國立交通大學

應用數學系

碩士論文

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研究生：施政成　　Student：Jeng-cheng Shih

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中文摘要

對一 $n \times n$ 方陣 M 而言，其「值距」$\varphi(M)$ 通常定義為 M 的最大與最小特徵值的差距，也就是

$$\varphi(M) := \max_{i,j} |\rho_i - \rho_j| 。$$

上式的最大值是對任兩個 M 的特徵值差考慮，不過有時特徵值 0 被排除。我們考慮圖論上被廣泛使用的三種方陣：鄰接方陣、拉普拉斯方陣、正拉普拉斯方陣。我們探討圖與此三種值距的關係，特別研究點數固定時，能得到最大或最小值距的圖。

Spectral Spread of Graphs

Student: Jeng-cheng Shih　　　　Advisor: Chih-wen Weng

Department of Applied Mathematics

National Chiao Tung University

Abstract

Given an $n \times n$ matrix M, the spread, $\varphi(M)$, is essentially the diameter of its spectrum:

$$\varphi(M) := \max_{i,j} |\rho_i - \rho_j|,$$

where the maximal is taken over all pairs of eigenvalues (or nonzero eigenvalues in some cases) of M. We consider adjacent matrices, Laplacian and signless Laplacian matrices which are commonly used in graph theory. After discussing relatedness on the graphs and their corresponding spreads, we discover the boundary which affects the spread, and use this result to find the graphs that may have the maximal or minimal spread.

Contents

1

Introduction

The spread of a graph is the difference between the largest eigenvalue and the least eigenvalue of its adjacency matrix. In order to let someone read these kinds of articles more conveniently, the purpose of the thesis as to conform some interested papers to get the target. We review the history in the beginning. In [1], Petrović determined all minimal graphs whose spreads do not exceed 4. In [2] and [3], some lower and upper bounds for the spread of a graph were given. Particularly, they give the maximal and minimal spreads among the graphs. After then, the Laplacian spread of the graph is considered as the difference between the largest and the second smallest eigenvalues of Laplacian matrix, as the smallest one always equals zero. In [11], the authors showed that among all trees of fixed order, the star is the unique one with maximal Laplacian spread and the path is the unique one with the minimal. And in [12], [16] the unique unicyclic graph with maximal Laplacian spread is obtained from a star by adding an edge between two pendant vertices and the cycle is the unique one with the minimal. In [17], there exist exactly two bicyclic graphs with maximal Laplacian spread among all bicyclic graphs of fixed order, which are obtained from a star by adding two incident edges and by adding two non-incident edges between the pendent vertices of the star, respectively. In [18], there are only five types of tricyclic graphs with maximal Laplacian spread among all tricyclic graphs of fixed order. In [12], [16] and [17], they do not show the detail for searching the characteristic polynomial, and we give two different methods in such Proposition 5.1.2 and Lemma 6.1.1. After this we give an conjecture of a connected graph with fixed order whose have the maximal Laplacian spread. Finally, the signless Laplacian matrices has become more popular recently. In [20], some upper and lower bounds for the signless Laplacian spreads have considered, and then determine the unique unicyclic graph with maximal signless Laplacian spread among the class of connected unicyclic graphs of fixed order. And they give the remarks for some open problems, and the conjecture for the maximal signless Laplacian spread.

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Preliminaries

We shall recall three theorems in the matrix theory with their proof in this chapter, the Perron-Frobenius theorems, the eigenvalue interlacing theorem and the Geršgorin's Theorem. First we give some notations.

Definition 2.0.1. (i) For two matrices M, N of the same sizes, we write $M \leq N$ if $M_{ij} \leq N_{ij}$ for all i, j ; write $M < N$ if $M_{ij} < N_{ij}$; write $M \lneqq N$ if $M \leq N$ and $M \neq N$ for all i, j.

(ii) $|M|$ is the matrix with entries $|M_{ij}|$.

(iii) An $n \times n$ matrix M is associated with a digraph Γ_M with vertex set $V\Gamma = \{1, 2, \ldots, n\}$ and arcs (i, j) whenever $M_{ij} \neq 0$.

(iv) A digraph Γ is *strong connected* if for any two vertices x, y there exists a walk in Γ from x to y.

(v) A nonnegative matrix M is *irreducible* if Γ_M is strong connected.

(vi) For an $n \times n$ matrix M, the number that takes the maximal $|\lambda|$ among all eigenvalues $\lambda \in \mathbb{C}$ is called the *spectral radius* of M.

2.1 Perron-Frobenius theorems

We introduce Perron-Frobenius theorems and their proof in this section. First we give an observation.

Remark 2.1.1. (i) If M is an $n \times n$ nonnegative irreducible matrix then $(I + M)^{n-1} > 0$.

(ii) $x \lneqq y \Rightarrow (I + M)^{n-1}x < (I + M)^{n-1}y$ for $x, y \in \mathbb{R}^n$.

Definition 2.1.2. Let $B := \{x \in \mathbb{R}^n | x \geq 0, x \neq 0\}$. For $x \in B$, define

$$\lambda(x) := \min\{\frac{(Mx)_i}{x_i} | 1 \leq i \leq n, x_i \neq 0\},$$

and note that

$$\lambda(x) = \sup\{\eta \in \mathbb{R} | \eta x \leq Mx\}.$$

The following lemma is crucial in the proof of Perron-Frobenius theorem.

Lemma 2.1.3. *$\lambda((I + M)^{n-1}x) > \lambda(x)$ for $x \in B$ with $\lambda(x)x \lneqq Mx$.*

Proof. Since

$$\lambda(x)[(I + M)^{n-1}x] = (I + M)^{n-1}\lambda(x)x < (I + M)^{n-1}Mx = M[(I + M)^{n-1}x],$$

we have $\lambda((I + M)^{n-1}x) > \lambda(x)$. □

The following theorem is the main part of Perron-Frobenius theorems.

Theorem 2.1.4. *Let M be an $n \times n$ nonnegative irreducible matrix and define $\lambda_1 := \sup_{x \in B} \lambda(x) \in \mathbb{R} \cup \infty$. Then $\lambda_1 = \lambda(x_0)$ for some $x_0 > 0$. Moreover λ_1 is an eigenvalue and x_0 is its associated eigenvector.*

Proof. Let $C = \{x \in B | x_1 + x_2 + \ldots + x_n = 1\}$, and note that $\sup_{x \in B} \lambda(x) = \sup_{x \in C} \lambda(x)$. Despite C is compact, λ is not necessary to be continuous on C. Set $D = (I + M)^{n-1}C$ and note that λ is continuous on D. Now

$$\sup_{x \in C} \lambda(x) = \sup_{x \in B} \lambda(x) \geq \sup_{x \in D} \lambda(x) = \lambda(x_0) \geq \sup_{x \in C} \lambda(x)$$

for some $x_0 \in D$ as $D \subseteq B$ and D is compact. Hence $\lambda(x_0) \geq 0$ is an eigenvalue of M with eigenvector $x_0 > 0$. □

The above x_0 is indeed unique by the following theorem. We refer x_0 as the *Perron-Frobenius vector* of M.

Theorem 2.1.5. *As the notation in Theorem 2.1.4, the eigenvalue $\lambda_1 = \sup_{x \in B} \lambda(x)$ is the spectral radius of M. Moveover the geometric multiplicity of λ_1 is 1, i.e. the eigenspace of λ_1 has dimension 1.*

Proof. Let $\lambda \in \mathbb{C}$ be another eigenvalue with eigenvector $x \in \mathbb{C}^n$. That is $Mx = \lambda x$. Then $|\lambda||x| = |\lambda x| = |Mx| \leq M|x|$. Hence $|\lambda| \leq \lambda(|x|)$. This not only implies $|\lambda| \leq \lambda_1$ but also implies that if $\lambda = \lambda_1$ then $|x|$ is also an eigenvector of λ_1. Since $M|x| = \lambda_1|x| \neq 0$, if $|x|_i = 0$ then $\sum_{k=1}^n M_{ik}|x|_k = 0$, equivalently $|x|_k = 0$ for $M_{ik} > 0$. By strong connectivity of Γ_M, $|x|_i \neq 0$ for all i. If λ_1 has two independent eigenvectors, it is always possible to have a linear combination of them to have some zero position. Hence $x = cx_0$ for some $c \in \mathbb{C}$. □

The following Theorem shows that the largest eigenvalue λ_1 of M is characterized by its eigenvector.

Theorem 2.1.6. *Let M be an $n \times n$ nonnegative irreducible matrix with $\lambda_1 = \sup_{x \in B} \lambda(x)$. Suppose that $\lambda \in \mathbb{C}$ is an eigenvalue of M whose associated eigenvector $x \in B$. Then $\lambda = \lambda_1$.*

Proof. Applying the above proof to left eigenvector, we have $y_0^T M = \lambda_1 y_0^T$ for maximal eigenvalue λ_1 with eigenvector $y_0 > 0$. Since $\lambda_1 y_0^T x = y_0^T M x = y_0^T \lambda x$ and $y_0^T x > 0$, we have $\lambda = \lambda_1$. □

The following two theorems are useful in the sequel.

Theorem 2.1.7. *Let M be an $n \times n$ irreducible nonnegative matrix, then*

1. *If $0 \neq x \geq 0$ and $Mx \geq px$, for some $p > 0$, then $p \leq \lambda_1(M)$, and equality holds if and only if $x > 0$ is an eigenvector of λ_1.*

2. *If* $0 \neq x \geq 0$ *and* $Mx \leq px$*, for some* $p > 0$*, then* $p \geq \lambda_1(M)$*, and equality holds if and only if* $x > 0$ *is an eigenvector of* λ_1*.*

Proof. As before, let λ_1 be the maximal eigenvalue with left eigenvector $y_0 > 0$. Suppose that $Mx \leq px$ for some $p > 0$ and $0 \neq x \geq 0$. Then $\lambda_1 y_0^T x = y_0^T Mx \leq y_0^T px$. Since $y_0^T x > 0$, we have $p \leq \lambda_1$. Note that $p = \lambda_1$ iff $Mx = px$. The other statement is similar. □

Theorem 2.1.8. *Let* M *be an* $n \times n$ *irreducible nonnegative matrix with spectral radius* λ_1*. Let* S *be a complex matrix with* $|S| \leq M$ *and* λ *be an eigenvalues of* S*. Then* $|\lambda| \leq \lambda_1$*, and equality holds iff* $|S| = M$ *and there are a diagonal matrix* E *with diagonal entries of absolute value* 1 *and a constant* c *of absolute value* 1*, such that* $S = cEME^{-1}$*.*

Proof. Suppose $s \neq 0$ and $Ss = \lambda s$. Then

$$M|s| \geq |S||s| \geq |Ss| = |\lambda s| = |\lambda||s|. \tag{2.1.1}$$

By theorem 2.1.7, $\lambda_1 \geq |\lambda|$, and equality holds iff $|s| > 0$ is an eigenvector of M. In this case, both of the equalities in (2.1.1) hold. The first equality implies $M_{ij}s_j = |S_{ij}s_j|$. The second equality implies for each i, $S_{ij}s_j$ is in the same direction e_i of the complex plane, where $|e_i| = 1$, i.e. $S_{ij}s_j = e_i|S_{ij}s_j|$ for all j. By setting $E_{ii} = e_i$ and $c = |s_j|e_j/s_j$, we have $S_{ij} = e_i M_{ij} e_j |s_j|/(s_j e_j) = cE_{ii}M_{ij}E_{jj}^{-1}$. □

2.2 The eigenvalue interlacing theorem

We consider the interlacing property between a matrix and its submatrix or quotient matrix. For $m < n$, the sequence $\eta_1 \geq \eta_2 \geq \dots \eta_m$ is said to *interlace* the sequence $\lambda_1 \geq \lambda_2 \geq \dots \lambda_n$, if $\lambda_i \geq \eta_i \geq \lambda_{n-m+i}$, for $1 \leq i \leq m$.

Lemma 2.2.1. *(Rayleigh's principle) Let* M *be a real symmetric matrix of order* n *with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ *and respectively orthonormal eigenvectors* $u_1, u_2, \dots, u_n$*. Then*

1. $\frac{u^TMu}{u^Tu} \geq \lambda_i$, *for any* $u \in \langle u_1, u_2, \ldots, u_i \rangle$, *and equality holds if and only if* u *is a* λ_i*-eigenvector.*

2. $\frac{u^TMu}{u^Tu} \leq \lambda_{i+1}$, *for any* $u \in \langle u_1, u_2, \ldots, u_i \rangle^{\perp}$, *and equality holds if and only if* u *is a* λ_{i+1}*-eigenvector.*

Proof. Let $u = c_1u_1 + \ldots c_iu_i$ for some c_i is real. Then

$$\frac{u^TMu}{u^Tu} = \frac{c_1^2\lambda_1 + \ldots + c_i^2\lambda_i}{c_1^2 + \ldots + c_i^2} \geq \lambda_i.$$

And the second is similarly true. □

Lemma 2.2.2. *Let* S *be real* $n \times m$ *matrix such that* $S^TS = I$, *where* $m < n$. *And* M *be a real symmetric matrix of order* n *with eigenvalues* $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, *and respectively orthonormal eigenvectors* $u_1, u_2, \ldots, u_n$. *Define* $N = S^TMS$ *and let* N *has eigenvalues* $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_m$ *and respectively orthonormal eigenvectors* $v_1, v_2, \ldots, v_m$. *Then the eigenvalues of* N *interlace those of* M.

Proof. For all $1 \leq i \leq m$, chose a nonzero vector

$$s_i \in \langle v_1, v_2, \ldots, v_i \rangle \cap \langle S^Tu_1, S^Tu_2, \ldots, S^Tu_{i-1} \rangle^{\perp}.$$

Note that $(Ss_i)^Tu_j = 0$, for $1 \leq j \leq i-1$, hence $Ss_i \in \langle u_1, u_2, \ldots, u_{i-1} \rangle^{\perp}$ and by Rayleigh's principle,

$$\lambda_i \geq \frac{(Ss_i)^TM(Ss_i)}{(Ss_i)^T(Ss_i)} = \frac{s_i^TNs_i}{s_i^Ts_i} \geq \eta_i.$$

And similarly by applying the above inequality to $-M$ and $-N$, we get $\lambda_{n-m+i} \leq \eta_i$. □

Given an $n \times n$ matrix M and an ordered partition $(X_1, \ldots, X_m)$ of the ordered set $\{1, 2, \ldots, n\}$, M can be presented as a matrix in block form:

$$M = \begin{pmatrix} M_{1,1} & \cdots & M_{1,m} \\ \vdots & \ddots & \vdots \\ M_{m,1} & \cdots & M_{m,m} \end{pmatrix}$$

where $M_{i,j}$ has X_i as the set of its row numbers and X_j as the set of its column numbers. We always use Q_M hereafter to denote the *quotient matrix* of the partition matrix M, which is defined to be the $m \times m$ matrix whose entries are the average row sums of the blocks $M_{i,j}$; that is, the (i, j)-entry of the matrix Q_M is obtained by dividing the sum of all row sums of $M_{i,j}$ by $|X_i| = n_i$, where $1 \leq i, j \leq m$. Let

$$D = \begin{pmatrix} n_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & n_m \end{pmatrix}$$

and

$$S = \begin{pmatrix} e_{n_1}/\sqrt{n_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e_{n_m}/\sqrt{n_m} \end{pmatrix}$$

is an $n \times m$ matrix, where e_{n_i} is the all one vector with n_i entries, for $1 \leq i \leq m$. Then it is easy to check that $Q_M = DS^TMSD^{-1}$.

Lemma 2.2.3. *Suppose that Q_M is a quotient matrix of a symmetric matrix M. Then the eigenvalues of Q_M interlace the eigenvalues of M.*

Proof. Note that $S^TS = I$. By Lemma 2.2.2, the eigenvalues of Q_M interlace the eigenvalues of M. □

2.3 Geršgorin's Theorem

The following theorem is called Geršgorin's Theorem.

Theorem 2.3.1. *Any eigenvalue λ of a matrix A is located in one of the closed discs of the complex plane centered at a_{ii} and having the radius:*

$$\rho_i = \sum_{j=1, j\neq i}^{j=n} |a_{ij}|.$$

In other words, for all $\lambda \in \sigma(A)$, for some i such that

$$|\lambda - a_{ii}| \leq \sum_{j=1, j\neq i}^{j=n} |a_{ij}|,$$

where $\sigma(A)$ is the spectra of A.

Proof. Let x be an eigenvector associated with an eigenvalue λ and let m be the index of the component of largest modulus in x. Scale x so that $|\xi_m| = 1$ and $|\xi_i| \leq 1$ for $i \neq m$. Since x is an eigenvector, then

$$(\lambda - a_{mm})\xi_m = \sum_{j=1, j\neq i}^{j=n} a_{ij}\xi_j,$$

which gives

$$|\lambda - a_{mm}| \leq \sum_{j=1, j\neq m}^{j=n} |a_{mj}||xi_j| \leq \sum_{j=1, j\neq m}^{j=n} |a_{mj}| = \rho_m.$$

This completes the proof. □

3

The adjacency spread of a graph

For an $n \times n$ matrix M, the spread, $\varphi(M)$, of M is defined as the diameter of its spectrum: $\varphi(M) := \max_{i,j} |\lambda_i - \lambda_j|$, where the maximal is taken over all pairs of eigenvalues of M. Suppose M is Hermitian. In that case, the eigenvalues $\lambda_i = \lambda_i(M)$ of M are real and may always be assumed to be in non-increasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Then $\varphi(M) = \lambda_1 - \lambda_n$, the distance between the extreme eigenvalues λ_1, λ_n. Also, for unit vectors x, y

$$\lambda_1 \geq x^* M x \quad and \quad \lambda_n \leq y^* M y, \tag{3.0.1}$$

with equality if and only if x is a unit eigenvector associated with λ_1 and y a unit eigenvector associated with λ_n, respectively. Thus,

$$\varphi(M) = \max_{x,y}(x^* M x - y^* M y) = \max_{x,y} \sum_{i,j} m_{i,j}(\bar{x}_i x_j - \bar{y}_i\, y_j), \tag{3.0.2}$$

where the maximal is taken over all pairs of unit vectors. If $M \neq O$, the maximal is attained by orthonormal eigenvectors of M corresponding to the eigenvalues λ_1, λ_n, respectively.

The spread, $\varphi_A(G)$, of a graph G will be that of its adjacency matrix $A = A(G)$, where $a_{i,j} = 1$ if i, j are adjacent in G and $a_{i,j} = 0$ otherwise. In (3.0.1), taking x to be a unit vector with equal entries gives the lower bound $\lambda_1 \geq 2e/n$ with equality if and only if G is regular. And we have

$$0 = tr(A) = \sum_i \lambda_i \quad and \quad 2e = \sum_{i,j} a_{i,j}a_{j,i} = tr(A^2) = \sum_i {\lambda_i}^2. \tag{3.0.3}$$

Example 3.0.2. (i) The complete graph K_n of order n has spectrum: $n-1, \overbrace{-1, \ldots, -1}^{n-1}$. Hence

$$\varphi_A(K_n) = (n-1) - (-1) = n.$$

(ii) The complete bipartite graph $K_{a,b}$ with a vertices in one part and b in the other has spectrum: $\sqrt{ab}, \overbrace{0, \ldots, 0}^{a+b-2}, -\sqrt{ab}$. Hence

$$\varphi_A(K_{a,b}) = \sqrt{ab} - (-\sqrt{ab}) = 2\sqrt{ab}.$$

(iii) The cycle C_n and the path P_n has spectrums:

$$2\cos\frac{2\pi i}{n}, 1 \leq i \leq n, \quad 2\cos\frac{\pi i}{n+1}, 1 \leq i \leq n$$

respectively. Hence both of them have spread does not exceed 4. The graphs G with $\varphi_A(G) \leq 4$ has all been classified by *Petroviċ* [1].

3.1 The upper bound

When G is a graph of order n, let n_0 be the number of non-isolated vertices of G and let G_0 denote the subgraph of order n_0 obtained by deleting the isolated vertices of G.

Theorem 3.1.1. *[2]*

For a graph G with n vertices and e edges,

$$\varphi_A(G) \leq \lambda_1 + \sqrt{2e - {\lambda_1}^2} \leq 2\sqrt{e}. \tag{3.1.1}$$

Equality holds throughout if and only if equality holds in the first inequality ; equivalently, if and only if $e = 0$ or $G_0 = K_{a,b}$ for some a, b with $e = ab$ and $a + b \leq n$.

Proof. From (3.0.3), ${\lambda_1}^2 + {\lambda_n}^2 \leq 2e$, so $\varphi_A(G) = \lambda_1 - \lambda_n \leq \lambda_1 + \sqrt{2e - {\lambda_1}^2}$. Equality holds if and only if $\lambda_2 = \lambda_3 = \ldots = \lambda_{n-1} = 0$, that is, if and only if $A = O$ or rank(A)= 2; equivalently, if and only if the non-isolated vertices of G have at most two distinct neighbor sets. Thus, equality holds if and only if $e = 0$ or $G_0 = K_{a,b}$ for some a, b where, necessarily, $a + b = n_0 \leq n$ and $e = ab$. If the latter case holds, then, by (3.0.3), $\lambda_1 = -\lambda_n = \sqrt{ab}$ and so equality holds in the second inequality in (3.1.1). The second inequality in (3.1.1) holds because $\lambda_1 + \sqrt{2e - {\lambda_1}^2}$ is a strictly increasing function of λ_1 when $\lambda_1 \leq \sqrt{e}$; it is strictly decreasing when $\lambda_1 \geq \sqrt{e}$. □

Remark 3.1.2. When $e > \lfloor n^2/4 \rfloor$, the bound(s) in Theorem 3.1.1 cannot be attained since a bipartite graph with n vertices has at most $\lfloor n^2/4 \rfloor$ edges. However, if $e > \lfloor n^2/4 \rfloor$, then $\lambda_1 \geq 2e/n > \sqrt{e}$ and so the bound $\varphi_A(G) \leq 2\sqrt{e}$ in Theorem 3.1.1 can be improved to

$$\varphi_A(G) \leq \frac{2e}{n} + \sqrt{2e - (\frac{2e}{n})^2}, \tag{3.1.2}$$

when $e > \lfloor n^2/4 \rfloor$. Unfortunately, when $e > \lfloor n^2/4 \rfloor$, this bound cannot be attained either; for if it could, then $\lambda_1 = 2e/n$, equality would hold in 3.1.1 and so, by Theorem 3.1.1, G would be bipartite.

A *complete p-partite graph* is a simple graph, whose vertex set can be partitioned into p subsets (the vertex parts) so that vertices are adjacent, if and only if they belong to different parts. Vertex parts are usually allowed to be empty. Here a complete p-partite graph is assumed to have precisely p non-empty parts.

Theorem 3.1.3. *[2] Let G be a graph with n vertices, e edges, and precisely k negative eigenvalues, $1 \leq k \leq n$. Then*

$$\varphi_A(G) \leq \frac{k+1}{k}\lambda_1 + \sqrt{2e\frac{k-1}{k} - \frac{k^2-1}{k^2}\lambda_1^2}. \tag{3.1.3}$$

Equality holds if and only if G has at most three distinct non-zero eigenvalues: $\lambda_1, \beta, \lambda_n$, where $\lambda_1 > 0 > \beta \geq \lambda_n$ and β has multiplicity $k-1$ if $\beta > \lambda_n$ and multiplicity k if $\beta = \lambda_n$. Equivalently, equality holds if and only if G_0 is a complete

$(k+1)$-partite graph and, when $k+1 \geq 4$, the k smallest parts of G_0 all have equal size (necessarily, $-\beta = (\lambda_1 + \lambda_n)/(k-1)$.)

Proof. Since the deletion of isolated vertices does not affect any of the parameters in (3.1.3), we may assume that $G = G_0$. When $k = 1$, (3.1.3) becomes the well-known inequality $\lambda_1 \geq -\lambda_n$. If $k = 1$, then by the trace equation (3.0.3), $\lambda_1 = -\lambda_n$ if and only if $\text{rank}(G) = 2$, that is, if and only if G has precisely two different neighbor sets. Thus, when $k = 1$, equality holds in (3.1.3) if and only if G is complete bipartite.

Suppose now that $G = G_0$ has precisely k negative eigenvalues, $k \geq 2$. Let $\lambda_1, \alpha_1, \ldots, \alpha_{p-1}$ be the positive eigenvalues of G and let $\lambda_n, \beta_1, \ldots, \beta_{k-1}$ be the negative eigenvalues. By (3.0.3),

$$2e - \lambda_1^2 - \lambda_n^2 \geq \sum \beta_i^2 \geq \frac{(\sum \beta_i)^2}{k-1} = \frac{(\lambda_1 + \lambda_n + \sum \alpha_i)^2}{k-1} \geq \frac{(\lambda_1 + \lambda_n)^2}{k-1}. \qquad (3.1.4)$$

The second inequality follows from the Cauchy-Schwarz inequality and so equality holds there if and only if the β_i are all equal. Equality holds in the last inequality if and only if G has precisely one positive eigenvalue. By (3.1.4),

$$k\lambda_n^2 + 2\lambda_1\lambda_n + k\lambda_1^2 - 2e(k-1) \leq 0. \qquad (3.1.5)$$

The quadratic in λ_n has one positive and one negative root, and it follows that

$$-\lambda_n \leq \frac{1}{k}\lambda_1 + \sqrt{\frac{2e(k-1)}{k} - \frac{k^2-1}{k^2}\lambda_1^2}. \qquad (3.1.6)$$

Since $\varphi_A(G) = \lambda_1 - \lambda_n$, (3.1.3) follows and equality holds if and only if it holds throughout (3.1.4) to (3.1.6); that is, if and only if G has $k+1$ non-zero eigenvalues: $\lambda_1, \beta_1, \ldots, \beta_{k-1}, \lambda_n$, with $\beta_1 = \ldots = \beta_{k-1} = \beta$, where $\beta = -(\lambda_1 + \lambda_n)/(k-1)$, since the eigenvalues sum to zero.

Suppose now that $G = G_0$ is a graph with k negative eigenvalues and that equality holds in (3.1.3). Then the eigenvalues satisfy the conditions required. In particular, G has only one positive eigenvalue, and so must be complete multipartite [3, p. 163]. It's straightforward to check that the number of distinct rows of the adjacency matrix of a complete multipartite graph is equal to the number of parts, and that the distinct rows are linearly independent. Thus, G must be complete multipartite with $\text{rank}(G) = k + 1$ parts. Suppose that G has m_i parts of size n_i, $i = 1, \ldots, t$, where $n_1 < n_2 < \ldots < n_t$. Then $\sum m_i = k + 1$, the total number of parts, and $\sum n_i m_i = n$, the total number of vertices. By [3, p. 74] we have the characteristic polynomial of (the adjacency matrix of) G is

$$\lambda^{n-k-1}(1 - \sum_{i=1}^{t} \frac{n_i m_i}{\lambda + n_i}) \prod_{i=1}^{t} (\lambda + n_i)^{m_i}. \tag{3.1.7}$$

It follows that G has a negative eigenvalue in each of the $t - 1$ open intervals $(-n_{i+1}, -n_i)$, $i = 1, \ldots, t - 1$ and that $-n_i$ is a negative eigenvalue of multiplicity $m_i - 1$ whenever $m_i > 1$. The only remaining eigenvalue, λ_1, is the unique positive zero of the middle factor of the characteristic polynomial (3.1.7). Thus, if s is the number of part sizes of G that occur more than once, then $s + t \leq 3$.

If $k = 2$, then G must be complete tripartite. Also, every such graph G has $\text{rank}(G) = 3$ non-zero eigenvalues, $\lambda_1 > \beta \geq \lambda_n$, when $\beta = -(\lambda_1 + \lambda_n)$. Thus, when $k = 2$, equality holds in (3.1.3) for all complete tripartite graphs.

If $k \geq 3$, then G must be complete $(k + 1)$-partite with four or more parts. Since $s + t \geq 3$, G cannot have two different part sizes each occurring more than once. Thus either all the part sizes of G must be equal or some part size occurs exactly k times. In the latter case, the part sizes are $n_1 < n_2$ and we must have $-n_2 < \lambda_n < -n_1 = \beta$, so it is the smaller part size that occurs k times. Thus if equality holds in (3.1.3) and $k \geq 3$, then the k smallest parts of G must all have equal size $n_1 = -\beta = (\lambda_1 + \lambda_n)/(k - 1)$.

Conversely, if G is a complete $(k + 1)$-partite graph and if the k smallest parts of G all have equal size when $k + 1 \geq 4$, then by (3.1.7), G has at most three distinct non-zero eigenvalues: $\lambda_1, \beta, \lambda_n$, where $\lambda_1 > 0 > \beta \geq \lambda_n$ and β has multiplicity $k - 1$ if $\beta > \lambda_n$ and multiplicity k if $\beta = \lambda_n$. □

3.2 The maximal spread $\varphi_A(n)$

We shall show that $\varphi_A(H)$ is a lower bound of $\varphi_A(G)$ for any induced subgraph H of G.

Corollary 3.2.1. *If H is a subgraph of G, then $\lambda_1(H) \leq \lambda_1(G)$ with strict inequality if G is connected and H is a proper subgraph of G.*

Proof. Apply $0 < A(H) \leq A(G)$ Theorem 2.1.8. □

If we take $S = [I\ O]^T$ in Lemma 2.2.2, then $N = A(H)$ is just a principle submatrix of $M = A(G)$. Then we have the following corollary.

Corollary 3.2.2. *If G is a graph with an induced subgraph H, then the eigenvalues of H interlace the eigenvalues of G.*

Lemma 3.2.3. *If H is an induced subgraph of G, then $\lambda_n(G) \leq \lambda_t(H)$, where $t = |H|$. Thus $\varphi_A(G) \geq \varphi_A(H)$ with strict inequality if G is connected and H is a proper induced subgraph of G.*

Proof. If U is a proper subset of the vertex set of G, then the adjacency matrix of $H = G\backslash U$ is a principal submatrix of the adjacency matrix of G. Thus, by eigenvalues interlacing, $\lambda_n(G) \leq \lambda_t(G\backslash U)$. Also, by Corollary 3.2.1, $\lambda_1(G) \geq \lambda_1(G\backslash U)$ with strict inequality if G is connected and U is proper and non-empty. Thus, $\varphi_A(G) \geq \varphi_A(H)$ with strict inequality if H is a proper induced subgraph of G and G is connected. □

The *join* of two vertex disjoint graphs G_1, G_2 is the graph G_1, G_2 obtained from their union by including all edges between the vertices in G_1 and the vertices in G_2. There are graphs G with $\varphi_A(G) > n$. For integer $1 \leq k \leq n-1$, let $G(n,k) = K_k \vee \overline{K}_{n-k}$, the join of K_k, the complete graph of order k, with the $n-k$ independent vertices of $\overline{K}_{n-k}$, the complement of K_{n-k}. The characteristic polynomial of $G(n,k)$ is $\lambda^{n-k-1}(\lambda+1)^{k-1}[\lambda^2 - (k-1)\lambda - k(n-k)]$ [3, p. 57]. It follows that

$$\varphi_A(G(n,k)) = ((k-1)^2 + 4k(n-k))^{\frac{1}{2}}.$$

It is straightforward to check that $\varphi_A(G(n,k)) > n$ when $(n+1)/3 < k < n-1$ and that $\varphi_A(G(n,k))$ is maximal when $k = \lfloor 2n/3 \rfloor$. If $G = K_n$ and $H = G(n, \lfloor 2n/3 \rfloor)$, then $\varphi_A(H) > n = \varphi_A(G)$ when $n \geq 4$, and so the monotonicity property may fail for graph spread. The inequality $\varphi_A(H) \leq \varphi_A(G)$ does hold for some classes of graph H of G.

Let $\varphi_A(n)$ be the maximal possible spread for all graphs on n vertices. The following conjecture has been checked by [2] for the graph of order $n \leq 9$ and is supported by some observation. If H is a graph on $n-1$ vertices and G is any connected graph on n vertices having H as an induced subgraph, then $\varphi_A(G) > \varphi_A(H)$ by Lemma 3.2.3 Therefore, $\varphi_A(n)$ is strictly increasing.

Conjecture 3.2.4. The maximal spread $\varphi_A(n)$ of the graphs of order n is attained only by $G(n, \lfloor 2n/3 \rfloor)$; that is $\varphi_A(n) = \sqrt{\lfloor (4/3)(n^2 - n + 1) \rfloor}$ and so

$$(\frac{1}{\sqrt{3}})(2n-1) < \varphi_A(n) < (\frac{1}{\sqrt{3}})(2n-1) + \frac{\sqrt{3}}{4n-2}.$$

The complete multipartite graphs G giving equality in Theorem 3.1.3 are natural candidates for graphs with maximal spread $\varphi_A(n)$. As supporting evidence for Conjecture 3.2.4, we now verify that if G is one of these graphs on n vertices and G has maximal spread, then $G = G(n, \lfloor 2n/3 \rfloor)$. If $k = 1$, then G is complete bipartite and so, by Theorem 3.1.1, $\varphi_A(G) = 2\sqrt{e} \leq n < \varphi_A(n)$ when $n \geq 3$, and $G = K_2 = G(n, \lfloor 2n/3 \rfloor)$ when $n = 2$.If $k = 2$, then G is (complete) tripartite and by the following Proposition 3.2.7 implies that $\varphi_A(G) < \varphi_A(n)$ when $n \geq 35$. Also, [2] shows that if G is complete tripartite, then $\varphi_A(G) < \varphi_A(n)$ when $5 \leq n \leq 34$ and, when $n = 3, 4$, it is easy to check that $G = G(n, \lfloor 2n/3 \rfloor)$. If $k = 3$, the extremal graphs G in Theorem 3.1.3 are the complete $(k+1)$-partite graphs with k parts of size n_1 and a single part of size $n_2 \geq n_1$. Denote such a graph by $G(n, k, n_1)$. For this case, we first show that $n_1 = 1$. Since $\varphi_A(n)$ is strictly increasing, only graphs without isolated vertices needed to be examined. Thus, $n = kn_1 + n_2$. It follows from the discussion in the proof of Theorem 3.1.3 that the extreme eigenvalues λ_1, λ_n of $G(n, k, n_1)$ are the zeros of the middle factor of the characteristic polynomial (3.1.7) or, equivalently, they are the roots of the quadratic equation $\lambda^2 - n_1(k-1)\lambda - kn_1n_2 = 0$. Thus, $G(n,k,n_1)$ has spread

$$\lambda_1 - \lambda_n = (n_1^2(k-1)^2 + 4kn_1n_2)^{1/2}. \tag{3.2.1}$$

Since $kn_1 = n - n_2$ and $n_1(k-1) \leq n - n_1 - 1$ with equality if and only if $n_1 = 1$, it follows that, for $k \geq 3$, the spread is largest when $n_1 = 1$, as required. When $n_1 = 1$, $G(n,k,1) = G(n,k)$. Taking $n_1 = 1$ in (3.2.1)gives $\varphi_A(G(n,k)) = ((k-1)^2 + 4k(n-k))^{1/2}$. This quadratic is maximal when k is an integer closest to $(2n-1)/3$, that is, when $k = \lfloor 2n/3 \rfloor$, as claimed at the outset. As already mentioned in Conjecture 3.2.4

$$\varphi_A(n) \geq \varphi_A(G(n, \lfloor \frac{2n}{3} \rfloor)) > \frac{2n-1}{\sqrt{3}} \approx 1.1547n - 0.5774.$$

On the other hand, because $\lambda_1 \geq 2e/n$, Theorem 3.1.1 implies that

$$\varphi_A(G) \leq \lambda_1 + \sqrt{2e - \lambda_1^2} \leq \lambda_1 + \sqrt{n\lambda_1 - \lambda_1^2} \leq \frac{1}{2}(1+\sqrt{2})n.$$

For all graphs of order n. Thus, $\varphi_A(n) < 1.2072n$. This compares favorably with the conjectured value of $\varphi_A(n)$ (roughly, $1.1547n - 0.5774$) in Conjecture 3.2.4. Now, we conclude with some necessary conditions that a graph G on n vertices must satisfy if it has maximal spread $\varphi_A(n)$.

Lemma 3.2.5. *[2] Let G be a graph with e edges and let $\alpha \geq 1$. If $\varphi_A(G) > \alpha n$, then e must satisfy the quadratic inequality $8e^2 - (4\alpha+2)n^2e + \alpha^2n^2 < 0$.*

Proof. Since $\varphi_A(G) > n$, Theorem 3.1.1 implies that $e > n^2/4$. Thus, $\alpha n - 2e/n < (2e - (2e/n)^2)^{1/2}$ by (3.1.2). Since $\alpha n \geq n > 2e/n$, taking squares preserves the inequality. The quadratic inequality then follows by rearranging terms. □

Remark 3.2.6. Lemma 3.2.5 asserts that if $\varphi_A(G) > \alpha n \geq n$, then the number e of edges in G must lie between the roots of the quadratic $8x^2 - (4\alpha+2)n^2x + \alpha^2n^2$. For example, if $\varphi_A(G) > 2n/\sqrt{3}$ (an approximation to the conjectured value of $\varphi_A(n)$), then $0.346n^2 < e < 0.481n^2$. By comparison $G(n, \lfloor 2n/3 \rfloor)$, the graph that is conjectured to attain $\varphi_A(n)$, has roughly $0.444n^2$ edges.

Proposition 3.2.7. *[2] If $\varphi_A(G) = \varphi_A(n)$ and $n \geq 35$, then G is not tripartite.*

Proof. If $\varphi_A(G) = \varphi_A(n)$, then $\varphi_A(G) \geq \varphi_A(G(n, \lfloor 2n/3 \rfloor)) > \alpha n$ with $\alpha = (2n - 1)/n\sqrt{3} > 1$ when $n \geq 4$. The quadratic inequality in Lemma 3.2.5 then implies that $e > n^2(2\alpha + 1 - (4\alpha + 1 - 4\alpha^2)^{1/2})/8$. If G is tripartite, then $e \leq n^2/3$ [4, p. 6]. Thus, to show that G is not tripartite, it is sufficient to show that $n^2(2\alpha + 1 - (4\alpha + 1 - 4\alpha^2)^{1/2})/8 > n^2/3$. This simplifies to $6\alpha - 5 < (4\alpha + 1 - 4\alpha^2)^{1/2}$. Since $6\alpha - 5 > 0$, we may square and simplify to get $9\alpha^2 - 12\alpha + 2 > 0$. This will hold when α is greater than the largest root of the quadratic, that is, when $(2n - 1)/n\sqrt{3} \geq (2 + \sqrt{2})/3$, or $n > 34.72$. □

Proposition 3.2.8. *[2] If $\varphi_A(G) = \varphi_A(n)$, then G must be connected.*

Proof. Suppose that G is not connected. Then $G = G_1 \cup G_2$ for some vertex disjoint subgraphs G_1, G_2. Thus, $\lambda_n(G) = \min\{\lambda_n(G_1), \lambda_n(G_2)\}$. Let $\widehat{G} = G_1 \vee G_2$, the graph obtained from G by inserting all edges between the vertices in G_1 and the vertices in G_2. Then G is a proper subgraph of the connected graph $\widehat{G}$ and so $\lambda_1(G) < \lambda_1(\widehat{G})$. Since G_1, G_2 are induced subgraphs of $\widehat{G}$, by Lemma 3.2.3, $\lambda_n(\widehat{G}) \leq \min\{\lambda_n(G_1), \lambda_n(G_2)\} = \lambda_n(G)$. Thus

$$\varphi_A(\widehat{G}) = \lambda_1(\widehat{G}) - \lambda_n(\widehat{G}) > \lambda_1(G) - \lambda_n(G) = \varphi_A(G) = \varphi_A(n),$$

a contradiction. □

If A is the adjacency matrix of a graph G of order n, then by (3.0.2),

$$\varphi_A(G) = \max_{x,y} \sum_{i,j} a_{i,j}(x_i x_j - y_i y_j), \tag{3.2.2}$$

where the maximal is taken over all pairs x, y of unit vectors in $\mathbb{R}^n$ and is attained only for orthonormal eigenvectors of A corresponding to the eigenvalues λ_1, λ_n, respectively. The entries of x may always be assumed to be non-negative (and positive if G is connected). We call such an ordered pair of orthonormal eigenvectors x, y of G with $x \geq 0$ an *extremalpair* of eigenvectors of G. The following three lemmas are immediate results of (3.2.2) and Proposition 3.2.8.

Lemma 3.2.9. *[2] Suppose $\varphi_A(G) = \varphi_A(n)$ and x, y is an extremal pair of eigenvectors of G. Then distinct vertices i, j of G must be adjacent whenever $x_i x_j - y_i y_j > 0$ and non-adjacent whenever $x_i x_j - y_i y_j < 0$.*

For vectors $x, y \in \mathbb{R}^n$, let $G(x, y)$ be the graph, where distinct vertices i and j are adjacent, if and only if $x_i x_j - y_i y_j \geq 0$.

Lemma 3.2.10. *[2] $\varphi_A(n) = \varphi_A(G(x, y))$ for some graph $G(x, y)$ with $x, y \in \mathbb{R}^n$ orthonormal and x positive.*

For real numbers a, let a^+ equal a if $a \geq 0$ and 0 otherwise.

Lemma 3.2.11. *[2] $\varphi_A(n) = \max_{x,y} \sum_{i,j} (x_i x_j - y_i y_j)^+$, where the maximal is taken over all pairs x, y of orthonormal vectors in $\mathbb{R}^n$ with x positive.*

3.3 The lower bound

Lemmas 3.2.9 and 3.2.10 imply that in determining $\varphi_A(n)$, only graphs of the form $G = G_1 \vee G_2$ need to be considered, where G_1 is the subgraph of $G = G(x, y)$ induced by the vertices i with $y_i > 0$ and G_2 is the subgraph induced by the remaining vertices. For such graphs, the following lower bound on $\varphi_A(G)$, $3 \leq k \leq n-2$, follows from generalized interlacing [3, p. 19].

Proposition 3.3.1. *Let $G = G_1 \vee G_2$, where each G_i is a graph with n_i vertices, e_i edges and average degree $d_i = 2e_i/n_i$. Then $\varphi_A(G) \geq \sqrt{(d_1 - d_2)^2 + 4n_1 n_2}$.*

Remark 3.3.2. For $n = n_1 + n_2$ fixed, it is straightforward to check that the lower bound in Proposition 3.3.1 is maximal when $G = G(n, \lfloor 2n/3 \rfloor)$. This leads further support to Conjecture 3.2.4.

Now we consider the smallest possible spread for connected graphs. The next proposition shows that induced subgraphs are not the only subgraphs H of a graph G for which the monotonicity property, $\varphi_A(G) \geq \varphi_A(H)$, holds.

Proposition 3.3.3. *[2] If H is a bipartite subgraph of a graph G, then $\varphi_A(G) \geq \varphi_A(H)$.*

Proof. Since adding isolated vertices to H will not change $\varphi_A(H)$, we may assume that G and H each has n vertices. Also, by relabeling the vertices if necessary we may assume that the adjacency matrices of G and of H and a non-negative $\lambda_1(H)$ eigenvector of H are, respectively, of the form

$$A = \begin{pmatrix} A_1 & B \\ B^T & A_2 \end{pmatrix}, \; M = \begin{pmatrix} O & C \\ C^T & O \end{pmatrix}, \; x = \begin{pmatrix} u \\ v \end{pmatrix},$$

with $B \geq C$. By (3.0.1) $\varphi_A(G) \geq x^T Ax - y^T Ay = 4u^T Bv$. Since H is bipartite, $\lambda_n(H) = -\lambda_1(H)$, so $\varphi_A(H) = 2\lambda_1(H) = 2x^T Mx = 4u^T Cv \leq 4u^T Bv \leq \varphi_A(G)$. □

Remark 3.3.4. Equality need not be strict in Proposition 3.3.3. For example, if G and H are regular, H is bipartite and the complement of H is not connected, then $\varphi_A(G) = \varphi_A(H) = n$.

3.4 The minimal spread

We shall show that the path P_n of order n has the minimal spread among the connected graph of order n. Let $p_G(\lambda)$ be the *characteristic polynomial* denoted by $det(\lambda I - A(G))$, and if $e \in E(G)$, then $G - e$, $G - [e]$ denote the graphs arising from G by removing the edge e and the endpoints of e, respectively.

Lemma 3.4.1. *[5] If G is a tree (moreover, forest) and $e \in E(G)$, then*

$$p_G(\lambda) = p_{G-e}(\lambda) - p_{G-[e]}(\lambda).$$

Proof. As G is a tree we can label its vertices in such a way that e joins the points k and $k+1$ and there is no other edges between a point i $(1 \leq i \leq k)$ and a point j $(k+1 \leq j \leq n)$. Now the Laplacian expansion of the determinant $det(\lambda I - A(G))$ by its first k columns gives the equality of this lemma. □

Now introduce the following more complicated but better applicable notation: let $G' \prec G$ if and only if $p_{G'}(\lambda) \geq p_G(\lambda)$ for every $\lambda \geq \lambda_1(G)$. Obviously, $G' \prec G$ implies $\lambda_1(G') \leq \lambda_1(G)$.

Lemma 3.4.2. *[5] If G' is a subgraph of a tree G, then $G' \prec G$.*

Proof. We may assume $G' = G - e$. Let $\lambda \geq \lambda_1(G)$. By Corollary 3.2.1, $\lambda \geq \lambda_1(G - [e])$, thus $p_{G-[e]}(\lambda) \geq 0$, hence by Lemma 3.4.1,

$$p_G(\lambda) = p_{G-e}(\lambda) - p_{G-[e]}(\lambda) \leq p_{G-e}(\lambda).$$

□

Lemma 3.4.3. *[5] Let G, G' be trees (forests) of n points. $e \in E(G), e' \in E(G')$, and assume that $G' - e' \prec G - e$, $G - [e] \prec G' - [e']$. Then $G' \prec G$.*

Proof. Let $\lambda \geq \lambda_1(G)$. Then, by Corollary 3.2.1, $\lambda \geq \lambda_1(G - e)$ and thus by the assumption, $p_{G-e}(\lambda) \leq p_{G'-e'}(\lambda)$. Again, by Corollary 3.2.1, $\lambda \geq \lambda_1(G - e) \geq \lambda_1(G' - e') \geq \lambda_1(G' - [e'])$, hence $p_{G-[e]}(\lambda) \leq p_{G'-[e']}(\lambda)$. By Lemma 3.4.1,

$$p_G(\lambda) = p_{G-e}(\lambda) - p_{G-[e]}(\lambda) \leq p_{G'-e'}(\lambda) - p_{G'-[e']}(\lambda) = p_{G'}(\lambda).$$

□

Theorem 3.4.4. *[5] If G is a tree with n vertices then $P_n \prec G$.*

Proof. Consider a tree G such that there is no other tree G' such that $G' \prec G$; we have to prove $G = P_n$. Assume indirectly that there exist vertices of valency ≥ 3 in G. Let x be a point of valency ≥ 3 such that a certain component of $G - x$ does not contain further points having valency ≥ 3 in G. This component is a path $(a_1, \ldots, a_k)$, a_1 being joined to x. Let $e = (x, b)$ another edge incident with x and put $e' = (a_k, b)$, $G' = G - e \cup e'$. It is easy to see that G has more endpoints than G', hence $G \ncong G'$. Furthermore, $G - e = G' - e'$ and $G - [e]$ is isomorphic to a subgraph of $G' - [e']$. Hence by Lemmas 3.4.2 and 3.4.3 we obtain $G' \prec G$, a contradiction. □

Corollary 3.4.5. *If G is a connected graph of order n, then $\varphi_A(G) \geq \varphi_A(P_n)$. Equality holds if and only if $G = P_n$.*

Proof. Let T be a spanning tree of G. Since T is bipartite, $\varphi_A(G) \geq \varphi_A(T)$. Thus, to prove the result, it is sufficient to prove that if T is a tree other than a path, then $\varphi_A(T) > \varphi_A(P_n)$. Since T and P_n are bipartite, by Theorem 3.4.4, $\varphi_A(T) = 2\lambda_1(T) > 2\lambda_1(P_n) = \varphi_A(P_n)$. □

In the latter chapters, we consider the more well-known matrix, Laplacian matrix and signless Laplacian matrix. And some property is still useful to them.

4

The bounds of the Laplacian eigenvalues of a graph

Let $A(G)$ be the adjacency matrix of G and let $D(G)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Note that $L(G)$ is real symmetric and positive semi-definite. From this fact and Geršgorin's theorem, it follows that its eigenvalues are nonnegative real numbers. Moreover since its rows sum to zero, zero is the smallest eigenvalue of $L(G)$. Now, denote the eigenvalues of $L(G)$ by $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n = 0$.

4.1 Zero eigenvalues of Laplacian matrices

Lemma 4.1.1. *For any $n \times m$ matrix N, the two matrix N^T and NN^T have the same nullspace. i.e.* $\{x \in R^n | N^T x = 0\} = \{x \in R^n | NN^T x = 0\}$.

Proof. ($\subseteq$) It's clearly true.
($\supseteq$) Suppose $NN^T x = 0$. Then $||N^T x||^2 = (N^T x)^T (N^T x) = xNN^T x = 0$. □

Proposition 4.1.2. *Let G be a graph with c components. Then 0 is a Laplacian eigenvalue of G with multiplicity c.*

Proof. It suffices to prove the nullspace of N^T has dimension c. And $N^T 1 = 0$. Assume $c = 1$ first. (G is connected) To prove the vectors in the nullspace of N^T has the form $s1$, for some $s \in \mathbb{R}$. Let $x \in null(N^T)$ and suppose $x_i \neq x_j$, for some i, j. Choose such pair i, j with distance $\partial(i, j)$ in G is smallest. Note that i, j have an edge $ij = e$. Hence $(N^T x)e = \pm(x_i - x_j) \neq 0$, which is a contradiction. Then $\dim(null(N^T)) = 1$. In general, N^T has the block form $N^T = diag(N_1^T, N_2^T, \ldots, N_c^T)$, where N_i is the incidence matrix of the i-th component of G. Each N_i^T has the nullspace span by 1, which can be extended to a vector in $null(N^T)$ by filling zeros. Hence the nullspace of N^T is the linear combination of the c independent $(0, 1)$-vectors that form a partition of 1. □

4.2 Eigenvalues alternating property

In Lemmas 2.2.1, 2.2.2 and Corollary 3.2.2, we follow the same result for monotonicity property from adjacent spread. That is, if G is a graph, then the Laplacian eigenvalues of an induced subgraph of G interlace the Laplacian eigenvalues of G. And we have not only true for induced subgraph of G. The following is called *eigenvalues alternating property*.

Lemma 4.2.1. *For $e \in E(G)$, the Laplacian eigenvalues of $G' = G - e$ interlace those of G. i.e., $\mu_1(G) \geq \mu_1(G') \geq \mu_2(G) \geq \mu_2(G') \geq \ldots \geq \mu_n(G) = \mu_n(G') = 0$.*

Proof. Let N be the incidence matrix of an orientation G^σ and $L(G) = NN^T$. Let N' be the incidence matrix of an orientation $(G-e)^\sigma$ is obtained from N by deleting a column. Hence $N'^T N'$ is a principal sub-matrix of $N^T N$. By Corollary 3.2.2, the i-th largest eigenvalues of $N^T N$ is not less than that of $N'^T N'$. Since NN^T and $N^T N$ have same nonnegative eigenvalues, $\mu_{n-i}(G) \leq \mu_{n+1-i}(G') \leq \mu_{n+1-i}(G)$, we have $\mu_i(G) \geq \mu_i(G') \geq \mu_{i-1}(G)$. □

Remark 4.2.2. Use the same method, it's also true for the signless Laplacian eigenvalues.

Corollary 4.2.3. *Let G be a connected graph, and let H be a subgraph of G. Then, $\mu_1(H) \le \mu_1(G)$, and equality holds if and only if $H = G$.*

Proof. By the Corollary 3.2.2 and Lemma 4.2.1, the result follows. □

4.3 The bounds of $\mu_1(G)$ and $\mu_{n-1}(G)$

Define the degree of v is $d(v)$ and $m(v) = \sum_{u \in N(v)} d(u)/d(v)$, where $m(v)$ is the average of the degrees of the vertices adjacent to v. Denote $\Delta(G)$ be the maximal degree of G and N_i is the neighbor of the vertex v_i. In the next two sections, we will show the following equations $1 \sim 6$ which will be used in Chapters $5 \sim 7$ Chapters.

1. $\mu_1(G) \le n$,
2. $\mu_1(G) \le \max\{d(v_i) + d(v_j) : v_i v_j \in E(G)\}$,
3. $\mu_1(G) \le \max\{m(v_i) + d(v_i) : v_i \in V(G)\}$,
4. $\mu_1(G) \le \max\{d(v_i) + d(v_j) - |N_i \cap N_j| : 1 \le i \le j \le n, v_i v_j \in E(G)\}$,
5. $\mu_1(G) \ge \Delta(G) + 1$,
6. $0 < \mu_{n-1}(G) \le 1$.

And we also called $\mu_1(G)$ and $\mu_{n-1}(G)$ is called a *spectral radius* and *algebraic connectivity* of G, respectively.

Theorem 4.3.1. *Let G be a connected graph of order $n \ge 2$. Then*

$$\mu_1(G) \le n, \tag{4.3.1}$$

with equality if and only if the complement graph of G is disconnected.

Proof. Since a graph G is connected if and only if $\mu_{n-1} \ne 0$. And $L(G) + L(\bar{G}) = nI - J$, it implies that $\mu_i(G) = n - \mu_{n-i}(\bar{G})$, for $1 \le i \le n-1$. In particular, $\mu_1(G) = n - \mu_{n-1}(\bar{G}) \le n$. Therefore $\mu_1(G) \le n$ with equality if and only if $\bar{G}$ is disconnected. □

Lemma 4.3.2. *Let G be connected graph. If G is bipartite graph, then $L(G)$ and $|L(G)|$ are unitarily similar.*

Proof. If G is bipartite graph, then $L(G) = D(G) - A(G)$ and $|L(G)| = D(G) + A(G)$ are unitarily similar by a diagonal matrix D with diagonal entries ± 1. (that is, $|L(G)| = DL(G)D^{-1}$) □

Theorem 2.3.1 shows that $\mu_1 \leq 2\max\{d(v) : v \in V(G)\}$. Anderson and Morley improved this upper bound on the spectral radius by showing the following theorem.

Theorem 4.3.3. *[6] (Anderson and Morley(1985)) Let G be a graph. Then*

$$\mu_1(G) \leq \max\{d(v_i) + d(v_j) : v_i v_j \in E(G)\}. \tag{4.3.2}$$

If G is connected, then the equality holds if and only if G is bipartite and all vertices in the same part of the bipartition have the same valency. i.e., G is said biregular.

Proof. Since $N^T(G)N(G) - 2I$ is the adjacency matrix of the line graph of G, where $N(G)$ is the vertex-edge incident matrix of G. Note that $|L(G)| = N(G)N^T(G)$, since $N(G)N^T(G)$ and $N^T(G)N(G)$ have the same nonnegative eigenvalues. Since line graph of G has maximal degree at most $\max\{d(v_i) + d(v_j) : v_i v_j \in E(G)\} - 2$, which is larger than its largest eigenvalue known to be $\rho_1 - 2$, where ρ_1 is denoted by the largest signless Laplacian eigenvalue of G. The equality holds if and only if the line graph of G is regular. By Theorem 2.1.8, we have

$$\mu_1(G) \leq \rho_1(G) \leq \max\{d(v_i) + d(v_j) : v_i v_j \in E(G)\}.$$

And the equality holds through if and only if G is bipartite and the line graph is regular. □

Theorem 4.3.4. *[7] (Merris) If G is a connected graph, then*

$$\mu_1(G) \leq \max\{m(v_i) + d(v_i) : v_i \in V(G)\}. \tag{4.3.3}$$

Proof. If G has no edges, both sides of equation are zero. Otherwise, it suffices to prove the result for connected graphs, and the inequality follows by applying Geršgorin's theorem to the rows of $D^{-1}(G)|L(G)|D(G)$, the matrix whose (i,j)-entry is

$$\begin{cases} d(v_i) & \text{if } i=j \\ -d(v_j)/d(v_i) & \text{if } v_iv_j \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

Then

$$\begin{aligned} \mu_1(G) &\leq \max_i\{d(v_i) + \sum_{j=1,j\neq i}^{j=n} \frac{|-d(v_j)|}{d(v_i)} : v_iv_j \in E(G)\} \\ &= \max_i\{d(v_i)+m(v_i) : v_i \in V(G)\}. \end{aligned}$$

□

Remark 4.3.5. (4.3.3) improves (4.3.2) is clear.

Theorem 4.3.6. *[8] (Rojo) If G is a graph on vertex set $V=\{v_1,v_2,\ldots,v_n\}$, then*

$$\mu_1(G) \leq \max\{d(v_i)+d(v_j)-|N_i\cap N_j| : 1\leq i\leq j\leq n, v_iv_j\in E(G)\} \tag{4.3.4}$$

$|N_i\cap N_j|$ is the number of common neighbors of v_i and v_j. Moreover, this upper bound for $\mu_1(G)$ does not exceed n.

Proof. If G has no edge, both sides of (4.3.4) are zero. Otherwise, it suffices to prove the result for at least one edge in the graph G. Let x_k, $k=1,2,\ldots,n$ be the eigen-components of the eigenvector X corresponding to the eigenvalue $\mu_1(G)$ of the Laplacian matrix $L(G)$. Assume that one of the eigen-components (say x_i) is equal to 1 and the other eigen-components are less than or equal to 1 in magnitude. i.e., $x_i=1$ and $|x_k|\leq 1$ for all k. Also let $x_j=\min_k\{x_k : v_iv_k\in E(G)\}$. Let C_{ij} be the number of common neighbors of v_i and v_j. Therefore, $C_{ij}=|N_i\cap N_j|$. Since $x_j\leq x_k$ for all k such that $v_iv_k\in E(G)$,

$$\sum_k\{x_k : v_iv_k\in E(G), v_jv_k\notin E(G)\} \geq (d(v_i)-c_{ij})x_j,$$

and since $x_k \le 1$ for all k,

$$\sum_k \{x_k : v_jv_k \in E(G), v_iv_k \notin E(G)\} \le (d(v_j) - c_{ij}).$$

We have $LX = \mu_1 X$. This implies $\mu_1 x_i = d(v_i)x_i - \sum_k \{x_k : v_iv_k \in E(G)\}$, i.e., $\mu_1 = d(v_i) - \sum_k \{x_k : v_iv_k \in E(G)\, v_jv_k \in E(G)\} - \sum_k \{x_k : v_iv_k \in E(G), v_jv_k \notin E(G)\}$. From the j-th of $LX = \mu_1 X$, we have $\mu_1 x_j = d(v_j)x_j - \sum_k \{x_k : v_jv_k \in E(G)\}$, i.e., $\mu_1 x_j = d(v_j)x_j - \sum_k \{x_k : v_jv_k \in E(G), v_iv_k \in E(G)\} - \sum_k \{x_k : v_jv_k \in E(G), v_iv_k \notin E(G)\}$. By subtracting, we get

$$\begin{aligned} \mu_1(1 - x_j) &= d(v_i) - d(v_j)x_j - \sum_k \{x_k : v_iv_k \in E(G), v_jv_k \notin E(G)\} \\ &\quad + \sum_k \{x_k : v_jv_k \in E(G), v_iv_k \notin E(G)\} \\ &\le d(v_i) - d(v_j)x_j - (d(v_i) - c_{ij})x_j + (d(v_j) - c_{ij}) \\ &= (d(v_i) - d(v_j) + c_{ij})(1 - x_j). \end{aligned}$$

If $x_j = 1$, then $x_k = 1$ for all k such that $v_iv_k \in E(G)$. Therefore, $\mu_1 = d(v_i) - \sum_k \{x_k : v_iv_k \in E(G)\} = d(v_i) - d(v_i) = 0$. But it is not possible for at least one edge in the graph. Therefore, $x_j \ne 1$. And so $\mu_1 \le (d(v_i) - d(v_j) + c_{ij})$, where $v_iv_j \in E(G)$. Hence, $\mu_1 \le \max\{d(v_i) + d(v_j) - c_{ij} : 1 \le i \le j \le n, v_iv_j \in E(G)\}$, i.e., $\mu_1 \le \max\{d(v_i) + d(v_j) - |N_i \cap N_j| : 1 \le i \le j \le n, v_iv_j \in E(G)\}$. It's obvious that $\max\{d(v_i) + d(v_j) - |N_i \cap N_j| : 1 \le i < j \le n, v_iv_j \in E(G)\} \le \max\{d(v_i) + d(v_j) - |N_i \cap N_j| : 1 \le i \le j \le n\}$. □

Remark 4.3.7. $\max\{d(v_i) + d(v_j) - |N_i \cap N_j| : 1 \le i < j \le n, v_iv_j \in E(G)\} \le \max\{d(v_i) + d(v_j) : v_iv_j \in E(G)\}$. Hence the bound is better than (4.3.2).

Theorem 4.3.8. *(Grone and Merris (1994)) Let G be a graph of order $n \ge 2$ containing at least one edge. Then*

$$\mu_1(G) \ge \Delta(G) + 1 \tag{4.3.5}$$

where $\Delta(G)$ is the maximal degree of G. The equality holds if and only if $\Delta(G) = n-1$.

Proof. Since the star $K_{1,\Delta(G)}$ has the largest Laplacian eigenvalue $1 + \Delta(G)$ and it's a subgraph of G, then this follows from Corollary 4.2.3. □

A vertex v of a graph G, is called a *pendant vertex* of G, if v has exactly one neighbor. In the following theorem we consider the boundary on $\mu_{n-1}(G)$.

Theorem 4.3.9. *[9] Let G be a simple connected graph of order $n > 2$. If G has a pendant vertex v, then*

$$0 < \mu_{n-1}(G) \leq 1. \tag{4.3.6}$$

with equality if and only if the neighbor of v is adjacent to every vertex of G.

Proof. The highest degree of the complement graph of graph G is $n-2$. Since G has a pendant vertex and $n > 2$, therefore, the complement graph $\bar{G}$ has at least one edge. Therefore, the largest eigenvalue of $\bar{G}$ is $\mu_1(\bar{G}) \geq n-1$, from Theorem 4.3.8. And $L(G) + L(\bar{G}) = nI - J$, it implies that $\mu_i(G) = n - \mu_{n-i}(\bar{G})$, for $1 \leq i \leq n-1$. Then we get $\mu_{n-1}(G) = n - \mu_1(\bar{G}) \leq 1$. Let us construct a tree T of order n such that one isolated vertex connected to the pendant vertex of a star graph of order $n-1$. Using Theorem 4.3.8, we get $\mu_1(T) > n-1$. Since pendant vertex is not adjacent to the highest degree vertex (highest degree is $n-2$). Then T is a subgraph of $\bar{G}$. Therefore, $\mu_1(\bar{G}) \geq \mu_1(T) > n-1$, that is, $\mu_{n-1}(G) < 1$. □

Let W be the set of all column vectors x and e be the all 1 vector such that $x^T x = 1, x^T e = 0$. If L is positive semi-definite then the second smallest eigenvalue is equal to $\min_{x \in W} x^T L x$ by Rayleigh principle in Lemma 2.2.1. We use the principle for the other property.

Theorem 4.3.10. *[10] If G_1, G_2 are edge-disjoint graphs with the same set of vertices then $\mu_{n-1}(G_1) + \mu_{n-1}(G_2) \leq \mu_{n-1}(G_1 \cup G_2)$.*

Proof. We have $L(G_1 \cup G_2) = L(G_1) + L(G_2)$. Thus $\mu_{n-1}(G_1 \cup G_2) = \min_{x \in W}(x^T L(G_1)x + x^T L(G_2)x) \geq \min_{x \in W} x^T L(G_1)x + \min_{x \in W} x^T L(G_2)x = \mu_{n-1}(G_1) + \mu_{n-1}(G_2)$. □

Corollary 4.3.11. *The function* $\mu_{n-1}(G)$ *is non-decreasing for graphs with the same set of vertices. i.e.* $\mu_{n-1}(G_1) \leq \mu_{n-1}(G_2)$ *if* $G_1 \subseteq G_2$ *(and* G_1, G_2 *have the same set of vertices).*

In the latter chapter, we consider the Laplacian spread of a graph G, which is defined by $\varphi_L(G) = \mu_1(G) - \mu_{n-1}(G)$. Hence, for a graph G and H a subgraph with the same set of vertices of G, Laplacian spread doesn't have the monotonicity as the adjacency spread ($\varphi_A(G) \geq \varphi_A(H)$).

5

The Laplacian spread of trees

The Laplacian spread of graph G is defined to be $\varphi_L(G) = \mu_1(G) - \mu_{n-1}(G)$. Note that in the definition we consider the largest eigenvalue and the second smallest eigenvalue, as the smallest one always equals zero.

Example 5.0.12. (i) K_n has Laplacian spectrum: $0, \overbrace{n, \ldots, n}^{n-1}$.

$$\varphi_L(K_n) = (n) - (n) = 0.$$

(ii) Assume that $n < m$,

$K_{n,m}$ has Laplacian spectrum: $0, \overbrace{n, \ldots, n}^{m-1}, \overbrace{m, \ldots, m}^{n-1}, m+n$.

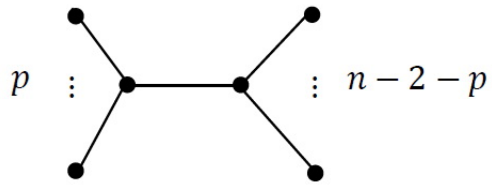
$$\varphi_L(K_{n,m}) = (m+n) - (n) = m.$$

In particular, $K_{1,n-1}$ has Laplacian spectrum: $0, \overbrace{1, \ldots, 1}^{n-1}, n$.

$$\varphi_L(K_{1,n-1}) = n - 1.$$

(iii) P_n has Laplacian spectrum: $2 - 2\cos(\frac{\pi k}{n}), 0 \le k \le n-1$.

$$\varphi_L(P_n) = 2\{1 + \cos(\frac{\pi}{n}) - [1 - \cos(\frac{\pi}{n})]\} = 4\cos(\frac{\pi}{n}).$$



A double star $T(n,p)$ with $n-2 \geq p \geq (n-2)/2$.

Fig 5.1.

5.1 The maximal Laplacian spread of trees

If G is disconnected, then $\mu_{n-1}(G) = 0$. We only consider connected graphs G in which case $\mu_{n-1}(G) > 0$. So we first consider the extremal Laplacian spread of trees. Let P_n, S_n be denoted by a path and a star of order n, respectively. Let T be the one with maximal Laplacian spread among all trees of order n. Now, we prove T is necessarily a double star of order n.

Lemma 5.1.1. *[11] Let T be the one with maximal Laplacian spread among all trees of order n. Then T is a double star $T(n,p)$, for some p with $n-2 \geq p \geq n-2/2$.*

Proof. Let T be a tree of order n, then for any edge uv of T, $d(u) + d(v) = |N(u) \cup N(v)| \leq n$, with equality if and only if $T = T(n, d(u)-1)$, [assume $d(u) \geq d(v)$]. In addition, the star $S_n = T(n, n-2)$ and $\varphi_L(S_n) = n-1$. For any tree T which is not a double star, then by the above discussion and Theorem 4.3.3, we have $\mu_1(T) \leq \max\{d(u) + d(v) : uv \in E(G)\} \leq n-1$, then $\varphi_L(T) = \mu_1(T) - \mu_{n-1}(T) < n-1$, as $\mu_{n-1}(T) > 0$. Then the result follows. $\square$

Proposition 5.1.2. *The characteristic polynomial of $L(T(n,p))$ is*

$$det(\lambda I - L(T(n,p))) = \lambda(\lambda-1)^{n-4}[(\lambda-n)(\lambda-1)^2 + p(n-2-p)\lambda].$$

Proof. We have the quotient matrix of $L(T(n,p))$ is

$$Q_{L(T(n,p))} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -p & p+1 & -1 & 0 \\ 0 & -1 & p+2-n & n-1-p \\ 0 & 0 & -1 & 1 \end{pmatrix},$$

then $det(\lambda I - Q_{L(T(n,p))}) = (\lambda - n)(\lambda - 1)^2 + p(n-2-p)\lambda$. Since 0 is an eigenvalue with multiplicity 1 and observe that $null(L+I) = n-4$, that is, -1 is an eigenvalue with multiplicity $n-4$. By Lemma 2.2.3 and above argument, we have $det(\lambda I - L(T(n,p))) = \lambda(\lambda-1)^{n-4}[(\lambda-n)(\lambda-1)^2 + p(n-2-p)\lambda]$. □

Remark 5.1.3. Denote

$$f(\lambda; n, p) := (\lambda - n)(\lambda - 1)^2 + p(n-2-p)\lambda. \tag{5.1.1}$$

Then the characteristic polynomial of $L(S_n)$ is $\lambda(\lambda-1)^{n-4} f(\lambda; n, n-2)$. For any double star $T(n,p)$ with $(n-2)/2 \le p \le n-3$ and $n \ge 5$, by Proposition 5.1.2, $(0 \le)\mu_{n-1}(T(n,p)) < 1$. And by Theorem 4.3.8, $\mu_1(T(n,p)) \ge d(T(n,p)) + 1 = p+2 \ge 4$. Hence the eigenvalue $\mu_1(T(n,p)), \mu_{n-1}(T(n,p))$ are both roots of the polynomial $f(\lambda; n, p)$. In addition, all roots of $f(\lambda; n, p)$ must be positive as they are nonzero eigenvalues of $L(T(n,p))$. In the following, we shall prove that for $(n-2)/2 \le p \le n-3$ and $n \ge 5$, $\varphi_L(T(n,p)) < \varphi_L(T(n,n-2)) = n-1$. By this inequality and Lemma 5.1.1 , we than get the result that the star is the unique tree with maximal Laplacian spread among all trees with given order. There are exactly two double stars $T(5,2), T(5,3)$ of order 5, and by the next lemma above inequality holds for $n = 5$. There are exactly three double stars $T(6,2), T(6,3), T(6,4)$ of order 6, $\varphi_L(T(6,3)) < \varphi_L(T(6,4))$. And $\varphi_L(T(6,2)) < \varphi_L(T(6,4))$ can be obtained by computation. By (5.1.1), $f(\lambda; 6, 2) = (\lambda-6)(\lambda-1)^2 + 4\lambda$, which has roots $(5 \pm \sqrt{17})/2, 3$. Therefore, $\varphi_L(T(6,2)) = \sqrt{17} < 6 - 1 = 5$.

Lemma 5.1.4. *For $n \ge 5$,*

$$\varphi_L(T(n,n-3)) < \varphi_L(T(n,n-2)) = \varphi_L(S_n) = n-1.$$

Proof. By Proposition 5.1.2, the eigenvalues $\mu_{n-1}(T(n, n-3)), \mu_1(T(n, n-3))$ are both roots of the polynomial $f(\lambda; n, n-3) = \lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n$. Note that

$$\begin{aligned} f(\frac{1}{3}; n, n-3) &= -\frac{23+3n}{27} < 0, \\ f(n-\frac{2}{3}; n, n-3) &= \frac{4-39n+9n^2}{27} > 0, \end{aligned}$$

if $n \geq 5$. If there is a $\lambda' > n - 2/3$, such that $f(\lambda'; n, n-3) \leq 0$ then $f(\lambda; n, n-3)$ has two roots both greater than $n-2/3$, and hence the sum of its root is greater than $2n - 4/3$. However, the sum of all roots (necessarily be positive) of $f(\lambda; n, n-3)$ is $r + 2 < 2n - 4/3$, which is contradiction, for $n \leq 4$. So, $\mu_1(T(n, n-3)) < n - 2/3$. Similarly, we get $\mu_{n-1}(T(n, n-3)) > 1/3$. Hence, $\varphi_L(T(n, n-3)) < (n-2/3) - 1/3 = n - 1$. □

Next, we consider the Laplacian spread of $T(n, p)$ with $(n-2)/2 \leq p \leq n-4$.

Lemma 5.1.5. *[11] For $(n-2)/2 \leq p \leq n-4$ and $n \geq 6$.*

$$\varphi_L(T(n, p)) < \varphi_L(T(n, n-2)) = \varphi_L(S_n) = n - 1.$$

Proof. Denote $\mu_1(T(n, p)), \mu_{n-1}(T(n, p))$ by μ_1, μ_{n-1}, respectively. Observe that $\varphi_L(T(n, n-2)) - \varphi_L(T(n, p)) = (n-1) - (\mu_1 - \mu_{n-1}) = (n - \mu_1) - (1 - \mu_{n-1})$. By (5.1.1), if $\lambda > 0$, the image of $f(\mu; n, p)$ is obtain from $f(\lambda; n, n-2)$ by adding a positive function $p(n-2-p)\lambda$. By Mean Value Theorem,

$$\begin{aligned} n - \mu_1 &= \frac{f(n; n, p) - f(\mu_1; n, p)}{f'(\xi_1; n, p)} = \frac{np(n-2-p)}{f'(\xi_1; n, p)} \\ 1 - \mu_{n-1} &= \frac{f(1; n, p) - f(\mu_{n-1}; n, p)}{f'(\xi_2; n, p)} = \frac{p(n-2-p)}{f'(\xi_2; n, p)}, \end{aligned}$$

for some $\xi_1 \in (\mu_1, n)$ and $\xi_1 \in (\mu_{n-1}, 1)$, where $f'(\lambda; n, p)$ denote the derivative of $f(\lambda; n, p)$ with respect to λ. If we can show $np(n-2-p)/f'(\xi_1; n, p) > p(n-2-p)/f'(\xi_2; n, p)$, or $nf'(\xi_2; n, p) > f'(\xi_1; n, p)$, the result will follow. Note that $f'(\lambda; n, p) = 3\lambda^2 - 2(n+2)\lambda + 2n + 1 + p(n-2-p)$. Thus $f'(\lambda; n, p)$ is strictly decreasing on the open interval $(0,(n+2)/3)$ and is strictly increasing on $((n+2)/3,\infty)$. Note that $0<\xi_2<1<(n+2)/3$, and by Theorem 4.3.10, $n>\xi_1>\mu_1\geq p+2\geq(n-2)/2+2>(n+2)/3$. Therefore, $nf'(\xi_2;n,p)>nf'(1;n,p)=np(n-2-p)$, $f'(\xi_1;n,p)>f'(n;n,p)=(n-1)^2+p(n-2-p)$. Then $f'(\xi_2;n,p)-f'(\xi_1;n,p)>(n-1)[p(n-2-p)-(n-1)]$. As $(n-2)/2\leq p\leq n-4$, $p(n-2-p)-(n-1)\geq 2(n-4)-(n-1)=n-7$. So, if $n\geq 7$, the result follows. If $n=6$, then $p=2$ and this case verified prior to Lemma 5.1.4. □

By Lemmas 5.1.1, 2.2.3 and 5.1.4, we get the main result.

Theorem 5.1.6. *For $n\geq 5$, the star is the unique tree with maximal Laplacian spread among all trees of order n.*

5.2 The minimal Laplacian spread of trees

The line graph of the tree T, denoted by T^l, is the graph whose vertices are exactly the edges of T with two vertices being adjacent if and only if the corresponding edges in T are incident. Note that T^l is connected, and $P_n^l=P_{n-1}$. Also, we denote the eigenvalues of $A(G)$ by $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$.

Lemma 5.2.1. *[11] For any tree T of order $n\geq 3$, the Laplacian spread of T is exactly the (adjacency) spread of T^l, i.e., $\varphi_L(T)=\varphi_A(T^l)$.*

Proof. As T is bipartite, the matrix $|L(T)|=N(T)N^T(T)=D(T)+A(T)$ is unitarily similar to $L(T)=D(T)-A(T)$, and hence they have the same spectra. Note that $N^T(T)N(T)$ and $N(T)N^T(T)$ have the same set of nonzero eigenvalues, and $N^T(T)N(T)=A(T^l)+2I_{n-1}$. Hence, the eigenvalues of $A(T^l)$ are $\lambda_1(T)-2,\lambda_2(T)-2,\ldots,\lambda_{n-1}(T)-2$, and the Laplacian spread of T is exactly the (adjacency) spread of T^l. □

Theorem 5.2.2. *[11] For $n\geq 5$, the path is the unique tree with minimal Laplacian spread among all trees of order n.*

Proof. Let T be any tree of order $n \geq 5$, which is not a path. Then T^l is a connected graph of order $n-1$ which is not a path. Then by Lemma 5.2.1 and Corollary 3.4.5, we have

$$\varphi_L(T) = \varphi_A(T^l) > \varphi_A(P_{n-1}) = \varphi_A(P_n^l) = \varphi_L(P_n).$$

The result follows. $\square$

6

The Laplacian Spread of Unicyclic graphs

In this chapter, continue the work on the Laplacian spread of graphs, and determine the unique unicyclic graph with maximal Laplacian spread among all unicyclic graphs of fixed order, which is obtained from a star by adding one edge between two pendent vertices. And we also determine the minimal Laplacian spread among all unicyclic graphs of fixed order. Note that a graph is called unicyclic if it contains exactly one cycle. And $|V(G)| = |E(G)|$, throughout this chapter we always assume that all unicyclic graphs are connected.

6.1 Graphs with a cut edge

Let $G = G_1u : vG_2$ be the graph obtained by joining the vertex u of the graph G_1 to the vertex v of the graph G_2 by an edge. Note that uv is a edge of G. Let the characteristic polynomial $det(xI - L(G))$ is denoted by $p(L(G))$. If $v \in V(G)$, let $L_v(L(G))$ be the principal submatrix of $L(G)$ obtained by deleting the row and column corresponding to the vertex v. In order to search the characteristic polynomial of some special graphs. We need the following lemma.

Lemma 6.1.1. *[13] Let $G = G_1u : vG_2$ be the graph obtained by joining the vertex u of the graph G_1 to the vertex v of the graph G_2 by an edge. Then*

$$p(L(G)) = p(L(G_1))p(L(G_2)) - p(L(G_1))p(L_v(G_2)) - p(L(G_2))p(L_u(G_1)).$$

Proof. Let $L(G_1^*)$ $(L(G_2^*))$ be the principal submatrix obtained by deleting the row and column corresponding to vertex v (u) from $L(G_1u : v)$ $(L(G_2v : u))$, where $G_1u : v$ is the graph formed from G_1 by joining a new pendent vertex v to u. Without loss of generality, we may assume that

$$L(G) = \begin{pmatrix} L(G_1^*) & -E_{11} \\ -E_{11}^T & L(G_2^*) \end{pmatrix}$$

where E_{11} is the $|V(G_1)|$-by-$|V(G_2)|$ matrix whose only non-zero entry is a 1 in position $(1, 1)$. By the Laplace expansion Theorem, we have

$$p(L(G)) = p(L(G_1^*))p(L(G_2^*)) - p(L_u(G_1))p(L_v(G_2)).$$

Since

$$\begin{aligned} p(L(G_1^*)) &= p(L(G_1)) - p(L_u(G_1)), \\ p(L(G_2^*)) &= p(L(G_2)) - p(L_v(G_2)). \end{aligned}$$

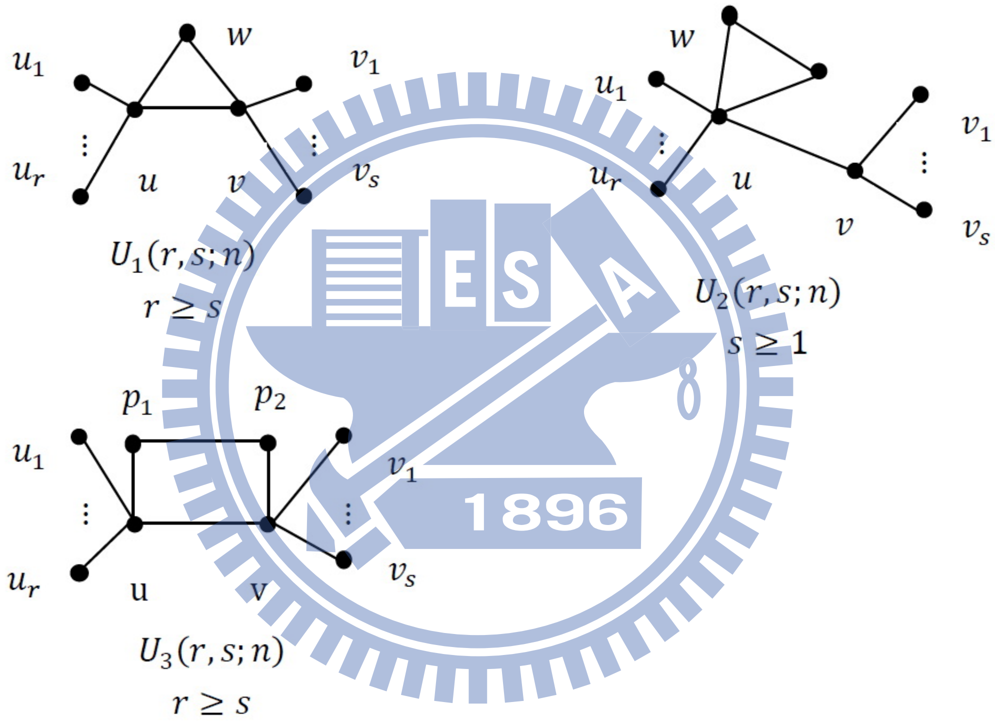
By combining all the equation, we have

$$p(L(G)) = p(L(G_1))p(L(G_2)) - p(L(G_1))p(L_v(G_2)) - p(L(G_2))p(L_u(G_1)).$$

□

6.2 The maximal Laplacian spread

We introduce three unicyclic graphs of order n in Fig 6.1: $U_1(r, s; n), r \geq s$; $U_2(r, s; n), s \geq 1$; $U_3(r, s; n), r \geq s$. Here r, s are nonnegative integers, which are respectively the number of pendant vertices adjacent to u and v; moreover parameters n, r, s are related by $n = r + s + 3, n = r + s + 4$.



u_1
w
v_1
u_r
u
v
v_s
$U_1(r,s;n)$
$r \geq s$
w
u_1
v_1
u_r
u
v
v_s
$U_2(r,s;n)$
$s \geq 1$
p_1
p_2
u_1
v_1
u_r
u
v
v_s
$U_3(r,s;n)$
$r \geq s$

Fig 6.1

Lemma 6.2.1. *[12] Let G be the graph with maximal Laplacian spread among all unicyclic graphs of order $n \geq 7$. Then G is among the graph $U_1(n-3,0;n), U_1(n-4,1;n), U_2(n-5,1;n)$ and $U_3(n-4,0;n)$.*

Proof. Let v_iv_j be an edge of G. Then $d(v_i)+d(v_j)-|N(v_i)\cap N(v_j)| = |N(v_i)\cup N(v_j)| \leq n$, with equality if and only if G is one of graphs in Fig 6.1 for some r or s. Therefore, if G is not a graph in Fig 6.1 , then by Theorem 4.3.6, $\mu_1(G) \leq n-1$ and hence $\varphi_L(G) = \mu_1(G) - \mu_{n-1}(G) < n-1$, as $\mu_{n-1}(G) > 0$. In addition, $\varphi_L(U_1(n-3,0;n)) = n-1$. So G must be one graph in Fig 6.1. Assume that $n \geq 7$ in the following discussion. For the graph $U_1(r,s;n)$, by Theorem 4.3.4 ,

$$\mu_1(U_1(r,s;n)) \leq \max\{r+2+\frac{n+1}{r+2}, s+2+\frac{n+1}{s+2}\} := \alpha.$$

Note that $r \geq s$ and hence $r+2 \geq (n-3)/2+2 > \sqrt{n+1}$. If $r \leq n-5$, then

$$\mu_1(U_1(r,s;n)) \leq \alpha \leq \max\{2+\frac{n+1}{2}, n-3+\frac{n+1}{n-3}\} < n-1,$$

and hence $\mu_1(U_1(r,s;n)) < n-1$.
For the graph $U_2(r,s;n)$ of Fig 6.1. By Theorem 4.3.4,

$$\mu_1(U_2(r,s;n)) \leq \max\{s+1+\frac{n-1}{s+1}, r+3+\frac{n+1}{r+3}\}.$$

As $n-4 \geq 5 \geq 1$, then

$$s+1+\frac{n-1}{s+1} \leq \max\{2+\frac{n-1}{2}, n-3+\frac{n+1}{n-3}\} < n-1.$$

If $(0 \leq) r \leq n-6$, then

$$r+3+\frac{n+1}{r+3} \leq \max\{3+\frac{n+1}{3}, n-3+\frac{n+1}{n-3}\} < n-1.$$

Hence, for $n \geq 7$, $r \leq n-6$ and arbitrary s, $\mu_1(U_2(r,s;n)) \leq n-1$ and hence $\varphi_L(U_2(r,s;n)) < n-1$.
For the graph $U_3(r,s;n)$ of Fig 6.1. By Theorem 4.3.4,

$$\mu_1(U_3(r,s;n)) \leq \max\{r+2+\frac{n}{r+2}, s+2+\frac{n}{s+2}\} := \beta.$$

Note that $r \geq s$ and hence $(n-4)/2 \leq r \leq n-4$. If $r \leq n-5$, then

$$\mu_1(U_3(r,s;n)) \leq \beta \leq \max\{2+\frac{n}{2}, n-3+\frac{n}{n-3}\} < n-1.$$

and hence $\varphi_L(U_3(r,s;n)) < n-1$. By the above discussion, if G is a graph with maximal Laplacian spread among all unicyclic graphs of order $n \geq 7$, then G is among the graphs $U_1(n-3,0;n), U_1(n-4,1;n), U_2(n-5,1;n)$ and $U_3(n-4,0;n)$ with the Laplacian spread value $n-1$. The result follows. □

Lemma 6.2.2. *[12] For $n \geq 7$, $\varphi_L(U_1(n-4,1;n)) < \varphi_L(U_1(n-3,0;n)) = n-1$.*

Proof. Write $\mu_1(U_1(n-4,1;n))$, $\mu_{n-1}(U_1(n-4,1;n))$ as μ_1, μ_{n-1}, respectively. Use Lemma 6.1.1, the characteristic polynomial of $L(U_1(n-4,1;n))$ is $p(U_1(n-4,1;n)) = \lambda(\lambda-1)^{n-5}[\lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n]$. By Theorems 4.3.1, 4.3.8, $n > \mu_1 \geq n-1 \geq 6$, and by Theorem 4.3.9, $\mu_{n-1} < 1$. So μ_1, μ_{n-1} are both roots of the polynomial

$$f_1(\lambda) := \lambda^4-(n+5)\lambda^3+(6n+3)\lambda^2-(9n-5)\lambda+3n.$$

The derivative

$$f_1'(\lambda) := 4\lambda^3-3(n+5)\lambda^2+2(6n+3)\lambda-(9n-5),$$

And the second derivative

$$f_1''(\lambda) := 12\lambda^2-6(n+5)\lambda+2(6n+3).$$

Observe that $\mu_L(U_1(n-3,0;n)) - \mu_L(U_1(n-4,1;n)) = (n-\mu_1)-(1-\mu_{n-1})$. If we can show $n-\mu_1 > 1-\mu_{n-1}$, the result will follow. By the Mean Value Theorem, $f_1(n)-f_1(\mu_1) = (n-\mu_1)f_1'(\xi_1)$, for some $\xi_1 \in (\mu_1, n)$. As $f_1'(x)$ is positive and strictly increasing on the interval $(\mu_1, +\infty)$ and $\mu_1 < n$,

$$n-\mu_1 = \frac{f_1(n)-f_1(\mu_1)}{f_1'(\xi_1)} > \frac{n^3-6n^2+8n}{f_1'(n)} = \frac{n(n-2)(n-4)}{(n-1)(n^2-2n-5)} > \frac{n-4}{n-1}.$$

By the Lagrange Remainder Theorem,

$$f_1(\mu_{n-1}) = f_1(1)+f_1'(1)(\mu_{n-1}-1)+\frac{f_1''(\xi_2)}{2!}(\mu_{n-1}-1)^2,$$

for some $\xi_2 \in (\mu_{n-1}, 1)$. As $f_1'(1) = 0$, $f_1(1) = 4 - n$, and $f_1''(x)$ is positive and strictly decreasing on the open interval $(0, 1)$,

$$(1 - \mu_{n-1})^2 = \frac{2(n-4)}{f_1''(\xi_2)} < \frac{2(n-4)}{f_1''(1)} = \frac{n-4}{3(n-2)}.$$

If $n \geq 7$, $(n-4)/(n-1) > \sqrt{(n-4)/3(n-2)}$, and hence $n - \mu_1 > 1 - \mu_{n-1}$, the result follows. □

Lemma 6.2.3. *[12] For $n \geq 6$, $\varphi_L(U_2(n-5, 1; n)) < \varphi_L(U_1(n-3, 0; n)) = n - 1$.*

Proof. Write $\mu_1(U_2(n-5, 1; n))$, $\mu_{n-1}(U_2(n-5, 1; n))$ as μ_1, μ_{n-1}, respectively. Use Lemma 6.1.1, the characteristic polynomial of $L(U_2(n-5, 1; n))$ is $p(U_2(n-5, 1; n)) = \lambda(\lambda-1)^{n-5}[\lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n]$. By Theorems 4.3.1, 4.3.8, $n > \mu_1 \geq n-1 \geq 5$, and by Theorem 4.3.9, $\mu_{n-1} < 1$. So μ_1, μ_{n-1} are both roots of the polynomial

$$f_2(\lambda) := \lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n.$$

To show that $n - \mu_1 > 1 - \mu_{n-1}$. By the Mean Value Theorem,

$$n - \mu_1 = \frac{f_2(n) - f_2(\mu_1)}{f_2'(\xi_1)} > \frac{n^2 - 3n}{f_2'(n)} = 1 - \frac{2n-2}{n^2 - n - 2},$$

for some $\xi_1 \in (\mu_1, n)$, where the inequality holds as $\mu_1 < n$ and $f_2'(\lambda) = 3\lambda^2 - 2(n+2)\lambda + (3n-2)$ is positive and strictly increasing on $(\mu_1, +\infty)$. Note that the function $g(x) := (2x-2)/(x^2 - x - 2)$ is strictly decreasing on the whole real axis. Hence

$$(n - \mu_1) - (1 - \mu_{n-1}) > \mu_{n-1} - g(n) \geq \mu_{n-1} - g(6) = \mu_{n-1} - \frac{5}{14}.$$

In addition, $f_2(5/14) = -2535/2744 - 11n/196$. So $\mu_{n-1} > 5/14$, and the result follow. □

Lemma 6.2.4. *[12] For $n \geq 5$, $\varphi_L(U_3(n-4, 0; n)) < \varphi_L(U_1(n-3, 0; n)) = n - 1$.*

Proof. We simply write $\mu_1(U_3(n-4, 0; n))$, $\mu_{n-1}(U_3(n-4, 0; n))$ as μ_1, μ_{n-1}, respectively. Use Lemma 6.1.1, the characteristic polynomial of $L(U_3(n-4, 0; n))$ is

$p(U_3(n-4,0;n)) = \lambda(\lambda-1)^{n-5}(\lambda-3)[\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-2n]$. By Theorems 4.3.1, 4.3.8, $n > \mu_1 > n-1 \geq 4$, and by Theorem 4.3.9, $\mu_{n-1} < 1$. So μ_1, μ_{n-1} are both roots of the polynomial

$$f_3(\lambda) := \lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n.$$

By the Mean Value Theorem , for some $\xi_1 \in (\mu_1, n)$ and $\xi_2 \in (\mu_{n-1}, 1)$,

$$\begin{aligned} n - \mu_1 &= \frac{f_3(n) - f_3(\mu_1)}{f_3'(\xi_1)} > \frac{n^2-4n}{f_3'(\xi_1)}, \\ 1 - \mu_{n-1} &= \frac{f_3(1) - f_3(\mu_{n-1})}{f_3'(\xi_2)} = \frac{n-4}{f_3'(\xi_2)}. \end{aligned}$$

If we can show $n/f_3'(\xi_1) > 1/f_3'(\xi_2)$, the result will follow. Note that $f_3'(\lambda) = 3\lambda_2 - 2(n+3)\lambda + 4n - 2$. As $f_3'(\lambda)$ is positive and strictly decreasing on the interval $(0,1)$, and is positive and strictly increasing on $(\mu_1, +\infty)$. $nf_3'(\xi_2) > nf_3'(1) = 2(2n-5)$, $f_3'(\xi_1) < f_3'(n) = n^2 - 2n - 2$. Then $nf_3'(\xi_2) - f_3'(\xi_1) > n^2 - 3n - 2 > 0$. The result follows. □

By Lemmas 6.2.1 to 6.2.4 and Fig 6.2, we get the main result.

Theorem 6.2.5. *For $n \geq 4$, the graph $U_1(n-3,0;n)$ of Fig 6.1 is the unique graph with maximal Laplacian spread among all unicyclic graphs of order n.*

6.3 The minimal Laplacian spread

In this section, we characterize the unique unicyclic graph with minimal Laplacian spread among all connected unicyclic graphs of given order. By the definition of Laplacian spread and the property of the complement which from the proof of Theorem 4.3.1, it is clearly to check that

$$\varphi_L(G) = \mu_1(G) + \mu_1(\bar{G}) - n. \tag{6.3.1}$$

Lemma 6.3.1. *Let G be a graph of order n with minimal degree $\delta(G)$ and maximal degree $\Delta(G)$. Then*

$$\varphi_L(G) \geq \Delta(G) - \delta(G) + 1. \tag{6.3.2}$$

n=4

Graphs	Spread
•$U_1(1{,}0;4)$	•3
•$U_2(0{,}0;4)$	•2

n=5

Graphs	Spread
•$U_1(2{,}0;5)$	•4
•$U_1(1{,}1;5)$	•$\sqrt{13}$
•$U_2(0{,}1;5)$	•≈ 3.65128
•$U_3(1{,}0;5)$	•<4 by lemma 3.8

n=6

Graphs	Spread
•$U_1(3{,}0;6)$	•5
•$U_1(2{,}1;6)$	•≈4.47575
•$U_2(1{,}1;6)$	•<5by lemma3.7
•$U_2(0{,}2;6)$	•$\sqrt{17}$
•$U_3(1{,}1;6)$	•≈4.15653
•$U_3(2{,}0;6)$	•<5 by lemma3.8

Fig 6.2

Proof. By Theorem 4.3.8 and (6.3.1). The lemma follows. □

Lemma 6.3.2. *Let C_n be a cycle with n vertices. Then $\varphi_L(C_n) < 4$.*

Proof. Note that $\mu_1(C_n) \leq 4$ by Theorem 4.3.3 and the equality holds if and only if n is even. Thus we have $\varphi_L(C_n) \leq 4 - \mu_{n-1}(C_n) < 4$. The result follows. □

Theorem 6.3.3. *Let G be an unicyclic graph of order n with $\Delta(G) \geq 4$. Then*

$$\varphi_L(G) \geq 4 > \varphi_L(C_n).$$

Proof. Let G be a unicyclic (connected) graph with $\Delta(G) \geq 4$, then $\delta(G) = 1$. By Lemmas 6.3.1 and 6.3.2, we have $\varphi_L(G) \geq 4 - 1 + 1 = 4 > \varphi_L(C_n)$. The result follows. □

Now, we assume that G is unicyclic graph with $\Delta(G) = 3$. And by the interlacing property, we have the following lemmas.

Lemma 6.3.4. *For $e \notin E(G)$, the Laplacian eigenvalues of G and $G' = G + e$ interlace. i.e., $\mu_1(G') \geq \mu_1(G) \geq \mu_2(G') \geq \mu_2(G) \geq \ldots \geq \mu_n(G') = \mu_n(G) = 0$.*

Proof. It follows from Lemma 4.2.1. □

Remark 6.3.5. In Lemma 6.3.4, if v is a pendent vertex of G and e the pendent edge incident with v, then $\mu_1(G - v) = \mu_1(G - e) \leq \mu_1(G)$.

Lemma 6.3.6. *[14] Let G be a connected graph of order n. If v is a pendent vertex of G, then*

$$\mu_i(G) \leq \mu_{i-1}(G - v), 2 \leq i \leq n.$$

In Particular, $\mu_{n-1}(G) \leq \mu_{n-1}(G - v)$.

Proof. Let $e = uv$ be the pendent edge of G, then $G - e = G' \cup v$, where $G' = G - v$, so by Lemma 6.3.4, we have $\mu_i(G) \leq \mu_{i-1}(G - e) = \mu_{i-1}(G' \cup v) = \mu_{i-1}(G') = \mu_{i-1}(G - v)(2 \leq i \leq n)$. Particularly, $\mu_{n-1}(G) \leq \mu_{n-1}(G - v)$. □

Lemma 6.3.7. *Let G be an unicyclic graph of order n with $\Delta(G) = 3$. Then*

$$\varphi_L(G) \geq \varphi_L(G - v),$$

where v is a pendent vertex of G.

Proof. Let G be a unicyclic (connected) graph with $\Delta(G) = 3$, then $\delta(G) = 1$. Let v be a pendent vertex. By Lemmas 6.3.4 and 6.3.6 , we have $\mu_1(G) \geq \mu_1(G - v)$ and $\mu_{n-1}(G) \leq \mu_{n-1}(G-v)$. Hence $\varphi_L(G) = \mu_1(G) - \mu_{n-1}(G) \geq \mu_1(G-v) - \mu_{n-1}(G-v) = \varphi_L(G - v)$. □

Let $C_k + v$ be the cycle C_k added a pendent vertex v. By Lemma 6.3.7, we have the following theorem.

Theorem 6.3.8. *Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be k. Then $\varphi_L(G) \geq \varphi_L(C_k + v)$.*

Remark 6.3.9. Note that: $\mu_{n-1}(C_n) = 2(1 - \cos(2\pi/n))$. Then by the calculation, we have the following lemma.

Lemma 6.3.10. *The algebraic connectivity of C_n is a decreasing function on n.*

Lemma 6.3.11. *[15] Let G be a simple graph with at least one edge, then $\mu_1(G)$ is at least the maximal of*

$$\sqrt{\frac{d_i^2 + 2d_i - 2d_j - 2 + \sqrt{(d_i^2 + 2d_i + 2d_j + 4)^2 + 4(d_i - c_{ij} - 1)(d_j - c_{ij} - 1)}}{2}} \tag{6.3.3}$$

where the maximal is taken from all i, j with $v_iv_j \in E(G)$, d_i and d_j are are the vertex of degrees of v_i and v_j respectively, and c_{ij} is the cardinality of the set of common neighbors between v_i and v_j. □

Lemma 6.3.12. *[16] If $k \geq 61$, then $\varphi_L(C_k + v) \geq 4 > \varphi_L(C_n)$, where $n(n \geq 3)$ is an arbitrary positive integer.*

Proof. Let u be the neighbor of v and let w be another neighbor of u. Then $d_i = deg(u) = 3$ and $d_j = deg(w) = 2$. Note that $c_{ij} = 0$. By Lemma 6.3.11, the right hand side of (6.3.3) is equal to $\sqrt{(9+\sqrt{537})/2} > 4.0408$. By Lemmas 6.3.6 and 6.3.10 and direct calculation we have $\mu_{n-1}(C_k+v) \leq \mu_{n-1}(C_k) \leq \mu_{n-1}(C_{61}) \approx 0.0106$, for $k \geq 61$. Thus, we have $\varphi_L(C_k+v) > 4 > \varphi_L(C_n)$. □

Lemma 6.3.13. *[16] If $9 \leq k \leq 60$, then $\varphi_L(C_k+v) > 4 > \varphi_L(C_n)$, where $n (n \geq 3)$ is an arbitrary positive integer.*

Proof. If $24 \leq k \leq 60$, then $\mu_1(C_{24}+v) \approx 4.38298$ and $\mu_{n-1}(C_k+v) \leq \mu_{n-1}(C_{24}+v) \approx 0.06251$. Thus, $\varphi_L(C_k+v) \geq \varphi_L(C_{24}+v) \approx 4.38298-0.0625 = 4.32047 > 4 > \varphi_L(C_n)$. If $9 \leq k \leq 23$, then $\varphi_L(C_k+v) \geq \varphi_L(C_9+v) \approx 4.37720 - 0.34891 > 4 > \varphi_L(C_n)$. The lemma follows. □

By Theorem 6.3.8 and Lemmas 6.3.12, 6.3.13. We have the following corollary.

Corollary 6.3.14. *Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be k. If $k \geq 9$, then $\varphi_L(G) > \varphi_L(C_n)$.*

Lemma 6.3.15. *[16] Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be $k = 6, 7, 8$. Then $\varphi_L(G) > \varphi_L(C_n)$.*

Proof. When $k = 8$, we consider two cases according to the order of G.
Case1 : $k = 8$ and $n = 9$.
Then $G \cong C_8 + v$ and $\varphi_L(G) \approx 4.39276 - 0.41309 > 3.87939 - 0.46791 \approx \varphi_L(C_9)$.
Case2 : $k = 8$ and $n \geq 10$.
Let $C_8 = v_1v_2 \dots v_8v_1$ and let G have a subgraph $C_8 + v_1v$. Since $n \geq 10$ and $\Delta(G) = 3$, G has a subgraph obtained by adding a vertex u to $C_8 + v_1v$. There exist five such non-isomorphic graphs. The graph which attains the minimal Laplacian spread among these five graphs is $C_8 + v_1v + v_5u$. By gradually deleting pendent vertices from G, G can be transformed into $C_8 + v_1v + v_5u$. By Lemma 6.3.7, we have $\varphi_L(G) \geq \varphi_L(C_8 + v_1v + v_5u) \approx 4.15632 > \varphi_L(C_n)$. When $k = 6, 7$, similar to the case $k = 8$, then the result follows. □

Lemma 6.3.16. *[16] Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be $k = 5$. Then $\varphi_L(G) > \varphi_L(C_n)$.*

Proof. If $n = 6$, then $G \cong C_5 + v$ for some v. Thus, we have $\varphi_L(G) \approx 4.30278 - 0.69722 > 3 = \varphi_L(C_6)$. When $n \geq 7$, let $C_5 = v_1v_2 \ldots v_5v_1$ and v be a vertex adjacent to v_1. Then $C_5 + v_1$ is a subgraph of G. Note that $n \geq 7$ and $\Delta(G) = 3$. A new vertex u may be adjacent to v, v_2, v_3, v_4, or v_5. We consider the following two case:
Case1 : u is not adjacent to v_3.
By computation, the minimal Laplacian spread value of $C_5 + v_1v + xu$, for $x \in \{v, v_2, v_4, v_5\}$ is attained when $x = v_2$ or v_5. By Lemma 6.3.7, we have $\varphi_L(G) \geq \varphi_L(C_5 + v_1v + v_2u) \approx 4.65109 - 0.62280 > 4 > \varphi_L(C_n)$.
Case2 : u is adjacent to v_3.
Subcase2.1. $n = 7$, then $G \cong C_5 + v_1v + v_3u$ and $\varphi_L(G) \approx 4.41421 - 0.51881 = 3.8954 > 3.04892 \approx \varphi_L(C_7)$.
Subcase2.2. $n \geq 8$, by computation, the minimal Laplacian spread value of $C_5+v_1v+v_3u + xy$, for $y \in \{v, v_2, u, v_4, v_5\}$ is attained when $y = v$ or u. By Lemma 6.3.7, we have $\varphi_L(G) \geq \varphi_L(C_5+v_1v+v_3u+xv) \approx 4.48119-0.32487 > 4 > \varphi_L(C_n)$. Thus this lemma follows. □

Lemma 6.3.17. *[16] Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be $k = 4$. Then $\varphi_L(G) > \varphi_L(C_n)$.*

Proof. Case1 : $n = 5$. Then $G \cong C_4 + v$ for some v and $\varphi_L(G) \approx 4.48119-0.82991 = 3.65128 > 2.36606 \approx \varphi_L(C_5)$.
Case2 : $n \geq 6$. Let $C_4 = v_1v_2 \ldots v_4v_1$ and v be a vertex adjacent to v_1. Then G contains the subgraph $C_4 + v_1v$. Since $n \geq 6$ and $\Delta(G) = 3$. A new vertex u may be adjacent to v, v_2, v_3, or v_4. By direct computation, the subgraph which attains the minimal Laplacian spread is $C_4 + v_1v + vu$, where the value is $\varphi_L(C_4 + v_1v + vu) \approx 4.56155 - 0.43845 > 4 > \varphi_L(C_n)$. By deleting pendent vertices from G, G can be transformed into C_4+v_1v+vu. Then by Lemma 6.3.7, $\varphi_L(G) \geq \varphi_L(C_4+v_1v+vu) > 4 > \varphi_L(C_n)$. □

Lemma 6.3.18. *[16] Let G be an unicyclic graph of order n with $\Delta(G) = 3$ and the length of the cycle be $k = 3$. Then $\varphi_L(G) > \varphi_L(C_n)$.*

Proof. If $n = 4$, then $G \cong C_3 + v$ for some v. Hence $\varphi_L(G) = 4-1 = 3 > 2 = \varphi_L(C_4)$. Let $C_3 = v_1v_2 \dots v_3v_1$ and v be a vertex adjacent to v_1. Then $C_3 + v_1v$ is a subgraph. If $n \geq 5$, a new vertex u may be adjacent to v_2, v_3, or v. According to the vertex induced subgraphs of G, we have

Case1 : $C_3 + v_1v + v_2u$ is a subgraph of G. Let $G_1 \cong C_3 + v_1v + v_2u$, $G_2 \cong C_3 + v_1v + v_2u + vx \cong C_3 + v_1v + v_2u + ux$, $G_3 \cong C_3 + v_1v + v_2u + v_3x$, for some x. If $n = 5$, then $G \cong G_1$ and $\varphi_L(G) \approx 4.30278 - 0.69722 = 3.60556 > 2.23606 \approx \varphi_L(C_5)$. If $n = 6$, then $G \cong G_i (i = 2, 3)$. By calculation, $\varphi_L(G_i) > \varphi_L(C_6) = 3$. Suppose $n \geq 7$. By direct computation, the minimal Laplacian spread value among all 7-vertex unicyclic graphs containing $C_3+v_1v+v_2u$ is $\varphi_L(C_3+v_1v+v_2u+vx+v_3y) \approx 4.0322424 > \varphi_L(C_n)$, for some x and y. By Lemma 6.3.7, we have $\varphi_L(G) \geq \varphi_L(C_3+v_1v+v_2u+vx+v_3y) \approx 4.0322424 > 4 > \varphi_L(C_n)$.

Case2 : $C_3 + v_1v + v_3u$ is a subgraph of G. Since v_2 and v_3 are symmetric in $C_3 + v_1v$, this case is similar to Case1.

Case3 : $C_3 + v_1v + vu$ is a subgraph of G. Let $G_4 \cong C_3 + v_1v + vu$, $G_5 \cong C_3 + v_1v + vu + ux$, $G_6 \cong C_3 + v_1v + vu + vx$, $G_7 \cong C_3 + v_1v + vu + v_2x \cong C_3 + v_1v + vu + v_3x$, for some x. If $n = 5$, then $G \cong G_4$ and $\varphi_L(G) \approx 3.65128 > 2.23606 \approx \varphi_L(C_5)$. If $n = 6$, then $G \cong G_j (j = 5, 6, 7)$. By calculation, we have $\varphi_L(G_j) > \varphi_L(C_5)$. When $n \geq 7$, similar to Case1 the graph $C_3 + v_1v + vu + ux + xy$ for some x and y attains the minimal Laplacian spread value among all 7-vertex unicyclic graphs containing $C_3 + v_1v + vu$. By Lemma 6.3.7, we have $\varphi_L(G) \geq \varphi_L(C_3 + v_1v + vu + ux + xy) \approx 4.22833 - 0.22538 > 4 > \varphi_L(C_n)$. All possible cases are exhausted, and the proof of lemma is complete. □

By Corollary 6.3.14 and Lemmas 6.3.15 to 6.3.18 , we have the following theorem.

Theorem 6.3.19. *Let G be a unicyclic graph with $\Delta(G) = 3$. Then $\varphi_L(G) > \varphi_L(C_n)$.*

Combining Theorems 6.2.5, 6.3.19, we arrive at the main result.

Theorem 6.3.20. *Let G be a unicyclic graph of order n. Then $\varphi_L(G) \geq \varphi_L(C_n)$ and the equality holds if and only if $G \cong C_n$.*

7

The Laplacian Spread of bicyclic graphs

In this chapter, we work on the Laplacian spread of graphs, and prove that there exist exactly two bicyclic graphs with maximal Laplacian spread among all bicyclic graphs of fixed order, which are obtained from a star by adding two incident edges and by adding two non-incident edges between the pendent vertices of the star, respectively.

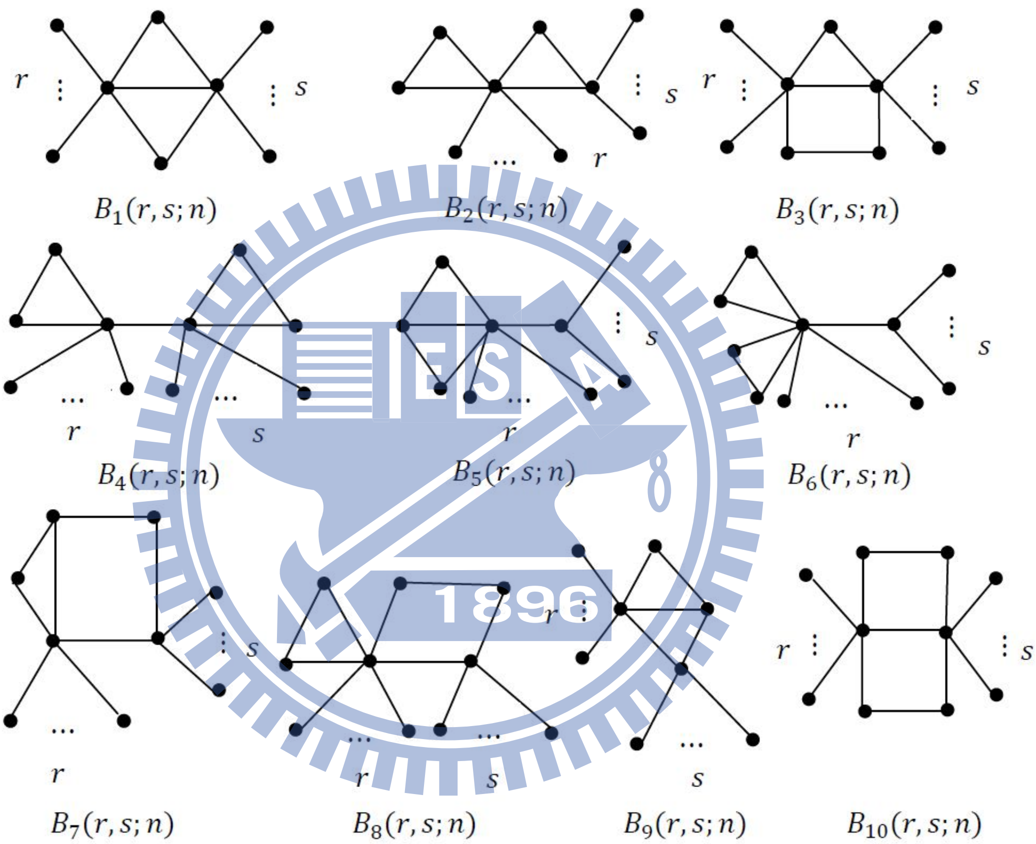
7.1 The maximal Laplacian spread

Lemma 7.1.1. *Let G be a graph $B_1(n-4,0;n)$ or $B_2(n-5,0;n)$. Then $\varphi_L(B_1(n-4,0;n)) = \varphi_L(B_2(n-5,0;n)) = n-1$.*

Proof. By Theorems 4.3.8 and 4.3.9, we can get the result easily. □

In the following, we will prove that the graph $B_1(n-4,0;n)$ and $B_2(n-5,0;n)$ are the only two bicyclic ones with maximal Laplacian spread. We first narrow down the possibility of the bicyclic graphs with maximal Laplacian spread.

Lemma 7.1.2. *[17] Let G be a graph with maximal Laplacian spread among all bicyclic graphs of order $n \geq 9$. Then G is among the graphs $B_1(n-4,0;n), B_1(n-$*



r
s
$B_1(r,s;n)$
s
r
$B_2(r,s;n)$
r
s
$B_3(r,s;n)$
r
s
$B_4(r,s;n)$
s
r
$B_5(r,s;n)$
s
r
$B_6(r,s;n)$
s
r
$B_7(r,s;n)$
r
s
$B_8(r,s;n)$
r
s
$B_9(r,s;n)$
r
s
$B_{10}(r,s;n)$

Fig 7.1.

$5, 1; n), B_2(n-5, 0; n), B_2(n-6, 1; n), B_3(n-5, 0; n), B_5(n-6, 1; n), B_6(n-7, 1; n), B_8(n-$ $6, 0; n), B_9(n-5, 1; n), B_9(0, n-4; n)$.

Proof. Let v_iv_j be an edge of G. Then

$$d(v_i) + d(v_j) - |N(v_i) \cap N(v_j)| = |N(v_i) \cup N(v_j)| \leq n,$$

with equality holding if and only if G is one graph in B_1 to B_{10} for some r or s. Therefore, if G is not a graph in B_1 B_{10}, then by Theorem 4.3.6, $\mu_1(G) \leq n-1$ and hence $\varphi_L(G) < n-1$, as $\mu_{n-1}(G) > 0$. However, by Theorem 4.3.9, $\varphi_L(B_1(n-4, 0; n)) = \varphi_L(B_2(n-5, 0; n)) = n-1$. So G must be one graph in B_1 B_{10}. For the graph $B_1(r, s; n)$ in Fig 7.1 with $0 \leq s \leq r \leq n-4$, by Theorem 4.3.4,

$$\mu_1(B_1(r, s; n)) \leq \max\{r + 3 + \frac{n+3}{r+3}, s + 3 + \frac{n+3}{s+3}\} := \alpha.$$

Note that $r + 3 \geq \frac{n-4}{2} + 3 > \sqrt{n+3}$. If $r \leq n-6$ and $n \geq 9$, then

$$\mu_1(B_1(r, s; n)) \leq \alpha \leq \max\{3 + \frac{n+3}{3}, n - 3 + \frac{n+3}{n-3}\} \leq n-1.$$

Hence, if $n \geq 9$ and $r \leq n-6$, then $\varphi_L(B_1(r, s; n)) < n-1$, as $\mu_{n-1}(G) > 0$.
For the graph $B_2(r, s; n)$ in Fig 7.1 with $0 \leq s, r \leq n-5$, by Theorem 4.3.4,

$$\mu_1(B_2(r, s; n)) \leq \max\{s + 2 + \frac{n+1}{s+2}, r + 4 + \frac{n+3}{r+4}\}.$$

For $n \geq 9$ and $r \leq n-7$, and an arbitrary s,

$$\begin{aligned} s + 2 + \frac{n+1}{s+2} &\leq \max\{2 + \frac{n+1}{2}, n - 3 + \frac{n+1}{n-3}\} \leq n-1, \\ r + 4 + \frac{n+3}{r+4} &\leq \max\{4 + \frac{n+3}{4}, n - 3 + \frac{n+3}{n-3}\} \leq n-1. \end{aligned}$$

Hence $\mu_1(B_2(r, s; n)) \leq n-1$, $\varphi_L(B_2(r, s; n)) < n-1$.
For the graph $B_3(r, s; n)$ in Fig 7.1 with $0 \leq s, r \leq n-5$, by Theorem 4.3.4,

$$\mu_1(B_3(r, s; n)) \leq \max\{r + 3 + \frac{n+2}{r+3}, s + 3 + \frac{n+2}{s+3}\}.$$

For $n \geq 8$ and $r \leq n-6$,

$$\mu_1(B_3(r, s; n)) \leq \max\{3 + \frac{n+2}{3}, n - 3 + \frac{n+2}{n-3}\} \leq n-1.$$

Hence $\varphi_L(B_3(r,s;n)) < n-1$.

For the graph $B_4(r,s;n)$ in Fig 7.1 with $0 \le s \le r \le n-6$, by Theorem 4.3.4,

$$\mu_1(B_4(r,s;n)) \le \max\{r+3+\frac{n+1}{r+3}, s+3+\frac{n+1}{s+3}\}.$$

For $n \ge 7$ and an arbitrary r, s,

$$\mu_1(B_4(r,s;n)) \le \max\{3+\frac{n+1}{3}, n-3+\frac{n+1}{n-3}\} \le n-1.$$

Hence $\varphi_L(B_4(r,s;n)) < n-1$.

For the graph $B_5(r,s;n)$ in Fig 7.1 with $1 \le s \le n-5$, $0 \le r \le n-6$ by Theorem 4.3.4,

$$\mu_1(B_5(r,s;n)) \le \max\{s+1+\frac{n-1}{s+1}, r+4+\frac{n+3}{r+4}\}.$$

For $n \ge 9$ and $r \le n-7$, and an arbitrary s,

$$\begin{aligned} s+1+\frac{n-1}{s+1} &\le \max\{2+\frac{n-1}{2}, n-4+\frac{n-1}{n-4}\} \le n-1, \\ r+4+\frac{n+3}{r+4} &\le \max\{4+\frac{n+3}{4}, n-3+\frac{n+3}{n-3}\} \le n-1. \end{aligned}$$

Hence $\varphi_L(B_5(r,s;n)) < n-1$.

For the graph $B_6(r,s;n)$ in Fig 7.1 with $1 \le s \le n-6$, $0 \le r \le n-7$ by Theorem 4.3.4,

$$\mu_1(B_6(r,s;n)) \le \max\{s+1+\frac{n-1}{s+1}, r+5+\frac{n+3}{r+5}\}.$$

For $n \ge 9$ and $r \le n-8$, and an arbitrary s,

$$\begin{aligned} s+1+\frac{n-1}{s+1} &\le \max\{2+\frac{n-1}{2}, n-5+\frac{n-1}{n-5}\} \le n-1, \\ r+5+\frac{n+3}{r+5} &\le \max\{5+\frac{n+3}{5}, n-3+\frac{n+3}{n-3}\} \le n-1. \end{aligned}$$

Hence $\varphi_L(B_6(r,s;n)) < n-1$.

For the graph $B_7(r,s;n)$ in Fig 7.1 with $1 \le s \le n-5$, $0 \le r \le n-6$ by Theorem 4.3.4,

$$\mu_1(B_7(r,s;n)) \le \max\{s+2+\frac{n}{s+2}, r+3+\frac{n+2}{r+3}\}.$$

For $n \geq 8$ and arbitrary r, s,

$$\begin{aligned} s+2+\frac{n}{s+2} &\leq \max\{3+\frac{n}{3}, n-3+\frac{n}{n-3}\} \leq n-1, \\ r+3+\frac{n+2}{r+3} &\leq \max\{3+\frac{n}{3}, n-3+\frac{n+2}{n-3}\} \leq n-1. \end{aligned}$$

Hence $\varphi_L(B_7(r,s;n)) < n-1$.

For the graph $B_8(r,s;n)$ in Fig 7.1 with $0 \leq s, r \leq n-6$, by Theorem 4.3.4,

$$\mu_1(B_8(r,s;n)) \leq \max\{s+2+\frac{n}{s+2}, r+4+\frac{n+2}{r+4}\}.$$

For $n \geq 8$ and $r \leq n-7$, and an arbitrary s,

$$\begin{aligned} s+2+\frac{n}{s+2} &\leq \max\{2+\frac{n}{2}, n-4+\frac{n}{n-4}\} \leq n-1, \\ r+4+\frac{n+2}{r+4} &\leq \max\{4+\frac{n}{4}, n-3+\frac{n+2}{n-3}\} \leq n-1. \end{aligned}$$

Hence $\varphi_L(B_8(r,s;n)) < n-1$.

For the graph $B_9(r,s;n)$ in Fig 7.1 with $0 \leq r \leq n-5, 1 \leq s \leq n-4$, by Theorem 4.3.4,

$$\mu_1(B_9(r,s;n)) \leq \max\{r+3+\frac{n+3}{r+3}, s+2+\frac{n+2}{s+2}\}.$$

For $n \geq 9$ and $r \leq n-6$, and $s \leq n-5$,

$$\begin{aligned} r+3+\frac{n+3}{r+3} &\leq \max\{3+\frac{n}{3}, n-3+\frac{n+3}{n-3}\} \leq n-1, \\ s+2+\frac{n+2}{s+2} &\leq \max\{3+\frac{n}{3}, n-3+\frac{n+2}{n-3}\} \leq n-1. \end{aligned}$$

Hence $\varphi_L(B_9(r,s;n)) < n-1$.

For the graph $B_{10}(r,s;n)$ in Fig 7.1 with $0 \leq s \leq r \leq n-6$, by Theorem 4.3.4,

$$\mu_1(B_{10}(r,s;n)) \leq \max\{r+3+\frac{n+1}{r+3}, s+3+\frac{n+1}{s+3}\}.$$

For $n \geq 7$ and arbitrary r, s,

$$\mu_1(B_{10}(r,s;n)) \leq \max\{3+\frac{n+1}{3}, n-3+\frac{n+1}{n-3}\} \leq n-1.$$

Hence $\varphi_L(B_{10}(r,s;n)) < n-1$.

By the above discussion, if G is one with maximal Laplacian spread of all bicyclic graphs of order $n \geq 9$, then G is among the graphs $B_1(n-4,0;n)$, $B_1(n-5,1;n)$, $B_2(n-5,0;n)$, $B_2(n-6,1;n)$, $B_3(n-5,0;n)$, $B_5(n-6,1;n)$, $B_6(n-7,1;n)$, $B_8(n-6,0;n)$, $B_9(n-5,1;n)$, $B_9(0,n-4;n)$. The result follows. □

Next, we show that except the graph $B_1(n-4,0;n)$ and $B_2(n-5,0;n)$, the Laplacian spreads of the other graph in Lemma 7.1.2 are all less than $n-1$ for a suitable n. Thus by a little computation in Fig 7.1 of small order $B_1(n-4,0;n)$ and $B_2(n-5,0;n)$ are proved to be the only two bicyclic graphs with maximal Laplacian spread among all bicyclic graphs of order $n \geq 5$. In the following Lemmas 7.1.3 to 7.1.10, for convenience we simply write $\mu_1(B_i(r,s;n)), \mu_{n-1}(B_i(r,s;n))$, for $1 \leq i \leq 10$, as μ_1, μ_{n-1}, respectively, if no confusions occur.

Lemma 7.1.3. *[17] For $n \geq 7$, $\varphi_L(B_1(n-5,1;n)) < n-1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_1(n-5,1;n)) = \lambda(\lambda-1)^{n-6}(\lambda-2)[\lambda^4-(n+6)\lambda^3+(7n+4)\lambda^2-(11n-6)\lambda+4n]$. By Theorems 4.3.1 and 4.3.8, $n > \mu_1 > n-1 \geq 6$, and by Theorem 4.3.9, $\mu_{n-1} < 1$. So μ_1, μ_{n-1} are both the roots of the following polynomial:

$$f_1(\lambda) := \lambda^4-(n+6)\lambda^3+(7n+4)\lambda^2-(11n-6)\lambda+4n,$$

with the derivative

$$f_1'(\lambda) := 4\lambda^3-3(n+6)\lambda^2+2(7n+4)\lambda-(11n-6),$$

and the second derivative

$$f_1''(\lambda) := 12\lambda^2-6(n+6)\lambda+2(7n+4).$$

Observe that $(n-1)-\varphi_L(B_1(n-5,1;n)) = (n-\mu_1)-(1-\mu_{n-1})$. If we can show that $n-\mu_1 > 1-\mu_{n-1}$, the result will follow. By Lagrange Mean Value Theorem, $f_1(n)-f_1(\mu_1) = (n-\mu_1)f_1'(\xi_1)$, for some $\xi_1 \in (\mu_1, n)$. As $f_1(x)$ is positive and strictly increasing on the interval $(\mu_1, +\infty)$ and $\mu_1 < n$, $n - \mu_1 = (f_1(n) - f_1(\mu_1))/f_1'(\xi_1) > (n^3 - 7n^2 + 10n)/f_1'(n) = n(n-2)(n-5)/(n-1)(n^2-3n-6) > (n-5)/(n-1)$. By Lagrange Remainder Theorem,

$$f_1(\mu_{n-1}) = f_1(1) + f_1'(1)(\mu_{n-1} - 1) + \frac{f_1''(\xi_2)}{2!}(\mu_{n-1} - 1)^2,$$

for some $\xi_2 \in (\mu_{n-1}, 1)$. As $f_1'(1) = 0$ and $f_1''(x)$ is positive and strictly decreasing on the open interval $(0,1)$, $(1-\mu_{n-1})^2 = 2(n-5)/f_1''(\xi_2) < 2(n-5)/f_1''(1) = (n-5)/4(n-2)$. If $n \geq 7$, $(n-5)/(n-1) > \sqrt{(n-5)/4(n-2)}$, and hence $n - \mu_1 > 1 - \mu_{n-1}$. □

Lemma 7.1.4. *[17] For $n \geq 7$, $\varphi_L(B_2(n-6,1;n)) < n-1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_2(n-6,1;n)) = \lambda(\lambda-1)^{n-6}(\lambda-3)[\lambda^4 - (n+5)\lambda^3 + (6n+3)\lambda^2 - (9n-5)\lambda + 3n]$. By a similar discussion to the proof of Lemma 7.1.3, both μ_1 and μ_{n-1} are the roots of the polynomial:

$$\begin{aligned} f_2(\lambda) &= \lambda^4 - (n+5)\lambda^3 + (6n+3)\lambda^2 - (9n-5)\lambda + 3n, \\ f_2'(\lambda) &= 4\lambda^3 - 3(n+5)\lambda^2 + 2(6n+3)\lambda - (9n-5), \\ f_2''(\lambda) &= 12\lambda^2 - 6(n+5)\lambda + 2(6n+3). \end{aligned}$$

And

$$n - \mu_1 = \frac{f_2(n) - f_2(\mu_1)}{f_2'(\xi_1)} > \frac{n^3 - 6n^2 + 8n}{f_2'(n)} = \frac{n(n-2)(n-4)}{(n-1)(n^2-2n-5)} > \frac{n-4}{n-1},$$

for some $\xi_1 \in (\mu_1, n)$. In addition, $f_2(\mu_{n-1}) = f_2(1) + f_2'(1)(\mu_{n-1} - 1) + f_2''(\xi_2)(\mu_{n-1} - 1)^2/2!$, for some $\xi_2 \in (\mu_{n-1}, 1)$. Note that $f_2'(1) = 0$, we have $(\mu_{n-1} - 1)^2 = 2(n-4)/f_2''(\xi_2) < 2(n-4)/f_2''(1) = (n-4)/3(n-2)$. If $n \leq 7$, $(n-4)/(n-1) > \sqrt{(n-4)/3(n-2)}$, and hence $n - \mu_1 > 1 - \mu_{n-1}$. The result follows . □

Lemma 7.1.5. *[17] For $n \geq 6$, $\varphi_L(B_3(n-5,0;n)) < n-1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_3(n-5,0;n)) = \lambda(\lambda-1)^{n-6}[\lambda^5 - (n+8)\lambda^4 + (9n+18)\lambda^3 - 3(9n+2)\lambda^2 + (31n-10)\lambda - 11n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_3(\lambda) = \lambda^5 - (n+8)\lambda^4 + (9n+18)\lambda^3 - 3(9n+2)\lambda^2 + (31n-10)\lambda - 11n,$$

and

$$n - \mu_1 = \frac{f_3(n) - f_3(\mu_1)}{f_3'(\xi_1)} > \frac{n^4 - 9n^3 + 25n^2 - 21n}{f_3'(n)} = 1 - \frac{4n^3 - 25n^2 + 40n - 10}{n^4 - 5n^3 + 19n - 10},$$

for some $\xi_1 \in (\mu_1, n)$. Note that the function

$$g_1(x) := \frac{4x^3 - 25x^2 + 40x - 10}{x^4 - 5x^3 + 19x - 10},$$

is strictly decreasing for $x \geq 6$. Hence $(n - \mu_1) - (1 - \mu_{n-1}) = \mu_{n-1} - g_1(n) > \mu_{n-1} - g_1(6) = \mu_{n-1} - 97/160$. Observe that a star of order n has eigenvalues : $0^1, n^1, 1^{n-2}$ and hence has $(n-1)$ eigenvalues not less than 1. As $B_3(n-5, 0; n)$ contains a star of order $n-1$, by Eigenvalues Interlacing Theorem (that is, $\lambda_i(G) \geq \lambda_i(G-e)$ for $i = 1, 2, \ldots, n$. If we delete an edge e from a graph of order n, $G_3(n-5, 0; n)$ has $(n-2)$ eigenvalues not less than 1. Now $f_3(97/160) \approx -5.2557 - 0.2595n < 0$. So $\mu_{n-1} > 97/160$; otherwise $\mu_{n-2} < \frac{97}{160} < 1$, a contradiction. The result follows . □

Lemma 7.1.6. *[17] For $n \geq 6$, $\varphi_L(B_5(n-6, 1; n)) < n - 1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_5(n-6, 1; n)) = \lambda(\lambda - 1)^{n-6}(\lambda - 2)(\lambda - 4)[\lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_4(\lambda) = \lambda^3 - (n+2)\lambda^2 + (3n-2)\lambda - n,$$

By Lagrange Mean Value Theorem,

$$n - \mu_1 = \frac{f_4(n) - f_4(\mu_1)}{f_4'(\xi_1)} > \frac{n^2 - 3n}{f_4'(n)} = 1 - \frac{2n - 2}{n^2 - n - 2},$$

for some $\xi_1 \in (\mu_1, n)$. Note that the function $g_2(x) := (2x-2)/(x^2 - x - 2)$ is strictly decreasing for all x. Hence $(n - \mu_1) - (1 - \mu_{n-1}) > \mu_{n-1} - g_2(n) \geq \mu_{n-1} - g_2(6) = \mu_{n-1} - 5/14$. By a similar discussion to those in the last paragraph of the proof of Lemma 7.1.5. As $f_4(5/14) = -(2535/2744) - (11n/196) < 0$, $\mu_{n-1} > 5/14$, and the result follows. □

Lemma 7.1.7. *[17] For $n \geq 7$, $\varphi_L(B_6(n-7, 1; n)) < n - 1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_6(n-7,1;n)) = \lambda(\lambda-1)^{n-6}(\lambda-2)(\lambda-3)[\lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_4(\lambda) = \lambda^3-(n+2)\lambda^2+(3n-2)\lambda-n,$$

which is the same as $f_4(\lambda)$ in the proof of Lemma 7.1.6. Hence, for $n \geq 7$, $n-\mu_1 > 1-\mu_{n-1}$. The result follows . □

Lemma 7.1.8. *[17] For $n \geq 6$, $\varphi_L(B_8(n-6,0;n)) < n-1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_8(n-6,0;n)) = \lambda(\lambda-1)^{n-6}(\lambda-2)(\lambda-3)[\lambda^3-(n+3)\lambda^2+(4n-2)\lambda-n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_5(\lambda) = \lambda^3-(n+3)\lambda^2+(4n-2)\lambda-n,$$

By Lagrange Mean Value Theorem,

$$\begin{aligned} n-\mu_1 &= \frac{f_5(n)-f_5(\mu_1)}{f_5'(\xi_1)} > \frac{n^2-4n}{f_5'(\xi_1)}, \\ 1-\mu_{n-1} &= \frac{f_5(1)-f_5(\mu_{n-1})}{f_5'(\xi_2)} = \frac{n-4}{f_5'(\xi_2)} \end{aligned}$$

for some $\xi_1 \in (\mu_1, n)$ and $\xi_2 \in (\mu_{n-1}, 1)$. If we can show $n/f_5'(\xi_1) > 1/f_5'(\xi_2)$, the result will follow. Note that $f_5'(\lambda) = 3\lambda^2-2(n+3)\lambda+4n-2$. As $f_5'(\lambda)$ is positive and strictly decreasing on the interval $(0,1)$, and is positive and strictly increasing on the interval $(\mu_1,+\infty)$. $nf_5'(\xi_2) > nf_5'(1) = n(2n-5)$. $f_5'(\xi_1) < f_5'(n) = n^2-2n-2$. Then $nf_5'(\xi_2)-f_5'(\xi_1) > n^2-3n+2 > 0$. The result follows. □

Lemma 7.1.9. *[17] For $n \geq 6$, $\varphi_L(B_9(n-5,1;n)) < n-1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_9(n-5,1;n)) = \lambda(\lambda-1)^{n-6}[\lambda^5-(n+8)\lambda^4+(9n+17)\lambda^3-(26n+2)\lambda^2+(27n-13)\lambda-8n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_6(\lambda) = \lambda^5-(n+8)\lambda^4+(9n+17)\lambda^3-(26n+2)\lambda^2+(27n-13)\lambda-8n,$$

And

$$n - \mu_1 = \frac{f_6(n) - f_6(\mu_1)}{f_6'(\xi_1)} > \frac{n^4 - 9n^3 + 25n^2 - 21n}{f_6'(n)} = 1 - \frac{4n^3 - 26n^2 + 44n - 13}{n^4 - 5n^3 - n^2 + 23n - 13}.$$

Note that the function

$$g_3(x) := \frac{4x^3 - 26x^2 + 44x - 13}{x^4 - 5x^3 - x^2 + 23x - 13}.$$

is strictly decreasing for $x \geq 6$, we have $(n - \mu_1) - (1 - \mu_{n-1}) \geq \mu_{n-1} - g_3(6) = \mu_{n-1} - 179/305$. As $f(179/305) \approx -5.17633 - 0.405628n < 0$, $\mu_{n-1} > 179/305$. The result follows. □

Lemma 7.1.10. *[17] For $n \geq 5$, $\varphi_L(B_{10}(0, n-4; n)) < n - 1$.*

Proof. Use Lemma 6.1.1, the characteristic polynomial $p(B_{10}(0, n-4; n)) = \lambda(\lambda - 1)^{n-5}(\lambda - 4)[\lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n]$. So μ_1 and μ_{n-1} are the roots of the polynomial:

$$f_7(\lambda) = \lambda^3 - (n+3)\lambda^2 + (4n-2)\lambda - 2n,$$

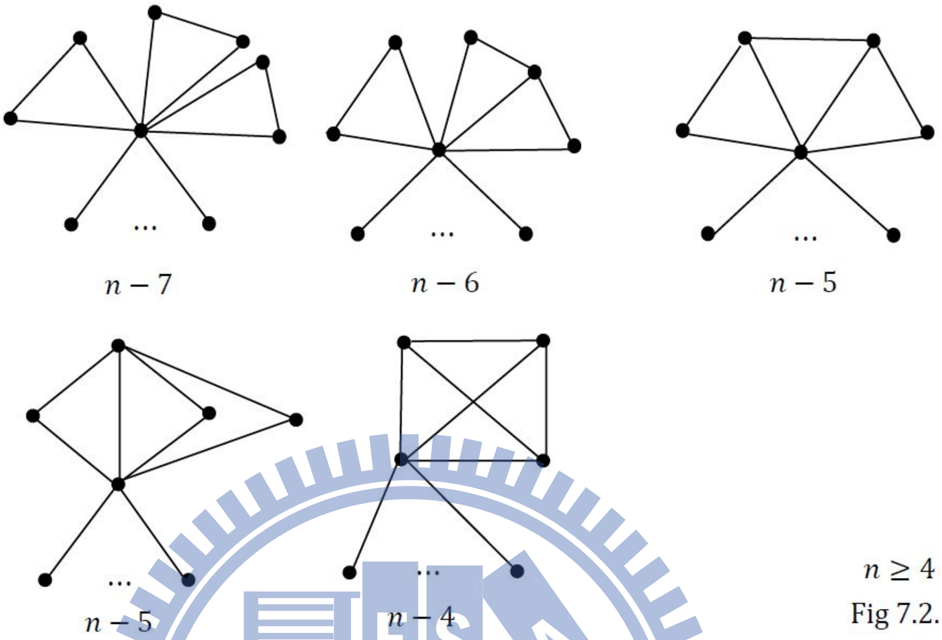
And

$$n - \mu_1 = \frac{f_7(n) - f_7(\mu_1)}{f_7'(\xi_1)} > \frac{f_7(n)}{f_7'(\xi_1)} = 1 - \frac{2n - 2}{n^2 - 2n - 2}.$$

Denote $g_4(x) := (2x - 2)/(x^2 - 2x - 2)$. Then we have $(n - \mu_1) - (1 - \mu_{n-1}) \geq \mu_{n-1} - g_4(6) = \mu_{n-1} - 5/11$. Noting that $f_7(5/11) = -(1910/1331) - (47n/121) < 0$. We have $\mu_{n-1} > 5/11$. The result follows . □

Let G be one with maximal Laplacian spread of all bicyclic graphs of order $n \geq 5$. From the first paragraph of the proof of Lemma 7.1.2, the graph G is necessarily among graphs in Fig 7.1. If the order $n \geq 9$, by Lemmas 7.1.2 to 7.1.10, G is the graph $B_1(n-4, 0; n)$ or $B_2(n-5, 0; n)$. For the order $n \geq 8$, the graph(s) with maximal Laplacian spread are among the graphs in Fig 7.1, and can be identified by a little computation, or by lemmas of this chapter.

Theorem 7.1.11. *For $n \geq 5$, $B_1(n-4, 0; n)$ and $B_2(n-5, 0; n)$ in Fig 7.1 are the only two graphs with maximal Laplacian spread among all bicyclic graphs of order n.*



$n \geq 4$
Fig 7.2.

7.2 Concluding Remarks

Remark 7.2.1. A tricyclic graph is connected graph in which the number of edges equals the number of vertices plus two. In the unicyclic and bicyclic cases, the maximal Laplacian spread are obtained from a star by adding edges. By the same ways, with the Theorems 4.3.1, 4.3.4, 4.3.6 and 4.3.9. We have the five graphs, with the maximal Laplacian spread is equal to $n-1$. [18]

Remark 7.2.2. It seems likely that the graphs which share the maximal Laplacian spread among all connected graphs of order n are the graph G with the induced subgraph $K_{1,n-1}$, and with the maximal value $n-1$.

Conjecture 7.2.3. Let G be a graph of order n, then $\varphi_L(G) = n-1$ only if $K_{1,n-1}$ is a subgraph of G.

8

The Signless Laplacian Spread

Research on signless Laplacian matrices has become popular recently. The signless Laplacian matrix $Q(G) = D(G) + A(G)$ is symmetric and nonnegative, and, when G is connected, it's irreducible. If N is the $n \times e$ vertex-edge incidence matrix of the (n, e) graph G, then $Q(G) = NN^T$. Thus $Q(G)$ is positive semi-definite and its eigenvalues can be arranged as: $\rho_1(G) \geq \rho_2(G) \geq \ldots \geq \rho_n(G) \geq 0$. Motivated by the definition of $\varphi_L(G)$, we define the signless Laplacian spread of the graph G, denoted by $\varphi_Q(G)$, as $\varphi_Q(G) = \rho_1(G) - \rho_n(G)$.

8.1 The bipartite graph case

We show in this section that when G is bipartite, $\varphi_Q(G) = \varphi_L(G) = \rho_1(G)$.

Proposition 8.1.1. *[19] If G is connected, then $\rho_n(G) = 0$ if and only if G is bipartite. Moreover, if G is bipartite, then $Q(G)$ and $L(G)$ share the same eigenvalues.*

Proof. Let $x^T = (x_1, x_2, \ldots, x_n)$. For a non-zero vector x we have $Qx = 0$ if and only if $N^T x = 0$, where N is the vertex-edge incidence matrix of a graph G. The later holds if and only if $x_i = -x_j$ for every edge, i.e. if and only if G is bipartite. Since the graph is connected, x is determined up to a scalar multiple by the value of its coordinate corresponding to any fixed vertex i. □

By Proposition 8.1.1, it immediately have the following proposition.

Proposition 8.1.2. *If G is a bipartite graph, then $\mu_1(G) = \rho_1(G) = \varphi_Q(G)$.*

8.2 The regular graph case

A graph G is called k-regular if $d_1 = d_2 = \ldots = d_n = k$. If G is k-regular, it is easy to see that $\lambda_1(G) = \rho_1(G) + k$ and $\lambda_n(G) = \rho_n(G) + k$. Thus, we have the following proposition.

Proposition 8.2.1. *If G is k-regular, then $\varphi_A(G) = \varphi_Q(G)$.*

8.3 The upper bound

We use the notation of majorization. Suppose $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ are two non-increasing sequences of real numbers, we say (x) is *majorized* by (y), denoted by $(x) \trianglelefteq (y)$, if and only if $\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$, and $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for all $j = 1, 2, \ldots, n$.

Proposition 8.3.1. *Let G be a graph with signless Laplacian spectrum $(\rho) = (\rho_1, \rho_2, \ldots, \rho_n)$ and the degree sequence $(d) = (d_1, d_2, \ldots, d_n)$. Then $(d) \trianglelefteq (\rho)$.*

Proof. It is well that the spectrum of a positive semi-definite Hermitian matrix majorizes its main diagonal (when both are rearranged in non-increasing order). □

Corollary 8.3.2. $\rho_n \leq d_n$.

Proof. By Proposition 8.3.1, it follows that $(d) \trianglelefteq (\rho)$, then $d_1 + d_2 + \ldots + d_{n-1} \leq \rho_1 + \rho_2 + \ldots + \rho_{n-1}$ and $d_1 + d_2 + \ldots + d_n = \rho_1 + \rho_2 + \ldots + \rho_n$. Hence $\rho_n \leq d_n$. □

Let $m(v) = \sum_{u \in N(v)} d(u)/d(v)$. The next result gives upper and lower bounds for $\rho_1(G)$.

Proposition 8.3.3. *[20] Let G be a connected graph on $n(n \geq 2)$ vertices. Then.*

$$\min\{d(v) + m(v) : v \in V(G)\} \leq \rho_1(G) \leq \max\{d(v) + m(v) : v \in V(G)\},$$

where equality holds in both of these inequalities if and only if G is regular or semi-regular bipartite.

Proof. The inequality follows by applying Geršgorin's theorem to the rows of the matrix $D^{-1}(G)Q(G)D(G)$, whose (i, j)-entry is

$$\begin{cases} d(v_i) & \text{if } i = j, \\ d(v_j)/d(v_i) & \text{if } v_iv_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$\rho_1(G) \leq \max\{d(v_i) + \sum_{j=1, j\neq i}^{j=n} \frac{d(v_j)}{d(v_i)} : v_iv_j \in E(G)\} = \max\{d(v) + m(v) : v \in V(G)\}.$$

The lower bound can be proved in a similar way. Suppose that the equality holds. Then, $\rho_1(G) = d(v_i) + m(v_i)$, for all $i = 1, 2, \ldots, n$. Since G is connected graph. G is regular or semi-regular bipartite [21]. □

Remark 8.3.4. If G is a connected bipartite graph, by Proposition 8.1.2 we can conclude that the bounds for $\rho_1(G)$ in Proposition 8.3.3 are also bounds for $\varphi_Q(G)$. Thus, Proposition 8.3.3 also gives bounds for $\varphi_Q(G)$ when G is a connected bipartite graph.

Remark 8.3.5. Consider the graph tree with the maximal and minimal signless Laplacian spread. Since tree is bipartite, by Proposition 8.1.2 and Theorem 4.3.1, the maximal signless Laplacian spread is $\varphi_Q(S_n) = \mu_1(S_n) = n$. And the minimal signless Laplacian spread is obtained from path, by Propositions 8.1.2, 8.3.3,

$$\varphi_Q(P_n) = \rho_1(P_n) \leq \max\{d(v) + m(v) : v \in V(P_n)\} = 3.$$

If G is a tree is not a path, that is, there is a vertex v, with $deg(v) \geq 3$. By Theorem 4.3.8 and Proposition 8.1.2, we have $\varphi_Q(G) = \mu_1(G) \geq 3 + 1 = 4$. Then the result follows.

Lemma 8.3.6. *[22] If G is a graph with at least one edge, then $\rho_1(G) \geq \mu_1(G) \geq \Delta(G) + 1$. If G is connected, the first equality holds if and only if G is bipartite, the second equality holds if and only if $\Delta(G) = n - 1$.*

Proof. Since $|L(G)| = D(G) + A(G) = Q(G)$, and G is connected, it follows that $A(G)$ and therefore $Q(G)$ is nonnegative and irreducible. By Theorem 2.1.8, we have $\rho_1(G) \geq \mu_1(G)$. Now suppose that $\rho_1(G) = \mu_1(G)$, then by Theorem 2.1.8, $D(G) - A(G) = U(D(G) + A(G))U^{-1}$, where U is a diagonal matrix with diagonal entries of absolute value 1. Assume that G is not bipartite. Then G has an odd cycle $u_1u_2 \ldots u_{2k}u_{2k+1}u_1$. Hence,

$$(D(G) - A(G))_{u_1u_2} = -1 = U_{u_1u_1} \times 1 \times U^{-1}_{u_2u_2}.$$

So, $U_{u_2u_2} = -U_{u_1u_1}$. Repeating this argument, one can obtain that $U_{u_3u_3} = -U_{u_2u_2} = U_{u_1u_1}, \ldots, U_{u_{2k+1}u_{2k+1}} = U_{u_1u_1}$ and $U_{u_{2k+1}u_{2k+1}} = -U_{u_1u_1}$, impossible. Thus G is bipartite.

Conversely suppose that G is a bipartite graph and S, T is a bipartition of $V(G)$. Then it is not to verify that $W(D(G) - A(G))W^{-1} = D(G) + A(G)$, where $W = diag(W_{uu} : u \in V(G))$, and $W_{uu} = 1$ if $u \in S$ and $W_{uu} = -1$ if $u \in T$. Thus $\mu_1(G) = \rho_1(G)$. □

Now, we consider some upper and lower bounds for $\varphi_Q(G)$, and determine the unique unicyclic graph with maximal signless Laplacian spread among the class of connected unicyclic graphs of order n.

The next result gives bounds for $\varphi_Q(G)$, when G is a connected graph.

Theorem 8.3.7. *If G is a connected graph, then*

$$d_1 - d_n + 1 < \varphi_Q(G) \leq \max\{d(v) + m(v) : v \in V(G)\},$$

where the upper bound holds if and only if G is regular bipartite or semi-regular bipartite.

Proof. Lemma 8.3.6 and Corollary 8.3.2 implies the strict lower bound. And the upper bound follows from Proposition 8.3.3. □

8.4 The lower bound

Let $G = (V, E)$, if $\emptyset \neq V_1 \subseteq V(G)$, by the average degree of V_1, say d_0, we mean that $d_0 = \sum_{v \in V(G)} d(v)/|V_1|$. Denote the (n, m) graph is a graph $G(V, E)$ with $|V| = n$ and $|E| = m$.

Theorem 8.4.1. *[20] Let G be a connected (n, m) graph with $n \geq 2$. Suppose G contains a nonempty set T of t independent vertices, the average degree of which is d_0. Then,*

$$\varphi_Q(G) \geq \frac{1}{n-t}\sqrt{(nd_0)^2 + 8(m - td_0)(2m - nd_0)}.$$

Proof. The t independent vertices give rise to a partition of $Q(G)$ with quotient matrix $B = \begin{pmatrix} d_0 & d_0 \\ \frac{td_0}{n-t} & \frac{4m-3td_0}{n-t} \end{pmatrix}$. The eigenvalues of B are

$$\beta_1, \beta_2 = \frac{4m + nd_0 - 4td_0}{2(n-t)} \pm \frac{1}{2(n-t)}\sqrt{(nd_0)^2 + 8(m - td_0)(2m - nd_0)}.$$

By Lemma 2.2.3, $\rho_1 \geq \beta_1\beta_2 \geq \rho_n$, which implies the required inequality. □

Remark 8.4.2. If G is k-regular, then $nd_0 = 2m$ and Theorem 8.4.1 gives $\varphi_A(G) = \varphi_Q(G) \geq nk/(n-t)$, where t and d_0 are denoted as in Theorem 8.4.1. Solving for t gives Hoffman's bound on t when G is k-regular:

$$t \leq \frac{n|\rho_n(G)|}{k - \rho_n(G)}.$$

Thus, Theorem 8.4.1 may be regarded as a generalization of Hoffman's bound to irregular graphs. There are may graphs for which the bound in Theorem 8.4.1 is attained. For if G is k-regular, the bound is attained if and only if G has a set T of independent vertices that attains Hoffman's bound. Also, if $G = G(X, Y)$ is bipartite and T is either of its two vertices parts, then $m - td_0 = 0$ and Theorem 8.4.1 gives $\rho_1 = \varphi_Q(G) \geq \ nm/t(n-t)$. Here, $\text{rank}(B) = 1$ in the proof of Theorem 8.4.1, and equality holds in the bound if and only if G is semi-regular. By Theorem 8.4.1, it immediately has the following corollary.

Corollary 8.4.3. *Let p be the number of pendent vertices of G. If G is a connected (n, m) graph with $n > p \geq 1$, then*

$$\varphi_Q(G) \geq \frac{1}{n-p}\sqrt{n^2 + 8(m-p)(2m-n)}.$$

Equality holds, for example, if $G \cong K_{1,n-1}$ and $p = n-1$.

If $d(u) = d_1$, then u is also an independent set of G. By Theorem 8.4.1, we have the following corollary.

Corollary 8.4.4. *If G is a connected (n, m) graph with $n \geq 2$, then*

$$\varphi_Q(G) \geq \frac{1}{n-1}\sqrt{(nd_1)^2 + 8(m-d_1)(2m-nd_1)}.$$

Equality holds, for example, if $G \cong K_n$.

By the proof of Theorem 8.4.1, we have the following remark.

Remark 8.4.5. If G is a connected (n, m) graph and contains $(1 \leq t < n)$ independent vertices, the average degree of which is d_a, then

$$\rho_1(G) \geq \frac{4m + nd_a - 4td_a}{2(n-t)} + \frac{1}{2(n-t)}\sqrt{(nd_a)^2 + 8(m-td_a)(2m-nd_a)}.$$

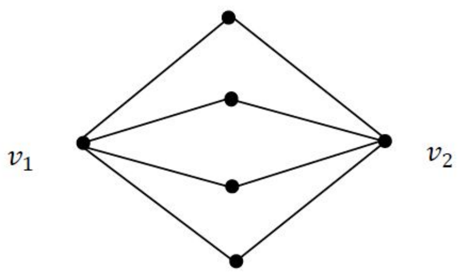
Also, with the same method as Corollary 8.4.4, we have the following remark.

Remark 8.4.6. If G is a connected (n, m) graph with $n \geq 2$, then

$$\rho_1(G) \geq \frac{4m + nd_1 - 4d_1}{2(n-1)} + \frac{1}{2(n-1)}\sqrt{(nd_1)^2 + 8(m-d_1)(2m-nd_1)}.$$

Let G be a connected (n, m) graph. Suppose G contains $(1 \leq t < n)$ independent vertices, the average degree of which is d_a. Then, the t independent vertices give rise to a partition of $L(G)$ with quotient matrix $B = \begin{pmatrix} d_a & -d_a \\ \frac{-td_a}{n-t} & \frac{td_a}{n-t} \end{pmatrix}$.

Lemma 8.4.7. *If G be a connected (n, m) graph and contains $(1 \leq t < n)$ independent vertices, the average degree of which is d_a. Then, $\mu_1 \geq nd_a/(n-t)$. In particular, if G is a connected k-regular graph, then $\mu_1 \geq nk/(n-t)$. Equality holds, for example, if $G \cong K_n$.*



The graph H. Fig 8.1.

As shown in the next example, the bounds in Remark 8.4.6 and Lemma 8.4.7 are sometimes better than the bounds in Lemma 8.3.6.

Example 8.4.8. Let H be the graph as shown in Fig 8.1. Clearly, $T = \{v_1, v_2\}$ is an independent vertex set, and $d_a = 4$. By Lemma 8.4.7, it follows that $\mu_1(H) \geq nd_a/(n-t) = 6 > 5 = d_1 + 1$. Actually, $\mu_1(H) = 6$. Thus, the bound in Lemma 8.4.7 can be attained. If we replace d_1 by 4 in Remark 8.4.6, then we have $\rho_1(G) > 5.78$, which is also better than $\rho_1(G) \geq d_1 + 1 = 5$ in Lemma 8.3.6.

Proposition 8.4.9. *[20] Suppose G has two induced subgraph G_1, G_2, where G_i has n_i vertices and e_i edges for $i = 1, 2$, $V(G_1) \cap V(G_2) = \emptyset$ and $n_1 + n_2 = n$. Let $a_1 = \sum_{v \in V(G_1)} d(v)/n_1$ and $a_2 = \sum_{v \in V(G_2)} d(v)/n_2$, then*

$$\varphi_Q(G) \geq \sqrt{(a_1 + a_2 + \frac{2e_1}{n_1} + \frac{2e_2}{n_2})^2 - 16(\frac{a_2 e_1}{n_1} + \frac{a_1 e_2}{n_2})}.$$

Proof. Note that $Q(G)$ has B as it quotient matrix, where $B = \begin{pmatrix} a_1 + \frac{2e_1}{n_1} & a_1 - \frac{2e_1}{n_1} \\ a_2 - \frac{2e_2}{n_2} & a_2 + \frac{2e_2}{n_2} \end{pmatrix}$

Obviously, B has two eigenvalues

$$\beta_1, \beta_2 = \frac{1}{2}[a_1 + a_2 + \frac{2e_1}{n_1} + \frac{2e_2}{n_2} \pm \sqrt{(a_1 + a_2 + \frac{2e_1}{n_1} + \frac{2e_2}{n_2})^2 - 16(\frac{a_2 e_1}{n_1} + \frac{a_1 e_2}{n_2})}]$$

Then Lemma 8.4.7 implies the result. $\square$

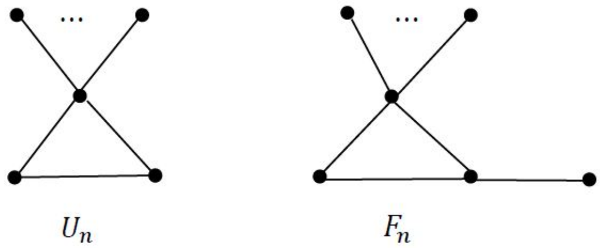


Fig 8.2.

The *join* of two vertex disjoint graph G_1, G_2 is the graph $G_1 \vee G_2$ obtained from their union by including all edges between the vertices in G_1 and the vertices in G_2.

Corollary 8.4.10. *Suppose $G = G_1 \vee G_2$, where each G_i is a graph has n_i vertices and e_i edges for $i = 1, 2$. Then*

$$\varphi_Q(G) \geq \sqrt{(n + \frac{4e_1}{n_1} + \frac{4e_2}{n_2})^2 - 16(e_1 + e_2 + \frac{4e_1e_2}{n_1n_2})}.$$

Equality holds, for example, if $G \cong K_n$.

Proof. Note that $G = G_1 \vee G_2$, then $a_1 - 2e_1/n_1 = n_2$ and $a_2 - 2e_2/n_2 = n_1$. By Proposition 8.4.9, the conclusion follows. When $G \cong K_n$, it is readily checked that equality holds because $\varphi_Q(K_n) = n$. □

In the following, let $\mathcal{U}_n$ denote the class of connected unicyclic graphs of order n. Let $U_1(n-3, 0; n), U_1(n-4, 1; n)$ be the unicyclic graphs as shown in Fig 8.2.

Lemma 8.4.11. *[23] If $n \geq 8$ and $G \in \mathcal{U}_n \backslash U_1(n-3, 0; n)$, then $\rho_1(G) \leq \rho_1(U_1(n-4, 1; n))$, where equality holds if and only if $G \cong F_n$.*

Theorem 8.4.12. *[20] If $n \geq 8$ and $G \in \mathcal{U}_n \backslash U_1(n-3, 0; n)$, then $\varphi_Q(U_1(n-3, 0; n)) > \varphi_Q(G)$.*

Proof. By a straightforward computation, we have

$$\begin{aligned} p(U_1(n-3, 0; n)) &= (x-1)^{n-3} f_1(x), \\ p(U_1(n-4, 1; n)) &= (x-1)^{n-5} f_2(x), \end{aligned}$$

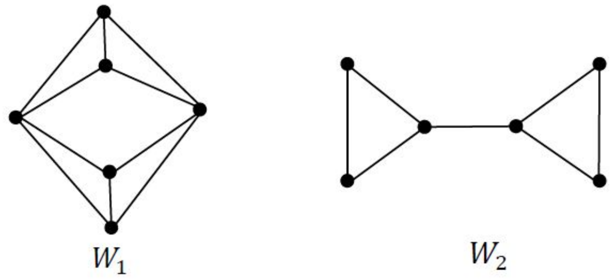


Fig 8.3.

where $f_1(x) = x^3 - (n+3)x^2 + 3nx - 4$, and $f_2(x) = x^5 - (n+5)x^4 + (6n+3)x^3 - (9n-1)x^2 + (3n+8)x - 4$. By Lemma 8.4.11, we only need to prove that $\varphi_Q(U_1(n-3,0;n)) > \rho_1(U_1(n-4,1;n))$, because $\rho_1(G) \leq \rho_1(U_1(n-4,1;n))$ and $\rho_n(G) \geq 0$. Since $f_1(0) = -4 < 0$, $f_1(0.2) = 0.56n - 4.112 > 0$, $f_1(n) = -4 < 0$, and $f_1(n+1) = n^2 - n - 6 > 0$, by the equality it follows that $0 < \rho_n(U_1(n-4,1;n) < 0.2$ and $n < \rho_1(U_1(n-3,0;n) < n+1$. Thus, $\varphi_Q(U_1(n-3,0;n)) = \rho_1(U_1(n-3,0;n)) - \rho_n(U_1(n-3,0;n)) > n - 0.2$. Since $f_2(0) = -4 < 0$, $f_2(0.3) = 0.2439n - 1.468 > 0$, $f_2(1) = 4 - n < 0$, $f_2(2) = 2n - 8 > 0$, $f_2(6) = 2024 - 306n < 0$, and $f_2(n-0.2) = 0.8n^4 - 5.44n^3 + 5.272n^2 + 7.1184n - 5.59232 > 0$, by the equality it follows that $6 < \rho_1(U_1(n-4,1;n)) < n-0.2$. Thus, $\rho_1(U_1(n-4,1;n) < n-0.2 < \varphi_Q(U_1(n-3,0;n)$. This completes the proof of this result. □

Remark 8.4.13. If G is a regular graph, then by Proposition 8.2.1 $\varphi_A(G) = \varphi_Q(G)$. By examining the spectrum of $A(G)$ and $Q(G)$ for graphs on five vertices (for example, see [3, p. 273-275]and [19]), we see that the inequality $\varphi_A(G) \leq \varphi_Q(G)$ often holds. But for the graph W_1 shown in Fig 8.3, we have $\varphi_A(W_1) > 5.744 > 5.657 > \varphi_Q(W_1)$. It is natural to consider when the strict inequality $\varphi_A(G) > \varphi_Q(G)$ is necessary and when it is sufficient.

Remark 8.4.14. In Proposition 8.1.2, it implies that $\varphi_L(G) \leq \varphi_Q(G)$ always holds for bipartite graphs G. But for the graph W_2 shown in Fig 8.3, we have $\varphi_L(W_2) >$

$4.123 > 4 = \varphi_Q(W_2)$. Thus, we could also consider the conditions for the inequality $\varphi_L(G) > \varphi_Q(G)$ to hold.

Conjecture 8.4.15. In Theorem 8.4.12, we determine the unicyclic graph with maximal signless Laplacian spread among all connected unicyclic graphs of order n. But the graphs which share the maximal signless Laplacian spread among all connected graphs of order n are still unknown. Let K_n^1 be the graph on n vertices obtained by attaching a pendant vertex to K_{n-1}. Then $\varphi_Q(K_n^1) = \sqrt{4n^2 - 20n + 33}$. So, $\varphi_Q(K_n^1) \leq 2n - 4$ when $n \geq 5$. A computer run [20] on connected graph G of order n for $3 \leq n \leq 8$ indicates that if $n \neq 4$, then $\varphi_Q(G) \leq \varphi_Q(K_n^1)$ and that, when $n = 6, 7, 8$, equality is attained only when $G = K_n^1$. Note that if G is disconnected, then it is straightforward to check that $\varphi_Q(G) \leq 2n - 4$ and the equality is attained only if $G = K_{n-1} + K_1$, which is the complete graph on $n-1$ vertices together with a single isolated vertex. Because of the computer run and because K_n^1 is obtained from the disconnected maximizer $K_{n-1} + K_1$ by adding a single edge, it seems likely that $\varphi_Q(G) \leq \varphi_Q(K_n^1)$ for connected graphs G of order $n \leq 5$.

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