AN INTRODUCTION TO SPECTRAL GRAPH THEORY

JIAQI JIANG

Abstract. Spectral graph theory is the study of properties of the Laplacian matrix or adjacency matrix associated with a graph. In this paper, we focus on the connection between the eigenvalues of the Laplacian matrix and graph connectivity. Also, we use the adjacency matrix of a graph to count the number of simple paths of length up to 3.

Contents

1. Introduction

The eigenvalues of the Laplacian matrix of a graph are closely related to the connectivity of the graph. Therefore, bounds for the smallest nonzero eigenvalue of the graph Laplacian give us intuition on how well connected a graph is. Thus, we focus on finding bounds for this eigenvalue. Additionally, the adjacency matrix of a graph provides information about paths contained in the graph. Therefore, it is also one of our goals to find a way to count the number of paths of different length contained in the graph using the adjacency matrix.

2. Background of Spectral Graph Theory

We introduce the basic concepts of graph theory and define the adjacency matrix and the Laplacian matrix of a graph.

Definition 2.1. A graph is an ordered pair G=(V,E) of sets, where

$$E \subset \{\{x, y\} \mid x, y \in V, x \neq y\}.$$

The elements of V are called *vertices* (or *nodes*) of the graph G and the elements of E are called *edges*. So in a graph G with vertex set $\{x_1, x_2, \ldots, x_n\}$, $\{x_i, x_j\} \in E$ if and only if there is a line in G which connects the two points x_i and x_j. The graph we defined above is called an undirected graph. A directed graph is similar to an undirected graph except the edge set $E \subset V \times V$. Unless specified, the graphs we deal with in this paper are all undirected and finite. Also, the vector spaces we are working on are all real vector spaces.

Now we will define the concept of adjacency.

Definition 2.2. In a graph $G = (V, E)$, two points $x_i, x_j \in V$ are *adjacent* or *neighbors* if $\{x_i, x_j\} \in E$.

If all the vertices of G are pairwise adjacent, then we say G is *complete*. A complete graph with n vertices is denoted as K^n. For example, the graph of a triangle is K^3, the complete graph with three vertices.

Definition 2.3. The *degree* $d(v)$ of a vertex v is the number of vertices in G that are adjacent to v.

There are two matrices we can get from a graph G. One is called adjacency matrix, which we denote as A_G. The other is called Laplacian matrix, which we denote as L_G. Without loss of generality, assume a graph G has the vertex set $V = \{1, 2, \ldots, n\}$. Now we define the adjacency matrix and the Laplacian matrix of G as follows:

Definition 2.4. In the *adjacency matrix* A_G of the graph G, the entries $a_{i,j}$ are given by

$$a_{i,j} = \begin{cases} 1 & \text{if } \{i, j\} \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Definition 2.5. In the *Laplacian matrix* L_G of the graph G, the entries $l_{i,j}$ are given by

$$l_{i,j} = \begin{cases} -1 & \text{if } \{i, j\} \in E, \\ d(i) & \text{if } i = j, \text{and} \\ 0 & \text{otherwise.} \end{cases}$$

One use of the adjacency matrix of a graph is to calculate the number of walks of different length connecting two vertices in the graph. Before we define the concept of walk, we first introduce the concept of incident.

Definition 2.6. A vertex $v \in V$ is *incident* with an edge $\{v_i, v_j\} \in E$ if $v = v_i$ or $v = v_j$.

Now we define the concept of the walk.

Definition 2.7. A *walk* on a graph is an alternating series of vertices and edges, beginning and ending with a vertex, in which each edge is incident with the vertex immediately preceding it and the vertex immediately following it.

A walk between two vertices u and v is called a $u - v$ *walk*. The *length* of a walk is the number of edges it has. In a walk, we count repeated edges as many times as they appear.

Theorem 2.8. *For a graph G with vertex set $V = \{1, 2, \ldots, m\}$, the entry a^n_{ij} of the matrix A^n_G obtained by taking the nth power of the adjacency matrix A_G equals the number of $i - j$ walks of length n.*

Proof. We will prove the theorem by induction. When $n = 1$, the entry a_{ij} is 1 if $\{i, j\} \in E$. By definition, $i\,\{i, j\}\,j$ is then an $i - j$ walk of length 1 and this is the only one. So the statement is true for $n = 1$.

Now, we assume the statement is true for n and then prove the statement is also true for $n + 1$. Since $A_{ij}^{n+1} = A_{ij}^{n} \cdot A_{ij}$, therefore, $a_{ij}^{n+1} = \sum_{k=1}^{m} a_{ik}^{n} \cdot a_{kj}$. Because $a_{ki} = 0$ whenever $\{k, i\} \notin E$ and $a_{ki} = 1$ if $\{k, i\} \in E$, it follows that $a_{ik}^{n} \cdot a_{ki}$ represents the number of those $i - j$ walks that are $i - k$ walks of length n joined by the edge $\{k, j\}$. In particular, all walks from i to j of length $n + 1$ are of this form for some vertex k. Thus $a_{ij}^{n+1} = \sum_{k=1}^{m} a_{ik}^{n} \cdot a_{kj}$ indeed represents the total number of $i - j$ walks of length $n + 1$. This proves the statement for $n + 1$. Then by the principle of induction, we prove the statement for all natural numbers n. □

In a later section, we will discuss how to compute the number of paths (a walk in which vertices are all distinct from each other) of length up to 3 between i and j in a graph given the adjacency matrix of the graph.

3. Basic Properties of The Laplacian Matrix

One of the most interesting properties of a graph is its connectedness. The Laplacian matrix provides us with a way to investigate this property. In this section, we study the properties of the Laplacian matrix of a graph. First, we give a new way to define the Laplacian matrix for a graph, which turns out to be much more useful than the previous one.

Definition 3.1. Suppose $G = (V, E)$ is a graph with $V = \{1, 2, \ldots, n\}$. For an edge $\{u, v\} \in E$, we define an $n \times n$ matrix $L_{G_{\{u,v\}}}$ by

$$l_{G_{\{u,v\}}}(i, j) = \begin{cases} 1 & \text{if } i = j \text{ and } i \in \{u, v\}, \\ -1 & \text{if } i = u \text{ and } j = v, \text{ or vice versa}, \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to check that $L_{G_{\{u,v\}}}$ has the nice property that

$$\vec{x}^T L_{G_{\{u,v\}}} \vec{x} = (x_u - x_v)^2 \text{ for all } \vec{x} \in \mathbb{R}^n.$$

Now given the edge set E of a graph G, we are ready to give our new definition of the Laplacian matrix L_G of the graph.

Definition 3.2. For a graph $G = (V, E)$, $L_G = \sum\limits_{\{u,v\} \in E} L_{G_{\{u,v\}}}$.

It is readily seen that this new definition of the Laplacian matrix is indeed equivalent to the definition given in the previous section. However, we find that many elementary properties of the Laplacian matrix follow easily from the new definition. We see that the eigenvalues of the Laplacian matrix are all real by realizing that the Laplacian matrix of a graph is symmetric and consists of real entries. Thus, $L_G{=}L_G^*$ where L_G^* is the conjugate transpose of L_G. Therefore, L_G is self adjoint. By the following theorem, all the eigenvalues of L_G are thus real.

Theorem 3.3. *The eigenvalues of a self adjoint matrix are all real.*

Proof. Suppose λ is an eigenvalue of the self adjoint matrix L and v is a nonzero eigenvector of λ. Then

$$\begin{aligned}\lambda \|v\|^2 &= \lambda \langle v, v\rangle \\ &= \langle \lambda v, v\rangle \\ &= \langle Lv, v\rangle \\ &= \langle v, Lv\rangle \\ &= \langle v, \lambda v\rangle \\ &= \overline{\lambda} \langle v, v\rangle \\ &= \overline{\lambda} \|v\|^2\end{aligned}$$

Since $v \neq 0$, we have $\|v\|^2 \neq 0$. Therefore, $\lambda = \overline{\lambda}$. This proves that λ is real. □

In fact, the eigenvalues of the Laplacian matrix are not only real but also non-negative. Recall the definition of positive-semidefinite.

Definition 3.4. An $n \times n$ matrix M is called positive-semidefinite if $\vec{x}^T M \vec{x} \geqslant 0$ for all $\vec{x} \in \mathbb{R}^n$.

Since $\vec{x}^T L_{G_{\{u,v\}}} \vec{x} = (x_u - x_v)^2$ for all $\vec{x} \in \mathbb{R}^n$, we have

$$\vec{x}^T L_G \vec{x} = \sum_{\{u,v\} \in E} \vec{x}^T L_{G_{\{u,v\}}} \vec{x} = \sum_{\{u,v\} \in E} (x_u - x_v)^2 \geqslant 0.$$

Therefore, the Laplacian matrix of a graph is positive-semidefinite. It follows that all the eigenvalues of L_G is non-negative.

Theorem 3.5. *For a graph G, every eigenvalue of L_G is non-negative.*

Proof. Suppose λ is an eigenvalue and $\vec{x} \in \mathbb{R}^n$ is a nonzero eigenvector of λ. Then

$$\begin{aligned}\vec{x}^T L_G \vec{x} &= \vec{x}^T (\lambda \vec{x}) \\ &= \lambda (\vec{x}^T \vec{x})\end{aligned}$$

Since $\vec{x}^T L_G \vec{x} \geqslant 0$ and $\vec{x}^T \vec{x} > 0$, we have $\lambda \geqslant 0$. □

As we have noted, the Laplacian matrix L_G is self-adjoint and consists of real entries. Thus the Real Spectral Theorem states that L_G has an orthonormal basis consisting of eigenvectors of L_G. Therefore, for a graph G of n vertices, we can find n eigenvalues (not necessarily distinct) for L_G. We denote them as $\lambda_1, \lambda_2, \ldots, \lambda_n$. Since they are all real and non-negative, we assume that

$$0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n.$$

Now we prove some fundamental facts about Laplacians. Recall that in the previous section we mentioned that the eigenvalues of the Laplacian tell us how connected a graph is. Now, we define connectedness. First, we give the definition of a *path*.

Definition 3.6. A *path* is a non-empty graph $P = (V, E)$ of the form

$$V = \{x_0, x_1, \ldots, x_n\} \qquad E = \{\{x_0, x_1\}, \{x_1, x_2\}, \ldots, \{x_{n-1}, x_n\}\},$$

where all the vertices x_i are distinct.

Recall the definition of a walk, a path is in fact a walk with no repeating vertices.

Definition 3.7. A non-empty graph G is called *connected* if any two of its vertices are contained in a path in G.

Now we will see that the eigenvalue 0 is closely related to this connectedness.

Lemma 3.8. *For any graph G, $\lambda_1 = 0$ for L_G. If $G = (V, E)$ is a connected graph where $V = \{1, 2, \dots, n\}$, then $\lambda_2 > 0$.*

Proof. Let $\vec{x} = (1, 1, \dots, 1) \in \mathbb{R}^n$. Then the entry m_i of the matrix $M = L_G\vec{x}$ is

$$m_i = \sum_{k=1}^{n} l_{ik}.$$

Recall the definition of L_G given in the first section. It follows immediately that $m_i = 0$ since the row entries of L_G should add up to zero. So $L_G\vec{x} = 0$. Therefore, 0 is an eigenvalue of L_G. Since $0 \leqslant \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$, it follows that $\lambda_1 = 0$.

Now we want to show that $\lambda_2 > 0$ for a connected graph. Since 0 is an eigenvalue of L_G, let $\vec{z}$ be a nonzero eigenvector of 0. Then

$$\vec{z}^T L_G \vec{z} = \vec{z}^T \cdot 0 = 0.$$

So

$$\vec{z}^T L_G \vec{z} = \sum_{\{u,v\} \in E} (z_u - z_v)^2 = 0.$$

This implies that for any $\{u, v\}$ such that $\{u, v\} \in E$, $z_u = z_v$. Since G is connected, this means $z_i = z_j$ for all $i, j \in V$. Therefore,

$$z = \alpha \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix},$$

where α is some real number. So,

$$U_{\lambda_1} = \operatorname{Span}\left((1, 1, \dots, 1)\right),$$

where U_{λ_1} is the eigenspace of λ_1. Therefore, the multiplicity of eigenvalue 0 is 1. It follows that $\lambda_2 \neq 0$, so $\lambda_2 > 0$. □

In fact, the multiplicity of the eigenvalue 0 of L_G tells us the number of connected components in the graph G.

Definition 3.9. A *connected component* of a graph $G = (V, E)$ is a subgraph $G' = (V', E')$, $(V' \subset V,\ E' = \{\{x, y\} \in E \mid x, y \in V'\})$, in which any two vertices $i, j \in V'$ are connected while for any $i \in V'$ and $k \in V \setminus V'$, i, k are not connected .

Corollary 3.10. *Let $G = (V, E)$ be a graph. Then the multiplicity of 0 as an eigenvalue of L_G equals the number of connected components of G.*

Proof. Suppose $G_1 = (V_1, E_1), G_2 = (V_2, E_2), \dots, G_k = (V_k, E_k)$ are the connected components of G. Let $\vec{w_i}$ be defined by

$$(w_i)_j = \begin{cases} 1 & \text{if } j \in V_i, \\ 0 & \text{otherwise .} \end{cases}$$

Then, it follows from the previous lemma that if $\vec{x} \in \mathbb{R}^n$ is a non-zero eigenvector of 0, then $x_i = x_j$ for any $i, j \in V$ such that i, j are in the same connected component. So

$$U_{\lambda_1} = \text{Span}(\{\vec{w_1}, \vec{w_2}, \ldots, \vec{w_k}\}).$$

It is clear that $\vec{w_1}, \vec{w_2}, \ldots, \vec{w_k}$ are linearly independent. Therefore, the multiplicity of 0 as an eigenvalue of L_G is the number of connected components in G. $\square$

4. Eigenvalues and Eigenvectors of the Laplacians of Some Fundamental Graphs

Now we begin to examine the eigenvalues and the eigenvectors of the Laplacian of some fundamental graphs.

Definition 4.1. A complete graph on n vertices, K_n, is a graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$ and $E = \{\{i, j\} \mid i \neq j, i, j \in V\}$.

Proposition 4.2. *The Laplacian of K_n has eigenvalue 0 with multiplicity 1 and eigenvalue n with multiplicity $n - 1$.*

Proof. The first part of the proposition simply follows from Corollary 3.9.

To prove the second part of the proposition, consider the Laplacian of K_n. It is an $n \times n$ matrix defined by

$$a_{ij} = \begin{cases} -1 & \text{if } i \neq j, \\ n-1 & \text{if } i = j. \end{cases}$$

Therefore, $L_{K_n} - nI = M$ where M is the $n \times n$ matrix with entries all equal -1. Clearly, M is not invertible and has rank 1. Thus n is an eigenvalue of L_{K_n}. Then by Rank-nullity Theorem, $\text{null}(M) = n - 1$. It follows that the eigenvalue n has multiplicity $n - 1$. $\square$

Definition 4.3. The path graph on n vertices, P_n, is a graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$ and $E = \{\{i, i+1\} \mid 1 \leqslant i < n\}$.

Definition 4.4. The cycle graph on n vertices, C_n, is a graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$ and $E = \{\{i, i+1\} \mid 1 \leqslant i < n\} \cup \{\{1, n\}\}$.

Proposition 4.5. *The Laplacian of C_n has eigenvalues $2 - 2\cos(\frac{2\pi k}{n})$ and associated eigenvectors of the form*

$$x_i(k) = \sin\left(\frac{2\pi k i}{n}\right) \quad \textit{and,}$$
$$y_i(k) = \cos\left(\frac{2\pi k i}{n}\right),$$

where $x_i(k)$ denotes the ith component of the eigenvector for the kth eigenvalue and $k \leqslant \frac{n}{2}$.

Proof. Note the Laplacian matrix of C_n has the form

$$\begin{pmatrix} 2 & -1 & 0 & \cdots & -1 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ -1 & \cdots & 0 & -1 & 2 \end{pmatrix}.$$

Therefore, if λ is an eigenvalue of L_{C_n} and $\vec{x}$ is an associated eigenvector, then $\vec{x}$ should satisfy

$$2x_1 - x_2 - x_n = \lambda x_1 \tag{4.6}$$

$$-x_1 - x_{n-1} + 2x_n = \lambda x_n, \text{and,} \tag{4.7}$$

$$-x_{m-1} + 2x_m - x_{m+1} = \lambda x_m, \text{for all } 1 < m < n. \tag{4.8}$$

Also, from the form of L_{C_n}, we can see that if P is a cyclic permutation, then $P\vec{x}$ is also an eigenvector for λ. This means that $\vec{x}, P\vec{x}, \ldots, P^{n-1}\vec{x}$ are all eigenvectors of λ. However, the maximum dimension of any eigenspace is $n-1$ since 0 is an eigenvalue of multiplicity 1. This implies that

$$P^j\vec{x} \in \mathrm{Span}(\{\vec{x}, P\vec{x}, \ldots, P^{j-1}\vec{x}\})$$

for some j. This shall give us some idea about the possible form of $\vec{x}$. We might try the particular form corresponding to the case $j = 1$ such that

$$x_m = A^m, \tag{4.9}$$

where $A = x_1$ is some constant.

Plugging (4.9) into (4.6), (4.7) and (4.8), we get

$$\begin{aligned} 2 - A - A^{n-1} &= \lambda \\ 2 - A^{1-n} - A^{-1} &= \lambda \text{ and,} \\ 2 - A^{-1} - A &= \lambda \text{ for all } 1 < i < n. \end{aligned}$$

Combining these equations, we actually get that $A^n = 1$. This means

$$A_k = e^{\frac{2\pi k i}{n}}$$

for $1 \leqslant k \leqslant n$ are solutions. The associated eigenvalues $\lambda_k = 2 - 2\cos(\frac{2\pi k}{n})$ are indeed all real. Recall we are working on the real vector space, but so far the $\vec{x}$ we get by the form $x_m = A^m$ are complex as A_k is complex. However, if we write $x_m(k) = A^m$ using Euler's Formula, we can see that

$$z_m(k) = \cos(\frac{2\pi km}{n}) + i\sin(\frac{2\pi km}{n}).$$

Since $L_{C_n}z(k) = \lambda_k z(k)$ and both L_{C_n} and λ_k are real, this means that both the real part and the imaginary part of $z(k)$ are invariant under L_{C_n} because L_{C_n} consists of real entries. Therefore, $x_m(k) = \cos(\frac{2\pi km}{n})$ and $y_m(k) = \sin(\frac{2\pi km}{n})$ are both eigenvectors for $\lambda_k = 2 - 2\cos(\frac{2\pi k}{n})$. Then, for $k > \frac{n}{2}$,

$$x(k) \in \mathrm{Span}(\{x(1), x(2), \ldots, x(j)\}) \ \left(j \leqslant \frac{n}{2}\right), \text{ and,}$$

$$y(k) \in \mathrm{Span}(\{y(1), y(2), \ldots, y(j)\}) \ \left(j \leqslant \frac{n}{2}\right).$$

So the eigenvalues are $2-2\cos(\frac{2\pi k}{n})$ with $k \leqslant \frac{n}{2}$.

The list above is exhaustive since we have formed n independent eigenvectors correspondingly to these eigenvalues:
When n is odd, we have one eigenvector $x(0)$ for $\lambda_0 = 0$ ($y(0) = \vec{0}$), and two eigenvectors $x(k)$ and $y(k)$ for all $0 < k < \frac{n}{2}$.
When n is even, we have one eigenvector $x(0)$ for $\lambda_0 = 0$ ($y(0) = \vec{0}$) and two eigenvectors $x(k)$ and $y(k)$ for all $0 < k < \frac{n}{2}$ and one eigenvector $x(\frac{n}{2})$ for $\lambda_{\frac{n}{2}} = 4$ ($y(\frac{n}{2}) = \vec{0}$). □

Proposition 4.10. *The Laplacian of P_n has the same eigenvalues as C_{2n}, and the associated eigenvectors*

$$x_i(k) = \cos\left(\frac{\pi k i}{n} - \frac{\pi k}{2n}\right),$$

for $0 \leqslant k < n$.

Proof. In order to prove the proposition, we will treat P_n as a quotient of C_{2n} by identifying vertex i of P_n with both vertices i and $2n+1-i$ of C_{2n}. Then we find an eigenvector $\vec{v}$ of C_{2n} such that $v_i = v_{2n+1-i}$ for all vertices i of C_{2n}. Then,

$$\vec{x} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

is an eigenvector of P_n. First, I am going to show that $\vec{x}$ is an eigenvector of P_n. Notice that L_{P_n} has the form

$$\begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

So if $\vec{u}$ is an eigenvalue of P_n, then it must satisfy:

$$\begin{aligned} u_1 - u_2 &= \lambda u_1 \\ -u_{n-1} + u_n &= \lambda u_n, \text{and,} \\ -u_{i-1} + 2u_i - u_{i+1} &= \lambda u_i, \text{for all } 1 < i < n. \end{aligned}$$

Following immediately from the previous proof, our $\vec{x}$ satisfies the last condition. We only need to check whether it satisfies the first two conditions. As we notice,

$$\lambda u_1 = -u_{2n} + 2u_1 - u_2 = -u_1 + 2u_1 - u_2 = u_1 - u_2$$

$$\lambda u_n = -u_{n-1} + 2u_n - u_{n+1} = -u_{n-1} + 2u_n - u_n = -u_{n-1} + u_n.$$

So our $\vec{x}$ satisfies all the conditions.

Now, we want to make sure that there exists an eigenvector $\vec{v}$ of C_{2n} satisfying $v_i = v_{2n+1-i}$, so we can get our $\vec{x}$ from it. Fortunately, we only need to let

$$v_i(k) = \cos\left(\frac{\pi k i}{n} - \frac{\pi k}{2n}\right),$$

then

$$\begin{aligned} v_{2n+1-i}(k) &= \cos\left(\frac{\pi k(2n+1-i)}{n} - \frac{\pi k}{2n}\right) \\ &= \cos\left(\frac{\pi k(4n+2-2i-1)}{2n}\right) \\ &= \cos\left(\frac{4\pi kn}{2n} - \frac{\pi k(2i+1)}{2n}\right) \\ &= \cos\left(2\pi k - \frac{2\pi ki + \pi k}{2n}\right) \\ &= \cos\left(\frac{\pi ki}{n} - \frac{\pi k}{2n}\right) \\ &= v_i(k), \end{aligned}$$

which satisfies our definition for $\vec{v}$. Since

$$\begin{aligned} v_i(k) &= \cos\left(\frac{\pi ki}{n} - \frac{\pi k}{2n}\right) \\ &= \cos\left(\frac{\pi k}{2n}\right)\cos\left(\frac{2\pi ki}{2n}\right) + \sin\left(\frac{\pi k}{2n}\right)\sin\left(\frac{2\pi ki}{2n}\right), \end{aligned}$$

we have $\vec{v} \in \mathrm{Span}\left(\{x(k), y(k)\}\right)$, where $x(k)$ and $y(k)$ are the eigenvectors for C_{2n} following from proposition 4.5. The eigenvalues associated are thus $\lambda_k = 2 - 2\cos(\frac{2\pi k}{2n})$ where $1 \leqslant k \leqslant n$. □

5. The Bounding of λ

As noted above, the smallest non-zero eigenvalue of the Laplacian of a graph tells us how connected the graph is. Thus, it is important to find bounds for this value. First, we try to find a lower bound for the largest eigenvalue of the Laplacian of a graph. In order to do this, we introduce the Courant-Fischer Theorem.

Theorem 5.1 (Courant-Fischer)**.** *Let A be an $n \times n$ symmetric matrix and let $1 \leqslant k \leqslant n$. Let $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$ be the eigenvalues of A and $v_1, v_2, \ldots, v_n$ be the corresponding eigenvectors. Then,*

$$\begin{aligned} \lambda_1 &= \min_{x \neq 0} \frac{x^T A x}{x^T x} \\ \lambda_2 &= \min_{x \neq 0 \text{ and } x \perp v_1} \frac{x^T A x}{x^T x} \\ \lambda_n &= \max_{x \neq 0} \frac{x^T A x}{x^T x}. \end{aligned}$$

The proof of this theorem can be found in [5]. With Courant-Fischer Theorem, we can get some easy lower bounds for the largest eigenvalue λ_n of the Laplacian of a graph.

Lemma 5.2. *Let $G = (V, E)$ be a graph with $V = \{1, 2, \ldots, n\}$ and $u \in V$. If u has degree d, then*

$$\lambda_n(G) \geqslant d.$$

Proof. By Courant-Fischer Theorem,

$$\lambda_n(G) = \max_{\vec{x}\neq 0} \frac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}}.$$

Let $\vec{x} = \vec{e_u}$, where $\vec{e_1}, \vec{e_2}, \ldots, \vec{e_n}$ is the standard basis. Recall that

$$\vec{x}^T L_G \vec{x} = \sum_{\{u,v\}\in E} (x_u - x_v)^2.$$

Therefore, we have

$$\begin{aligned} \frac{\vec{e_u}^T L_G \vec{e_u}}{\vec{e_u}^T \vec{e_u}} &= \frac{\sum\limits_{\{u,v\}\in E} (x_u - x_v)^2}{\sum x_u^2} \\ &= \frac{d}{1} \\ &= d \end{aligned}$$

So $\lambda_n(G) \geqslant \dfrac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}} = d.$ □

In fact, we can slightly improve the bound.

Theorem 5.3. *Let $G = (V, E)$ be a graph with $V = \{1, 2, \ldots, n\}$ and $u \in V$. If u has degree d, then*

$$\lambda_n(G) \geqslant d + 1.$$

Proof. It follows the same idea as in the proof for the previous lemma. However, this time we will consider the vector $\vec{x}$ given by

$$x_i = \begin{cases} d & \text{if } i = u, \\ -1 & \text{if } \{i, u\} \in E, \\ 0 & \textit{otherwise}. \end{cases}$$

Then we have

$$\begin{aligned} \frac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}} &= \frac{\sum\limits_{\{u,v\}\in E} (x_u - x_v)^2}{\sum x_u^2} \\ &= \frac{d(d-(-1))^2}{d(-1)^2 + d^2} \\ &= \frac{d(d+1)^2}{d(d+1)} \\ &= d + 1 \end{aligned}$$

So $\lambda_n(G) \geqslant \dfrac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}} = d + 1.$ □

Now we turn our focus onto the bounding of λ_2. By Courant-Fischer Theorem, we can roughly get an upper bound for λ_2 of the path graph P_n.

Proposition 5.4. *Let P_n be the path graph, then $\lambda_2(P_n) = O\left(\dfrac{1}{n^2}\right)$.*

Proof. Consider the vector $\vec{u}$ such that $u_i = (n+1) - 2i$. Then

$$\vec{u} \cdot \vec{1} = \sum_i (n+1) - 2i = 0,$$

where $\vec{1} = (1, 1, \dots, 1)$. As we have shown before, $\vec{1}$ spans the eigenspace for the eigenvalue $\lambda_1 = 0$. Then by Courant-Fischer Theorem, we get

$$\begin{aligned} \lambda_2(P_n) &= \min_{\vec{x} \perp \vec{1}} \frac{\vec{x}^T L_{P_n} \vec{x}}{\vec{x}^T \vec{x}} \\ &\leqslant \frac{\vec{u}^T L_{P_n} \vec{u}}{\vec{u}^T \vec{u}} \end{aligned}$$

Recall that

$$\vec{x}^T L_G \vec{x} = \sum_{\{u,v\} \in E} (x_u - x_v)^2.$$

So

$$\begin{aligned} \frac{\vec{u}^T L_{P_n} \vec{u}}{\vec{u}^T \vec{u}} &= \frac{\sum\limits_{1 \leqslant i < n} (u_i - u_{i+1})^2}{\sum\limits_i (u_i)^2} \\ &< \frac{n2^2}{\sum\limits_{1 \leqslant i < n} (n+1-2i)^2} \end{aligned}$$

The denominator $\sum (n+1-2i)^2$ is of order n^3, therefore we can give a upper-bound of λ_2 by

$$\lambda_2 = O\left(\frac{1}{n^2}\right)$$

□

Now, we try to get a lower bound for λ_2 of P_n.

Definition 5.5. For two symmetric n by n matrices A and B, we write $A \succcurlyeq B$ if $A - B$ is positive semidefinite.

So if $A \succcurlyeq B$, then $\vec{x}^T A \vec{x} \geqslant \vec{x}^T B \vec{x}$ for all $\vec{x}$.

Lemma 5.6. *If G and H are both graphs with n vertices such that*

$$c \cdot L_G \succcurlyeq L_H,$$

then

$$c \cdot \lambda_2(G) \geqslant \lambda_2(H).$$

Proof. By Courant-Fischer Theorem,

$$\begin{aligned} c \cdot \lambda_2(G) &= \min_{\vec{x} \neq 0 \text{ and } \vec{x} \perp \vec{v_1}} \frac{c\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}} \\ &= \min_{\vec{x} \neq 0 \text{ and } \vec{x} \perp \vec{v_1}} \frac{\vec{x}^T (c \cdot L_G) \vec{x}}{\vec{x}^T \vec{x}} \end{aligned}$$

Assume when $\vec{x} = \vec{u}$, $\dfrac{\vec{x}^T(c \cdot L_G)\vec{x}}{\vec{x}^T\vec{x}}$ reaches minimum for $\vec{x} \neq 0$ and $\vec{x} \perp \vec{v_1}$. Since $c \cdot L_G \succcurlyeq L_H$, by definition,

$$\begin{aligned} c \cdot \lambda_2(G) &= \frac{\vec{u}^T(c \cdot L_G)\vec{u}}{\vec{u}^T\vec{u}} \\ &\geqslant \frac{\vec{u}^T(L_H)\vec{u}}{\vec{u}^T\vec{u}} \\ &\geqslant \min_{\vec{x}\neq 0 \text{ and } \vec{x}\perp\vec{v_1}} \frac{\vec{x}^T L_H \vec{x}}{\vec{x}^T\vec{x}} \\ &\geqslant \lambda_2(H). \end{aligned}$$

□

By using this lemma, we will be able to find a lower bound for $\lambda_2(P_n)$ by comparing it with $\lambda_2(K_n)$. Recall our previous definition of $L_{G_{\{u,v\}}}$ in definition 3.1. For convenience, I will denote $L_{G_{\{u,v\}}}$ simply as $L_{\{u,v\}}$ from now on.

Lemma 5.7. *For a graph G, let $c_1, c_2, \ldots, c_{n-1} > 0$. Then*

$$c \cdot \left(\sum_{i=1}^{n-1} c_i L_{\{i,i+1\}}\right) \succcurlyeq L_{\{1,n\}},$$

where

$$c = \sum_{i=1}^{n-1} \frac{1}{c_i}.$$

Proof. First, we should see the statement is equivalent to

$$\sum_{i=1}^{n-1} c_i L_{\{i,i+1\}} \succcurlyeq \frac{1}{\left(\sum_{i=1}^{n-1} \frac{1}{c_i}\right)} L_{\{1,n\}}.$$

We shall prove this equivalent statement by induction. When $n = 2$, it is trivial. Assume the statement is true for $n - 1$, then

$$\begin{aligned} \sum_{i=1}^{n-1} c_i L_{\{i,i+1\}} &= \sum_{i=1}^{n-2} c_i L_{\{i,i+1\}} + c_{n-1} L_{\{n-1,n\}} \\ &\succcurlyeq \frac{1}{\left(\sum_{i=1}^{n-2} \frac{1}{c_i}\right)} L_{\{1,n-1\}} + c_{n-1} L_{\{n-1,n\}}. \end{aligned}$$

Now, we want to show that

$$\frac{1}{\left(\sum_{i=1}^{n-2} \frac{1}{c_i}\right)} L_{\{1,n-1\}} + c_{n-1} L_{\{n-1,n\}} \succcurlyeq \frac{1}{\left(\sum_{i=1}^{n-1} \frac{1}{c_i}\right)} L_{\{1,n\}},$$

which is equivalent to showing that

$$M = \frac{1}{\left(\sum_{i=1}^{n-2} \frac{1}{c_i}\right)} L_{\{1,n-1\}} + c_{n-1} L_{\{n-1,n\}} - \frac{1}{\left(\sum_{i=1}^{n-1} \frac{1}{c_i}\right)} L_{\{1,n\}}$$

is positive semi-definite. As we know,

$$\vec{x}^T M \vec{x} = \frac{1}{\left(\sum\limits_{i=1}^{n-2} \frac{1}{c_i}\right)}(x_1 - x_{n-1})^2 + c_{n-1}(x_{n-1} - x_n)^2 - \frac{1}{\left(\sum\limits_{i=1}^{n-1} \frac{1}{c_i}\right)}(x_1 - x_n)^2.$$

Let $a_1 = \frac{1}{\sum\limits_{i=1}^{n-2} \frac{1}{c_i}}$ and $a_2 = c_{n-1}$ and let $y_1 = x_1 - x_{n-1}$ and $y_2 = x_{n-1} - x_n$, then

$$\begin{aligned}
\vec{x}^T M \vec{x} &= a_1 y_1^2 + a_2 y_2^2 - \frac{1}{a_1^{-1} + a_2^{-1}}(y_1 + y_2)^2 \\
&= \frac{1}{a_1^{-1} + a_2^{-1}}\left[\left(a_1^{-1} + a_2^{-1}\right)\left(a_1 y_1^2 + a_2 y_2^2\right) - (y_1 + y_2)^2\right].
\end{aligned}$$

By Cauchy-Schwartz Inequality, we get

$$\begin{gathered}
\left\| \begin{pmatrix} a_1^{-\frac{1}{2}} \\ a_2^{-\frac{1}{2}} \end{pmatrix} \right\|^2 \left\| \begin{pmatrix} a_1^{\frac{1}{2}} y_1 \\ a_2^{\frac{1}{2}} y_2 \end{pmatrix} \right\|^2 \geqslant \left| \begin{pmatrix} a_1^{-\frac{1}{2}} \\ a_2^{-\frac{1}{2}} \end{pmatrix} \cdot \begin{pmatrix} a_1^{\frac{1}{2}} y_1 \\ a_2^{\frac{1}{2}} y_2 \end{pmatrix} \right|^2 \\
\left(a_1^{-1} + a_2^{-1}\right)\left(a_1 y_1^2 + a_2 y_2^2\right) \geqslant (y_1 + y_2)^2.
\end{gathered}$$

Therefore, $\vec{x}^T M \vec{x} \geqslant 0$. So $M \succcurlyeq 0$. Thus, we have proved the statement for n. By principle of induction, we have proved the statement for all n. $\square$

Proposition 5.8. *For a path graph P_n, $\lambda_2 \geqslant \frac{6}{n^2}$.*

Proof. We will prove this proposition by comparing the path graph P_n to the complete graph K_n using the lemma we have just proved.
Suppose $K_n = (V, E)$ where $V = \{1, 2, \ldots, n\}$. For each edge $\{u, v\} \in E$ with $u < v$, we apply Lemma 5.10, with $c_1, c_2, \ldots, c_{n-1} = 1$. Then

$$(v - u)\sum_{i=u}^{v-1} L_{K_{n\{i,i+1\}}} \succcurlyeq L_{K_{n\{u,v\}}}.$$

Then summing over all pairs of u, v with $u < v$, we get

$$\sum_{1 \leqslant u < v \leqslant n} (v - u)\sum_{i=u}^{v-1} L_{K_{n\{i,i+1\}}} \succcurlyeq \sum_{1 \leqslant u < v \leqslant n} L_{K_{n\{u,v\}}} = L_{K_n}.$$

Notice that

$$\begin{aligned}
\sum_{1\leqslant u<v\leqslant n}(v-u) &= \sum_{i=1}^{n-1} i(n-i) \\
&= n\sum_{i=1}^{n-1} i - \sum_{i=1}^{n-1} i^2 \\
&= n\frac{n(n-1)}{2} - \frac{n(n-1)(2n-1)}{6} \\
&= \frac{n^3}{6} - \frac{n}{6} \\
&\leqslant \frac{n^3}{6}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\left(\frac{n^3}{6}\right) L_{P_n} = \left(\frac{n^3}{6}\right) \sum_{i=1}^{n-1} L_{K_{n\{i,i+1\}}} &\succcurlyeq \sum_{1\leqslant u<v\leqslant n}(v-u)\sum_{i=1}^{n-1} L_{K_{n\{i,i+1\}}} \\
&\succcurlyeq \sum_{1\leqslant u<v\leqslant n}(v-u)\sum_{i=u}^{v-1} L_{K_{n\{i,i+1\}}} \\
&\succcurlyeq L_{K_n}
\end{aligned}$$

So

$$\left(\frac{n^3}{6}\right) L_{P_n} \succcurlyeq L_{K_n}.$$

By Lemma 5.9, we have

$$\left(\frac{n^3}{6}\right) \lambda_2(P_n) \geqslant \lambda_2(K_n).$$

Proposition 4.2 implies that $\lambda_2(K_n) = n$, therefore

$$\left(\frac{n^3}{6}\right) \lambda_2(P_n) \geqslant n,$$

and so,

$$\lambda_2(P_n) \geqslant \frac{6}{n^2}.$$

□

We can readily see that this lower bound has the same order as our previous rough upper bound of $\lambda_2(P_n)$.

6. Further Discussion on Simple Path Counting Problem

In the previous section, we have shown that for a given graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$, the entry $a^k_{i,j}$ of the exponential of the adjacency matrix A^k_G tells us the number of $i - j$ walks of length k. However, from our definition, we can see these $i - j$ walks consist of repeating edges. It would be interesting to count the number of $i - j$ walks with no repeated vertices, which we will call simple paths.

Definition 6.1. Let $G = (V, E)$ be a graph and suppose $i, j \in V$. A *simple path* between $i - j$ in G is a subgraph which is a path connecting i and j. The length of the simple path is just the length of the subgraph path.

We can easily see that in a graph G all the $i-j$ walks of length 2 where $i \neq j$ are simple paths between $i-j$ of length 2. Thus the entries $a_{i,j}^2$ of A_G^2 where $i \neq j$ give us the correct number. Since any closed walk ($i-i$ walk for any $i \in V$) is not counted as a simple path, the number of simple path between i and i is always 0. Therefore, the matrix counting the number of simple paths of length 2 is

$$S_G^{(2)} = A_G^2 - D_G$$

where D_G is the degree matrix defined by

$$d_{i,j} = \begin{cases} d(i) & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

where $d(i)$ denotes the degree of vertex i.

Now we consider simple paths of length 3. A simple path of length 3 between i and j consists of a simple path of length 2 between i and a point u where $\{u, j\} \in E$. Thus, we would expect that

$$s_{i,j}^{(3)} = \sum_{p=1}^{n} s_{i,p}^{(2)} a_{p,j}$$

where $s_{i,p}^{(2)}$ is the number of simple path of length 2 between i, p and $a_{p,j}$ is the entry of adjacency matrix A_G. However, we should notice that if j is adjacent to i, then the formula above will include the number of $i-j$ walks which contain a closed walk at j . That is they are walks of the form $i-j-p-j$. Therefore, we have to subtract the number of such walks. We can easily see this number is given by $a_{i,j}(d(j)-1)$. So in fact

$$s_{i,j}^{(3)} = \sum_{p=1}^{n} s_{i,p}^{(2)} a_{p,j} - a_{i,j}(d(j)-1).$$

where $i \neq j$ and,

$$s_{i,i}^{(3)} = 0.$$

Therefore, we could see that

$$S_G^{(3)} = S_G^{(2)} A_G - A_G(D_G - I) - \mathrm{Diag}(S_G^{(2)} A_G)$$

where Diag denotes the matrix given by

$$\mathrm{Diag}(M)_{i,j} = \begin{cases} 0 & \text{if } i \neq j, \\ m_{i,j} & \text{if } i = j. \end{cases}$$

We can easily see this simply means that $S_G^{(3)}$ is obtained by changing the diagonals of $S_G^{(2)} A_G - A_G(D_G - I)$ to all 0s.

So far, I have only computed $S_G^{(k)}$ for up to 3 as the case for $k > 3$ is too complicated to compute. The problem may require different methods or tools to tackle in the future. However, we can reach a rough upper bound for the number of simple paths of length k. Consider the graph $G = (V, E)$ where $V = \{1, 2, \ldots, n\}$. It is obvious that the number m_G of simple paths of length k ($k \leqslant n$) contained in G is less than the number m_{K_n} of simple paths of length k contained in the complete graph K_n. We can easily compute m_{K_n},

$$\begin{aligned} m_{K_n} &= \frac{1}{2} n \cdot (n-1) \cdots (n-k+1) \\ &= \frac{P_{n,k}}{2}, \end{aligned}$$

where $P_{n,k}$ denotes $k-$ *permutations* of n. So,

$$m_G \leqslant m_{K_n} = \frac{P_{n,k}}{2}.$$

There still remains the possibility to get even finer bounds for certain families of graphs.

7. Acknowledgment

It is a pleasure to thank my mentor, Robin Walters, for introducing me to the topic of spectral graph theory and for his help throughout the paper writing process. I would not possibly have finished this paper without his advice and insights on the topic.

References

[1] Paul R. Halmos. Finite-Dimensional Vector Spaces. Springer-Verlag New York, Inc.1974.
[2] Sheldon Axler. Linear Algebra Done Right, Second Edition. Springer-Verlag New York, Inc.1997.
[3] Reinhard Diestel. Graph Theory. Springer-Verlag New York, Inc.2000.
[4] Dan Spielman. Spectral Graph Theory and its Applications. Online lecture notes. http://www.cs.yale.edu/homes/spielman/eigs/, 19 July 2012.
[5] Andre Wibisono (Scribe), Jonathan Kelner (Lecturer). Online lecture notes for course "18.409 Algorithmist's Toolkit". http://ocw.mit.edu/courses/mathematics/18-409-topics-in-theoretical-computer-science-an-algorithmists-toolkit-fall-2009/lecture-notes, 30 July 2012.