigenvalues are non-negative. We also get the following corollary which frees us from this annoying  $\mathbf{1}_S^T A \mathbf{1}_{V \setminus S}$  notation and is one of the reasons the Laplacian can be more natural to work with than the adjacency matrix.

**Corollary 1.2.** *Let  $S \subseteq V$ . Then,  $\mathbf{1}_S^T L \mathbf{1}_S = |\delta(S)|$ .*

*Proof.*

$$\mathbf{1}_S^T L \mathbf{1}_S = \sum_{\{v_i, v_j\} \in E} (\mathbb{I}\{v_i \in S\} - \mathbb{I}\{v_j \in S\})^2 = |\delta(S)|$$

since this quantity is 1 if and only if exactly one of  $v_i, v_j$  is in  $S$ . □

For vectors  $x \notin \{0, 1\}^n$ , this then gives us a kind of "fractional" cut.

**Fact 1.3.**  $\lambda_1 = 0$  for any Laplacian matrix  $L$ .

*Proof.*  $\mathbf{1}^T L \mathbf{1} = 0$  because the rows sum to 0, so  $L \mathbf{1}$  is the 0 vector. So,  $\lambda_1 = 0$ . □

So, the first eigenvalue is always 0. It turns out the second eigenvalue already tells us something interesting. Before we say this, let's prove a more general form of the Rayleigh quotient.

## 1.2 More on Eigenvalues

**Theorem 1.4.** *Given a symmetric matrix  $A \in \mathbb{R}^{n \times n}$  with eigenvalues  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$  with orthonormal eigenvectors  $v_1, \dots, v_n$ . Let  $O_k$  be the set of non-zero vectors that are orthogonal to the first  $k-1$  eigenvectors  $v_1, \dots, v_{k-1}$  (let  $O_1$  be all non-zero vectors). Then for any  $1 \leq k \leq n$ :*

$$\lambda_k = \min_{x \in O_k} \frac{x^T A x}{x^T x}$$

*Proof.* The proof of this is similar to the fact that  $\lambda_1 = \min_{x \neq 0 \in \mathbb{R}^n} \frac{x^T A x}{x^T x}$ , which you showed on your homework. In case you forget how that works, let's show that again. First we apply the spectral theorem so that  $A = \sum_{i=1}^n \lambda_i v_i v_i^T$  where  $v_1, \dots, v_n$  are an orthogonal basis of  $\mathbb{R}^n$ . So,  $x = c_1 v_1 + \dots + c_n v_n$  where  $c_i = \langle x, v_i \rangle$ . But now:

$$\begin{aligned} x^T A x &= (c_1 v_1 + \dots + c_n v_n)^T \left( \sum_{i=1}^n \lambda_i v_i v_i^T \right) (c_1 v_1 + \dots + c_n v_n) \\ &= (c_1 v_1 + \dots + c_n v_n) (\lambda_1 c_1 v_1 + \dots + \lambda_n c_n v_n) && \text{Since } v_i \text{ are orthonormal} \\ &= \sum_{i=1}^n \lambda_i c_i^2 \end{aligned}$$

Also, we have  $x^T x = (c_1 v_1 + \dots + c_n v_n)^T (c_1 v_1 + \dots + c_n v_n) = \sum_{i=1}^n c_i^2$ . Therefore:

$$\frac{x^T A x}{x^T x} = \frac{\sum_{i=1}^n \lambda_i c_i^2}{\sum_{i=1}^n c_i^2}$$

In other words,  $\frac{x^T A x}{x^T x}$  is a *convex combination* of the eigenvalues  $\lambda_1, \dots, \lambda_n$ . So, it is certainly at least  $\lambda_1$ , and we can pick the vector  $v_1$  to achieve  $c_1 = 1, c_i = 0$  for  $i > 1$ .

The more general proof is not very different. We know that the  $k$ th eigenvector is orthogonal to the others. So we have  $x \in O_k$ , and we must have  $c_1, \dots, c_{k-1} = 0$  since recall  $c_i = \langle x, v_i \rangle$ . So  $x \in O_k$  is a convex combination of  $\lambda_k, \dots, \lambda_n$  so to minimize it we should choose  $x = v_k$ . □

There is also a cleaner way to view things which is not tied to the eigenvectors.

**Theorem 1.5** (Courant-Fischer). *Let  $A$  be a symmetric matrix. Then:*

$$\lambda_k = \min_{S \subseteq \mathbb{R}^n: \dim(S)=k} \max_{x \in S} \frac{x^T A x}{x^T x}$$

This is quite similar to what we have already done, so we will leave the proof as an exercise.

### 1.3 $\lambda_2$ and Connectivity

Now that we understand eigenvalues a bit better, we can prove the following:

**Fact 1.6.**  *$G$  is connected if and only if  $\lambda_2 > 0$ .*

*Proof.* First suppose  $G$  is disconnected. Then, there is a set of vertices  $\emptyset \neq S \neq V$  so that  $|\delta(S)| = 0$ . So, by [Corollary 1.2](#),  $\mathbf{1}_S^T L \mathbf{1}_S = 0$ , and  $\mathbf{1}_S \neq \mathbf{0}$  which also implies  $L \mathbf{1}_S = 0 \cdot \mathbf{1}_S$ . But then we have two eigenvectors with eigenvalue 0,  $\mathbf{1}$  and  $\mathbf{1}_S$ . Furthermore, they are not linearly dependent. So by Courant-Fischer, we can pick  $S$  as the 2-dimensional space spanned by  $\mathbf{1}$  and  $\mathbf{1}_S$  and  $\lambda_1, \lambda_2$  are both 0, since  $x^T L x$  will be 0 for any vector in the span of  $\mathbf{1}$  and  $\mathbf{1}_S$ .

Second, suppose  $G$  is connected. Suppose that  $\lambda_2 = 0$ . Then there is a 2-dimensional space  $S$  with  $x^T L x = 0$  for all  $x \in S$ . There is therefore some  $x \in S$  which is not a multiple of the all 1s vector for which  $x^T L x = 0$ . Then,

$$\sum_{\{v_i, v_j\} \in E} (x_i - x_j)^2 = x^T L x = 0$$

That implies that  $x_i = x_j$  for all  $i, j$ . But then  $x$  would be a multiple of  $\mathbf{1}$ , contradiction.  $\square$

You might say now: who cares? We already know how to figure out if a graph is connected with much simpler methods. The reason we care is this:  $\lambda_2$  of  $L$  is actually a measure of *how connected the graph is*.

**Fact 1.7.** *For the complete graph, the second eigenvalue of the Laplacian is  $n$ .*

*Proof.* We have  $L = n \cdot I - \mathbf{1}\mathbf{1}^T$ . So:

$$Lx = (n \cdot I - \mathbf{1}\mathbf{1}^T)x = n \cdot x - \mathbf{1}\mathbf{1}^T x$$

but since the first eigenvector is  $\mathbf{1}$ , any eigenvector after the first is orthogonal to  $\mathbf{1}$ . So for any other eigenvector, we simply have  $Lx = nx$ . Therefore this matrix has  $\lambda_1 = 0$  and  $\lambda_i = n$  for all  $i \geq 2$ .  $\square$

This is big. So, the complete graph is "very" connected. But, if we want to have a concrete measure of connectedness, it's better for it not to depend on  $n$ . It would be nice to have a single number, say between 0 and 1, that measured the connectivity, where 0 was disconnected and 1 was super connected.

**Definition 1.8** (Normalized Adjacency Matrix and Normalized Laplacian). Given a graph  $G$ , the normalized adjacency matrix  $\tilde{A}$  is:

$$\tilde{A} = D^{-1/2} A D^{-1/2}$$

where  $D$  is the diagonal matrix of vertex degrees. In this way,  $\tilde{A}_{i,j} = \frac{A_{i,j}}{\sqrt{d_i d_j}}$ . The normalized Laplacian  $\tilde{L}$  is then equal to

$$\tilde{L} = I - \tilde{A}$$

**Fact 1.9.** The eigenvalues of  $\tilde{A}$  are between -1 and 1. The eigenvalues of  $\tilde{L}$  are between 0 and 2.

*Proof.* First, note that  $\tilde{L}$  is still PSD. This is because:

$$x^T \tilde{L} x = x^T D^{-1/2} L D^{-1/2} x = \sum_{e \in E} x^T D^{-1/2} L_e D^{-1/2} x = \sum_{\{v_i, v_j\} \in E} \left( \frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}} \right)^2 \geq 0$$

Also, 0 is still an eigenvalue of  $\tilde{L}$  because:

$$\tilde{L}(D^{1/2} \mathbf{1}) = (D^{-1/2} L D^{-1/2})(D^{1/2} \mathbf{1}) = D^{-1/2} L \mathbf{1} = \mathbf{0}$$

In other words, we have  $\tilde{L} = I - \tilde{A} \succeq 0$ . So  $\tilde{A} \preceq I$ , so its eigenvalues are at most 1. We leave the proof that its eigenvalues are at least -1 as an exercise.

So, the eigenvalues of  $\tilde{A}$  are between -1 and 1. But then the eigenvalues of  $I - \tilde{A}$  are between 0 and 2.  $\square$

It remains true that a graph is connected if and only if the second eigenvalue of  $\tilde{L}$  is greater than 0. And for the complete graph, we can see that  $\lambda_2 = \frac{n}{n-1}$ . This is because now  $\tilde{L} = \frac{n}{n-1} I - \frac{1}{n-1} \mathbf{1}\mathbf{1}^T$  since  $\tilde{A} = \frac{1}{n-1}$  on all off-diagonal entries and 0 on the diagonal. Furthermore, the first eigenvector (since the degrees are all equal) is the all 1s vector. So, for any  $x$  orthogonal to that we have:

$$\tilde{L}x = \left( \frac{n}{n-1} I - \frac{1}{n-1} \mathbf{1}\mathbf{1}^T \right) x = \frac{n}{n-1} x$$

Something perplexing here is that the complete graph is *not* maximally connected with respect to this measure  $0 \leq \lambda_2 \leq 2$  for  $\tilde{L}$ . That's a bit strange. It turns out that  $\lambda_2$  is 2 exactly when the graph is bipartite. We'll explore this next class.