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**ON DISTANCE SPECTRAL RADIUS  
AND  
LAPLACIAN MATRICES OF GRAPHS**

**A thesis submitted in partial fulfillment of the requirements  
for award of the degree of Doctor of Philosophy**

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## ABSTRACT

**Keywords.** Tree; Bipartite graph;  $\infty(p; l; q)$ -graph;  $\theta(p; t; q)$ -graph; Pockets; Edge-pockets; Matching number; Vertex Connectivity; Laplacian Matrix; Distance Matrix; Distance Spectral radius; Distance Laplacian Matrix.

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This thesis is the outcome of our study about the eigenvalues of the Laplacian and the distance matrices of a graph and their relation to the structure of the graph.

A generalization of the edge corona of graphs is defined and the corresponding Laplacian spectrum has been studied. The results are used to find an infinite family of Laplacian cospectral graphs.

Like many fields of mathematics, in graph theory also one is often interested in finding the maxima or minima of certain functions and identifying the points of optimality. We consider the function “distance spectral radius” and try to maximize and minimize it under different constraints and in different classes of graphs. Along this way, we have obtained the graph having maximal distance spectral radius among all trees with given matching number (resp. among all graphs with given number of pendent vertices) conjectured by Aleksandar Ilić in [Distance spectral radius of trees with given matching number, *Discrete Applied Mathematics* **158** (16), 1799–1806, 2010] (resp. by Yu et al. in [Some graft transformations and its applications on the distance spectral radius of a graph, *Applied Mathematics Letters* **25** (3), 315–319, 2012]).

The class of all connected graphs having connected complement (precisely a tree or a unicyclic graph) is considered and the second smallest distance Laplacian eigenvalue is studied. It has been proved that the largest distance Laplacian eigenvalue of path is simple and the structure of the corresponding eigenvector is described.

## DECLARATION

I do hereby declare that this thesis is the result of my own research work which has been carried out under the guidance and supervision of Dr. Milan Nath, Associate Professor, Department of Mathematical Sciences, Tezpur University, Assam. Also, I would like to declare that neither the thesis nor any part thereof has been submitted to this university or any other university/institution for any other degree.

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Place : Tezpur



## TEZPUR UNIVERSITY

### CERTIFICATE

This is to certify that the thesis entitled “**On Distance Spectral Radius and Laplacian Matrices of Graphs**” submitted to the School of Science, Tezpur University in partial fulfillment for the award of the degree of Doctor of Philosophy in Mathematics is a record of research work carried out by Somnath Paul under my supervision and guidance.

All help received by him from various sources have been duly acknowledged.

No part of this thesis has been submitted elsewhere for award of any other degree.

*MNB*  
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*Dedicated*  
*To*  
*my little angel*  
*“BIBHAB”*  
*(my two year old nephew)*  
*&*  
*his innocent childhood*

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# Chapter 1

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## Introduction

Algebraic graph theory is the study of many unexpected and many useful connections between two beautiful and apparently unrelated, parts of mathematics: algebra and graph theory. Some of the important problems in algebraic graph theory are matrix completion problems, minimum rank problems and problems in spectra of graphs. Spectral graph theory studies the relation between graph properties and the spectra of certain matrices associated to it. The associated matrices include the adjacency matrix, the Laplacian matrix, the distance matrix etc., and their normalized forms.

Spectral graph theory has a long history. In the early days, adjacency matrices of graphs were studied using matrix theory and linear algebra. Algebraic methods are especially effective in treating graphs which are regular and symmetric. In the past ten years, new spectral techniques have emerged and they are powerful and well-suited for dealing with general graphs. In a way, spectral graph theory has entered a new era.

This thesis is the outcome of our study about the eigenvalues of the Laplacian and the distance matrices of a graph and their relation to the structure of the graph. In literature, extensive study has been made on adjacency and Laplacian matrices. The distance matrix of a graph, while not as common as the more familiar adjacency matrix, has nevertheless come up in several different areas, including communication network design [30], graph embedding theory [23, 29], network flow algorithms [27] etc. Recently, the problem of finding all graphs with maximal or minimal distance spectral radius among a class of graphs has been studied extensively (see [36, 55, 57, 61, 62, 65]). This thesis is intended to fill some conspicuous gaps in the study of the distance spectral radius of graphs. The distance Laplacian matrix of a graph entered the scene of graph spectra as late as 2013. This thesis also attempts to answer certain questions on the distance Laplacian spectra of some graphs.

## 1.1 Graph terminologies

All graphs we consider in this thesis are finite, undirected, and simple, i.e., without loops and parallel edges. For a graph  $G = (V, E)$ , we write  $V(G)$  and  $E(G)$  for the vertex set  $V$  and the edge set  $E$  of  $G$ , respectively. By  $|G|$  (i.e., the *order* of  $G$ ) we mean the cardinality of the vertex set of  $G$  and  $d_G(v)$  is used to denote the *degree* (i.e., the number of incident edges) of a vertex  $v$  in  $G$ . An *isolated vertex* is a vertex of degree 0 and a *pendent vertex* is a vertex of degree 1. The vertex adjacent to a pendent vertex is called a *quasi-pendent vertex*. A *spanning subgraph* of  $G$  is a subgraph containing all the vertices of  $G$ . For a subset  $S$  of  $V(G)$ ,  $G[S]$  denotes the *induced subgraph* on  $S$  (i.e., the maximal subgraph of  $G$  on  $S$ ).

The *distance* between two vertices  $u, v \in V(G)$  is denoted by  $d_{uv}$  and is defined as the length of a shortest path between  $u$  and  $v$  in  $G$ . The distance, as a function on  $V \times V$ , satisfies the triangle inequality. Thus, for any three vertices  $u, v$  and  $w$ ,

$$d_{uw} \leq d_{uv} + d_{vw}.$$

The *diameter* (i.e., maximal distance between any two vertices) of  $G$  is denoted by  $d(G)$ .

We use the standard notations  $C_n$ ,  $K_n$ ,  $P_n$  and  $S_n$  for the cycle, the complete graph, the path and the star, respectively, on  $n$  vertices. An *empty graph* of order  $n$  is denoted by  $O_n$  and is defined as the complement of  $K_n$ , i.e., a graph having no edge.

If  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  are two graphs on disjoint sets of  $m$  and  $n$  vertices, respectively, then their *union* is the graph  $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$ . Their *join* is denoted by  $G_1 \vee G_2$  and consists of  $G_1 \cup G_2$  and all lines joining  $V_1$  and  $V_2$ .

A *tree* is a connected graph without a cycle. A *bipartite graph*  $G$  is a graph whose vertex set  $V(G)$  can be partitioned into two disjoint subsets  $V_1$  and  $V_2$  such that every edge of  $G$  joins a vertex of  $V_1$  with a vertex of  $V_2$ . If  $G$  contains every edge joining a vertex of  $V_1$  with a vertex of  $V_2$ , then it is a *complete bipartite graph* and is denoted by  $K_{m,n}$ , where  $m, n$  are the number of vertices in  $V_1$  and  $V_2$ , respectively.

An *edge independent set* of a graph  $G$  is a set of edges such that any two distinct edges of the set are not incident on a common vertex. The *edge independence number* of  $G$ , denoted by  $m(G)$ , is the maximum of the cardinalities of all edge independent sets. An edge independent set (resp. edge independence number) is usually called a *matching* (resp. *matching number*). For a connected graph  $G$  of order  $n$ , its matching number  $m(G)$  satisfies  $1 \leq m(G) \leq \lfloor \frac{n}{2} \rfloor$ .

For a set  $S$  of vertices and edges in a graph  $G$ ,  $G - S$  denotes the graph obtained from  $G$  by deleting all the elements of  $S$ . It is understood that when a vertex is deleted, all edges incident with it are deleted as well, but when an edge is deleted, the vertices incident with it are not.

The *vertex connectivity* of a graph  $G$ , denoted by  $\kappa(G)$ , is the minimum number of vertices whose deletion yields in a disconnected or a trivial graph. A *cut vertex* is a vertex whose removal increases the number of components of a graph. Thus for a graph  $G$  with a cut vertex,  $\kappa(G) = 1$ . The *neighbourhood*  $N_G(v)$  of a vertex  $v$  in  $G$  is  $\{u : uv \in E(G)\}$ . If  $v$  is a vertex of a tree  $T$ , then the components of  $T - v$  are called the *branches* of  $T$  at  $v$ . We say that a graph  $K$  is *attached* at a vertex  $v$  of  $G$  to mean that a new graph is obtained by joining  $v$  and a vertex of  $K$  by an edge. For other graph theoretic terms we follow [33].

A few words about the labels: the label of theorems, lemmas, corollaries, remarks, definitions, equations and examples are made like *c.s.n*; where  $c$  is the chapter number,  $s$  is the section number and  $n$  is the item number.

## 1.2 Schur complement and Kronecker product of matrices

Let  $M_1, M_2, M_3$  and  $M_4$  be respectively  $p \times p, p \times q, q \times p$  and  $q \times q$  matrices with  $M_1$  and  $M_4$  invertible. It is well known that

$$\begin{aligned} \det \begin{bmatrix} M_1 & M_2 \\ M_3 & M_4 \end{bmatrix} &= \det(M_4) \cdot \det(M_1 - M_2 M_4^{-1} M_3), \\ &= \det(M_1) \cdot \det(M_4 - M_3 M_1^{-1} M_2), \end{aligned}$$

where  $M_1 - M_2 M_4^{-1} M_3$  and  $M_4 - M_3 M_1^{-1} M_2$  are called the *Schur complements* of  $M_4$  and  $M_1$  respectively [63].

The *Kronecker product*  $A \otimes B$  of two matrices  $A = [a_{ij}]_{m \times n}$  and  $B = [b_{ij}]_{p \times q}$  is the  $mp \times nq$  matrix obtained from  $A$  by replacing each element  $a_{ij}$  by  $a_{ij}B$ . This is an associative operation with the property that  $(A \otimes B)^T = A^T \otimes B^T$  and  $(A \otimes B)(C \otimes D) = AC \otimes BD$  whenever the products  $AC$  and  $BD$  exist. The latter implies  $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$  for nonsingular matrices  $A$  and  $B$ . Moreover, if  $A$  and  $B$  are  $n \times n$  and  $p \times p$  matrices, then  $\det(A \otimes B) = (\det A)^p (\det B)^n$ . Other properties of the Kronecker product can be found in [34].

Throughout the thesis,  $J_{s \times t}$  (resp.  $\mathbf{0}_{s \times t}$ ) denotes the  $s \times t$  matrix with all entries equal to 1 (resp 0), where  $s, t \geq 2$ . Similarly,  $\mathbf{1}_s$  (resp.  $\mathbf{0}_s$ ) denotes the  $s \times 1$  vector with all entries equal to 1 (resp 0). The identity matrix of order  $k$  is denoted by  $I_k$ . (Though sometimes we omit the order if it is clear from the context).

### 1.3 The Laplacian matrix of a graph

Let  $V(G) = \{v_1, v_2, \dots, v_n\}$  be the vertex set of  $G$ . The *adjacency matrix* of  $G$ , is defined to be  $A(G) = [a_{ij}]_n$ , where

$$a_{ij} = \begin{cases} 1, & \text{if } v_i \text{ and } v_j \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases}$$

Being a real symmetric matrix, all the eigenvalues of  $A(G)$  are real and their algebraic multiplicities equal their geometric multiplicities [34].

The *matrix of vertex degrees* of  $G$  is the diagonal matrix  $\text{Deg}(G)$  of order  $n$ , whose  $i$ -th diagonal entry is the degree of the  $i$ -th vertex. The matrix  $L = L(G) = \text{Deg}(G) - A(G)$ , is the *Laplacian matrix* of  $G$ .

The *vertex-edge incidence matrix* [7]  $M$  of  $G$  is a matrix whose rows and columns are indexed by  $V(G)$  and  $E(G)$ , respectively. After giving any arbitrary orientation to the edges, the  $(i, j)$ -th entry of  $M$  is 0 if vertex  $i$  and edge  $e_j$  are not adjacent, and otherwise it is 1 or  $-1$  according as  $e_j$  originates or terminates at  $i$ , respectively.

The matrix  $L$  is symmetric, singular (because all row sums are 0) and positive semidefinite (because  $L = MM^T$ ). So all the eigenvalues of  $L$  are non-negative reals.

In 1847, Kirchoff proved a very important result involving the Laplacian matrix which put the study of the Laplacian matrix as an interesting subject in front of many researchers. The result is popularly known as *Kirchoff's Matrix Tree Theorem*. See [47] to collect some more references on this theorem.

**Theorem 1.3.1.** *Let  $G$  be a graph. Denote by  $L(i|j)$  the  $(n-1) \times (n-1)$  submatrix of  $L$  obtained by deleting its  $i$ -th row and  $j$ -th column. Then  $(-1)^{i+j} \det L(i|j)$  is the number of spanning trees in  $G$ .*

For a matrix  $M$  of order  $n$ ,

$$\phi(M; x) = \det(xI_n - M)$$

is the *characteristic polynomial* of  $M$ . In particular, for a graph  $G$ ,  $\phi(L(G); x)$  is called the *Laplacian characteristic polynomial* of  $G$ , and its roots are the Laplacian eigenvalues

of  $G$ . The collection of eigenvalues of  $L(G)$  together with their multiplicities is called the  $L$ -spectrum of  $G$  and is denoted by  $\sigma^L(G)$ . Two graphs are said to be  $L$ -cospectral, if they have the same  $L$ -spectrum.

Let  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq \mu_n = 0$  (we will use this ordering throughout the thesis) denote the Laplacian eigenvalues of  $G$ . The second smallest eigenvalue  $\mu_{n-1}$  of  $L$  is called the *algebraic connectivity*. The justification for the name is the fact that  $\mu_{n-1} = 0$  iff the graph is disconnected. An eigenvector corresponding to  $\mu_{n-1}$  is called a *Fiedler Vector*. The algebraic connectivity of a graph and the structure of a Fiedler vector is studied extensively in literature (see [24, 38–40, 47] and the references therein).

Let  $\overline{G}$  denote the complement of a graph  $G$ . Then, as observed in [1],

$$L(G) + L(\overline{G}) = L(K_n) = nI_n - J_n.$$

It follows that  $n - \mu_{n-1} \geq n - \mu_{n-2} \geq \dots \geq n - \mu_1 \geq 0$  are the Laplacian eigenvalues of  $\overline{G}$ .

Till now, many graph operations such as the disjoint union, the Cartesian product, the Kronecker product, the corona, the edge corona, the neighbourhood corona and the subdivision vertex (edge) neighbourhood corona have been introduced, and their  $L$ -spectra are computed (see [11, 15, 17, 18, 20, 28, 35, 42, 44]). These operations help to describe the spectrum of a relatively larger graph in terms of the spectra of some smaller graphs.

In Chapter 2, we define *graph with edge pockets* (see Definition 2.1.2) which generalizes the definition of edge-corona and discuss some results of their  $L$ -spectra. As an application, we show that these results enables us to construct infinitely many pairs of  $L$ -cospectral graphs.

## 1.4 The distance matrix and the distance spectral radius of a graph

The *distance matrix* of a connected graph  $G$  of order  $n$  is defined to be  $D(G) = [d_{ij}]_n$ , where  $d_{ij}$  is the distance between the vertices  $v_i$  and  $v_j$  in  $G$ . Thus,  $D(G)$  is a symmetric real matrix and have real eigenvalues [34]. The *distance spectral radius*  $\rho(G)$  of  $G$  is the largest eigenvalue of the distance matrix  $D(G)$ . Since  $D(G)$  is irreducible, by the Perron-Frobenius theory,  $\rho(G)$  is simple and is afforded by a positive eigenvector, called

the Perron vector [50]. If  $X(G) = (x_1, x_2, \dots, x_n)^T$  is the Perron vector of  $D(G)$ , then

$$\rho(G)x_i = \sum_{v_j \in V(G)} d_{ij}x_j.$$

Distance energy  $DE(G)$  is a newly introduced molecular graph-based analog of the total  $\pi$ -electron energy, and it is defined as the sum of the absolute eigenvalues of the molecular distance matrix. The distance spectral radius is a useful molecular descriptor in QSPR modelling, as demonstrated by Consonni and Todeschini in [16,59]. For more details on distance matrices and distance energy one may refer to [49,54,58].

Balaban et al. in [3] proposed the use of distance spectral radius as a molecular descriptor, while in [32] it was successfully used to infer the extent of branching and model boiling points of alkanes. In [66] and [68], Zhou and Trinajstić provided upper and lower bounds for  $\rho(G)$  in terms of the number of vertices, Wiener index and Zagreb index. Balasubramanian in [4,5] pointed out that the spectra of the distance matrices of many graphs such as the polyacenes, honeycomb and square lattice have exactly one positive eigenvalue, and he computed the spectrum of fullerenes  $C_{60}$  and  $C_{70}$ .

In the case of a tree, the distance matrix has some attractive properties. As for example, the determinant of the distance matrix of a tree depends only on the number of vertices, and not on the structure of the tree, as seen in the following result.

**Theorem 1.4.1.** [30] *Let  $T$  be a tree on  $n$  vertices, where  $n \geq 2$ , and  $D$  be the distance matrix of  $T$ . Then the determinant of  $D$  is given by*

$$\det D = (-1)^{n-1}(n-1)2^{n-2}.$$

It was also shown in [30] that the distance matrix of a non trivial tree has just one positive eigenvalue.

Let  $D$  be the distance matrix of a tree  $T$  with  $V(T) = \{1, 2, \dots, n\}$ . It follows from Theorem 1.4.1 that  $D$  is nonsingular. If  $\tau_i = 2 - d_T(i)$ ,  $i = 1, \dots, n$ , and  $\tau$  is the  $n \times 1$  vector with components  $\tau_1, \dots, \tau_n$ , then the following result connects the inverse of distance matrix of  $T$  with its Laplacian matrix.

**Theorem 1.4.2.** [29] *Let  $T$  be a tree with  $V(T) = \{1, 2, \dots, n\}$ . Let  $D$  be the distance matrix of  $T$  and  $L$  be the Laplacian matrix of  $T$ . Then*

$$D^{-1} = -\frac{1}{2}L + \frac{1}{2(n-1)}\tau\tau^T.$$

Merris in [46] obtained an interlacing inequality involving the distance and Laplacian eigenvalues of trees which is as follows.

**Theorem 1.4.3.** [46] *Let  $T$  be a tree of order  $n$ , where  $n \geq 2$ . Let  $D$  be the distance matrix and  $L$  be the Laplacian matrix of  $T$ . Let  $\lambda_1 > 0 > \lambda_2 \geq \dots \geq \lambda_n$  be the eigenvalues of  $D$  and  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$  be the eigenvalues of  $L$ . Then*

$$0 > -\frac{2}{\mu_1} \geq \lambda_2 \geq -\frac{2}{\mu_2} \geq \dots \geq -\frac{2}{\mu_{n-1}} \geq \lambda_n.$$

Various other connections between the distance matrix and the Laplacian matrix of a graph can be found in [6, 8].

Let  $e = uv$  be an edge of a connected graph  $G$  such that  $G' = G - e$  is also connected, and let  $D'$  be the distance matrix of  $G - e$ . As observed already in [57], the removal of  $e$  does not create shorter paths than the ones in  $G$ , and therefore,  $d_{ij} \leq d'_{ij}$  for all  $i, j \in V(G)$ , where  $d'_{ij}$  is the  $(i, j)$ -th entry of  $D'$ . Moreover,  $1 = d_{uv} < d'_{uv}$  and by the Perron-Frobenius theorem, one can conclude that

$$\rho(G) < \rho(G - e).$$

In particular, for any spanning tree  $T$  of  $G$ ,

$$\rho(G) \leq \rho(T). \quad (1.4.1)$$

Similarly, adding a new edge  $f = st$  to  $G$  does not increase distances, while it does decrease at least one distance; the distance between  $s$  and  $t$  is 1 in  $G + f$  and at least 2 in  $G$ . Again by the Perron-Frobenius theorem,

$$\rho(G + f) < \rho(G). \quad (1.4.2)$$

Inequality (1.4.2) tells us immediately that the complete graph  $K_n$  has the minimum distance spectral radius among the connected graphs on  $n$  vertices, while inequality (1.4.1) shows that the maximum distance spectral radius will be attained for a particular tree.

Ruzieh and Powers [55] proved that for  $n \geq 3$  the path  $P_n$  has the maximum distance spectral radius among trees on  $n$  vertices. Stevanović and Ilić [57] generalized this result, and proved that among trees with fixed maximum degree  $\Delta$ , the broom graph has maximum distance spectral radius and proved that the star  $S_n$  is the unique graph with minimal distance spectral radius among trees on  $n$  vertices. Zhang and Godsil [65]



studied the behaviour of the distance spectral radius when a graph is perturbed by grafting edges, and then, as applications, they determined the graph with  $k$  cut vertices (respectively,  $k$  cut edges) having the minimal distance spectral radius. Ilić [36] have determined the unique graph that minimizes the distance spectral radius among trees on  $n$  vertices with given matching number  $m$ . The unicyclic graphs having maximal and minimal distance spectral radii have been obtained by Yu et al. [62]. Das [21] obtained lower and upper bounds for the distance spectral radius of a connected bipartite graph and characterize those graphs for which these bounds are best possible. Indulal [37] has found sharp bounds on the distance spectral radius and the distance energy of graphs. More results on the distance spectral radius can be found in [22, 41, 43, 60, 64].

In Chapter 3, we determine the graphs having maximal (minimal) distance spectral radius in the class of all graphs with a given number of pendent vertices. The results proved in this chapter are proved in [12, 52].

In Chapter 4, we determine the graphs having maximal (minimal) distance spectral radius in the class of all graphs without a pendent vertex. The results proved in this chapter are proved in [14, 53].

In Chapter 5, we determine the unique graph with minimal distance spectral radius in the class of all bipartite graphs with a given matching number. We also characterize the graphs with minimal distance spectral radius in the class of all bipartite graphs with a given vertex connectivity. The results proved in this chapter are proved in [51].

## 1.5 The distance Laplacian matrix of a graph

The *transmission*  $Tr(v)$  of a vertex  $v$  is defined to be the sum of the distances from  $v$  to all other vertices in  $G$ , i.e.,

$$Tr(v) = \sum_{u \in V(G)} d_{uv}.$$

The *distance Laplacian matrix* of a connected graph  $G$  is defined as  $D^L = D^L(G) = Tr(G) - D(G)$ , where  $Tr(G)$  is the diagonal matrix, whose  $i$ -th diagonal entry is the transmission of the  $i$ -th vertex [2]. Let  $\delta_1 \geq \delta_2 \geq \dots \geq \delta_{n-1} \geq \delta_n$  (we will use this ordering throughout the thesis) denote the eigenvalues of  $D^L$ . It can be easily verified that  $D^L$  is a positive semidefinite matrix. Moreover, since sum of each row and column of  $D^L$  is 0, so  $\delta_n = 0$ .

The following important result is obtained by Aouchiche and Hansen [2].

**Theorem 1.5.1.** [2] *Let  $G$  be a connected graph on  $n$  vertices and  $m \geq n$  edges. Consider the connected graph  $\tilde{G}$  obtained from  $G$  by the deletion of an edge. Let  $\delta_1 \geq \delta_2 \geq \dots \geq \delta_{n-1} \geq \delta_n$  and  $\tilde{\delta}_1 \geq \tilde{\delta}_2 \geq \dots \geq \tilde{\delta}_{n-1} \geq \tilde{\delta}_n$  denote the distance Laplacian eigenvalues of  $G$  and  $\tilde{G}$  respectively. Then  $\tilde{\delta}_i \geq \delta_i$ , for all  $i = 1, \dots, n$ .*

The authors have also proved that for a connected graph  $G$  of order  $n$ , the second smallest distance Laplacian eigenvalue is at least  $n$ , where the equality holds if and only if  $\overline{G}$  is disconnected. In that case, the multiplicity of  $n$  as a distance Laplacian eigenvalue of  $G$  is one less than the number of components of  $\overline{G}$ . They have obtained a relation connecting the Laplacian and the distance Laplacian eigenvalues for graphs having diameter at most 2.

In Chapter 6, we study the second smallest distance Laplacian eigenvalue of a graph when its complement is connected. We also study the distance Laplacian spectrum of a path. We prove that the largest distance Laplacian eigenvalue of a path is simple and describe the structure of the corresponding eigenvector.

# Chapter 2

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## On the Laplacian spectra of graphs with edge-pockets

### 2.1 Introduction

Till now, many graph operations such as the disjoint union, the Cartesian product, the Kronecker product, the corona, the edge corona, the neighbourhood corona and the subdivision vertex (edge) neighbourhood corona have been introduced, and their  $L$ -spectra are computed. These operations help to describe the spectrum of a relatively larger graph in terms of the spectra of some smaller graphs. The following is such a graph operation, introduced by Barik [9].

**Definition 2.1.1.** [9] *Let  $F, H_v$  be graphs of order  $n$  and  $m$ , respectively, where  $m > 1$ ,  $v$  be a specified vertex of  $H_v$  and  $u_1, \dots, u_k \in F$ . Let  $G = G[F, u_1, \dots, u_k, H_v]$  be the graph obtained by taking one copy of  $F$  and  $k$  copies of  $H_v$ , and then attaching the  $i$ -th copy of  $H_v$  to the vertex  $u_i$ ,  $i = 1, \dots, k$ , at the vertex  $v$  of  $H$  (identify  $u_i$  with the vertex  $v$  of the  $i$ -th copy). Then the copies of the graph  $H_v$  that are attached to the vertices  $u_i$ ,  $i = 1, \dots, k$  are referred to as pockets, and  $G$  is described as a graph with  $k$  pockets.*

In [9], the author has described the  $L$ -spectrum of  $G[F, u_1, \dots, u_k, H_v]$  using the  $L$ -spectra of  $F$  and  $H_v$ , when  $d_{H_v}(v) = m - 1$ . In that case, if a copy of  $H_v$  is attached to every vertex of  $F$ , each at the vertex  $v$  of  $H_v$ , that is, if  $G$  has  $n$  pockets, then  $G = G[F, u_1, \dots, u_n, H_v]$  is nothing but the corona  $F \circ H$ , where  $H = H_v - \{v\}$ . Then in [11], the complete  $L$ -spectrum of  $G$  is described using the spectra of  $F$  and  $H$ .

For a subset  $S$  of  $E(G)$ ,  $G_S$  denotes the subgraph of  $G$  containing the edges in  $S$  only and vertices, which are the endpoints of the edges in  $S$ . Motivated by Definition 2.1.1, we define the following.

**Definition 2.1.2.** *Let  $F$  and  $H_{uv}$  be two graphs of order  $n$  and  $m$ , respectively, where  $n \geq 2$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  such that  $H_{uv} - \{u\}$  is isomorphic*

to  $H_{uv} - \{v\}$ , and  $S = \{e_1, \dots, e_k\} \subseteq E(F)$ . Let  $G = G[F_S, H_{uv}]$  be the graph obtained by taking one copy of  $F$  and  $k$  copies of  $H_{uv}$ , and then pasting the edge  $uv$  in the  $i$ -th copy of  $H_{uv}$  with the edge  $e_i \in S$ , where  $i = 1, \dots, k$ . We call the copies of the graph  $H_{uv}$  that are pasted to the edges  $e_i$ ,  $i = 1, \dots, k$  edge-pockets, and  $G$  is a graph with  $k$  edge-pockets.

Note that order of  $G[F_S, H_{uv}]$  is  $n + k(m - 2)$ ; and if  $F$  has  $l_1$  edges and  $H_{uv}$  has  $l_2$  edges, then  $G[F_S, H_{uv}]$  has  $l_1 + (l_2 - 1)k$  edges. The following example illustrates Definition 2.1.2.

**Example 2.1.3.** Let us consider the graphs  $F$  and  $H_{uv}$  shown in Fig. 2.1. Note that  $uv$  is an edge of  $H_{uv}$  such that  $H_{uv} - \{u\}$  is isomorphic to  $H_{uv} - \{v\}$ . If  $S = \{e_1, e_2\} \subseteq E(F)$ , then the graph  $G[F_S, H_{uv}]$  is shown in Fig. 2.1.

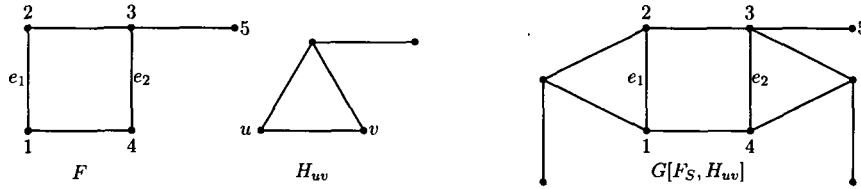


Figure 2.1: The graphs  $F$ ,  $H_{uv}$  and  $G[F_S, H_{uv}]$  of Example 2.1.3

This being a very general operation it is not possible to obtain the  $L$ -spectrum of  $G[F_S, H_{uv}]$  from the  $L$ -spectra of  $F$  and  $H_{uv}$ . But, a natural question remains is “how far can the  $L$ -spectrum of  $G[F_S, H_{uv}]$  be described by using the  $L$ -spectra of  $F$  and  $H_{uv}$ ?”

In Section 2.3, we show that the complete  $L$ -spectrum of  $G[F_S, H_{uv}]$  can be described in some particular cases. Finally, in a more general case, when  $F_S$  is a regular graph and  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$ , we describe all but  $n + k$  Laplacian eigenvalues of  $G[F_S, H_{uv}]$  using the Laplacian eigenvalues of  $H_{uv}$ . We also show that the remaining  $n + k$  Laplacian eigenvalues of  $G[F_S, H_{uv}]$  are independent of the graph  $H_{uv}$ . As an application, we show that these results enable us to construct infinitely many pairs of  $L$ -cospectral graphs.

## 2.2 Preliminaries

In this section, we give some preliminaries. The  $M$ -coronal  $\Gamma_M(x)$  of a matrix  $M$  of order  $n$  is defined [17, 44] to be the sum of the entries of the matrix  $(xI_n - M)^{-1}$ , that

is,

$$\Gamma_M(x) = \mathbf{1}_n^T (xI_n - M)^{-1} \mathbf{1}_n.$$

It is known [17, Proposition 2] that, if  $M$  is a matrix of order  $n$  with each row sum equal to a constant  $l$ , then

$$\Gamma_M(x) = \frac{n}{x-l} \quad (2.2.1)$$

In particular, since for any graph  $G$  on  $n$  vertices, each row sum of  $L(G)$  is equal to 0, we have

$$\Gamma_{L(G)}(x) = \frac{n}{x} \quad (2.2.2)$$

The following theorem of [48] will be needed to prove our main results of this chapter.

**Theorem 2.2.1.** [48] *Let  $G_1, G_2$  be two graphs on disjoint sets of  $m, n$ , vertices, respectively. If  $\sigma^L(G_1) = \{\mu_1(G_1), \dots, \mu_{m-1}(G_1), \mu_m(G_1) = 0\}$  and  $\sigma^L(G_2) = \{\mu_1(G_2), \dots, \mu_{n-1}(G_2), \mu_n(G_2) = 0\}$ , then  $\sigma^L(G_1 \vee G_2) = \{m+n, n+\mu_1(G_1), \dots, n+\mu_{m-1}(G_1), m+\mu_1(G_2), \dots, m+\mu_{n-1}(G_2), 0\}$ .*

## 2.3 Spectrum of $G[F_S, H_{uv}]$

In this section, we obtain the  $L$ -spectrum of  $G[F_S, H_{uv}]$  with the help of the coronal of a matrix. The 0-1 *vertex-edge incidence matrix*  $R(G) = [r_{i,e_j}]$  of a graph  $G$  is the matrix with rows and columns indexed by vertices and edges of  $G$ , respectively, where  $r_{i,e_j} = 1$  if the vertex  $i$  is incident with the edge  $e_j$  and 0 otherwise [7]. Thus, if  $G$  is a  $r$ -regular graph, then  $R(G)R(G)^T = A(G) + rI$ . Following is one of the main results of this section.

**Theorem 2.3.1.** *Let  $F$  and  $H_{uv}$  be two graphs of order  $n$  and  $m$ , respectively, where  $n \geq 2$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  and  $S$  be a  $k$ -element subset of  $E(F)$ , such that  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m-1$  and  $F_S$  is a spanning subgraph of  $F$ . If  $F_S$  is  $r$ -regular, then*

$$\phi(L(G[F_S, H_{uv}]); x) = \phi(L(H); x-2)^k \phi(M; x),$$

$$\text{where } H = H_{uv} - \{u, v\}$$

$$\text{and } M = r((m-2) + \Gamma_{L(H)}(x-2))I_n + L(F) + \Gamma_{L(H)}(x-2)A(F_S).$$

**Proof.** Since  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$ , so  $H_{uv}$  can be written as  $H_{uv} = (\{u, v\}, \{uv\}) \vee H$ . Thus, with a permutation similarity operation we can write

$$L(G[F_S, H_{uv}]) = \left[ \begin{array}{c|c} L(F) + r(m-2)I_n & \mathbb{1}_{m-2}^T \otimes -R(F_S) \\ \hline \mathbb{1}_{m-2} \otimes -R(F_S)^T & (L(H) + 2I_{m-2}) \otimes I_k \end{array} \right].$$

The Laplacian characteristic polynomial of  $G[F_S, H_{uv}]$  is given by

$$\begin{aligned} & \phi(L(G[F_S, H_{uv}]); x) \\ = & \det \left[ \begin{array}{c|c} xI_n - L(F) - r(m-2)I_n & \mathbb{1}_{m-2}^T \otimes R(F_S) \\ \hline \mathbb{1}_{m-2} \otimes R(F_S)^T & ((x-2)I_{m-2} - L(H)) \otimes I_k \end{array} \right] \\ = & \det \left( (x-2)I_{m-2} - L(H) \right)^k \cdot \det(S_1) \\ = & \phi(L(H); x-2)^k \cdot \det(S_1), \end{aligned} \tag{2.3.1}$$

$$\begin{aligned} \text{where } S_1 &= xI_n - L(F) - r(m-2)I_n - \Gamma_{L(H)}(x-2)R(F_S)R(F_S)^T \\ &= xI_n - L(F) - r(m-2)I_n - \Gamma_{L(H)}(x-2)(A(F_S) + rI_n) \\ &= xI_n - M \end{aligned} \tag{2.3.2}$$

is the Schur complement of  $((x-2)I_{m-2} - L(H)) \otimes I_k$ . Using (2.3.2) in (2.3.1) we have the result.  $\blacksquare$

A *factor* of a graph  $G$  is a spanning subgraph of  $G$  which is not empty [33]. A graph  $G$  is called the *sum of factors*  $G_i$  if it is their line-disjoint union, and such a union is called the *factorization* of  $G$ . A *k-factor* is regular of degree  $k$ . If  $G$  is the sum of  $k$ -factors, their union is called a *k-factorization* and  $G$  itself is *k-factorable*. In particular,  $K_{2k}$  is 1-factorable whereas  $K_{2k+1}$  is 2-factorable [33].

**Corollary 2.3.2.** *Let  $F = K_{2k}$  and  $H_{uv}$  be a graph of order  $m$ , where  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  and  $S$  be a  $k$ -element subset of  $E(F)$ , such that  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$  and  $F_S$  is a 1-factor of  $F$ . If  $\sigma^L(H_{uv}) = \{\mu_1(H_{uv}), \mu_2(H_{uv}), \dots, \mu_{m-1}(H_{uv}), \mu_m(H_{uv}) = 0\}$ , then  $\sigma^L(G[F_S, H_{uv}])$  consists of the eigenvalues*

- (a) 0,  $m$  with multiplicity 1;
- (b)  $\mu_j(H_{uv})$  with multiplicity  $k$ , for each  $j = 3, 4, \dots, m - 1$ ;
- (c)  $m + 2k - 2$  with multiplicity  $k$ ;

(d) two roots of the equation  $x^2 - (2k + m)x + 4k = 0$ , each with multiplicity  $k - 1$ .

**Proof.** By Theorem 2.3.1, we have

$$\phi(L(G[F_S, H_{uv}]); x) = (x - 2)^k \prod_{j=1}^{m-3} (x - 2 - \mu_j(H))^k \cdot \phi(M; x), \quad (2.3.3)$$

where  $H = H_{uv} - \{u, v\}$ ,

$\sigma^L(H) = \{\mu_1(H), \mu_2(H), \dots, \mu_{m-3}(H), \mu_{m-2}(H) = 0\}$  and

$$\begin{aligned} M &= ((m - 2) + \Gamma_{L(H)}(x - 2))I_{2k} + (2kI_{2k} - J_{2k}) \\ &\quad + \Gamma_{L(H)}(x - 2)(I_k \otimes A(K_2)) \\ &= \left( (m - 2) + \frac{m - 2}{x - 2} + 2k \right) I_{2k} - J_{2k} + \frac{m - 2}{x - 2} (I_k \otimes A(K_2)) \\ &\quad [\text{by (2.2.2)}]. \end{aligned}$$

Let  $M_1 = ((m - 2) + \frac{m-2}{x-2} + 2k) I_{2k} + \frac{m-2}{x-2} (I_k \otimes A(K_2))$  so that  $M = M_1 - J_{2k}$ .

$$\begin{aligned} \text{Now } \phi(M; x) &= \det(xI_{2k} - M) \\ &= \det(xI_{2k} - M_1 + J_{2k}) \\ &= \det(xI_{2k} - M_1) + \mathbb{1}_{2k}^T \text{adj}(xI_{2k} - M_1) \mathbb{1}_{2k} \\ &\quad [\text{where 'adj' is the adjoint of a matrix}] \\ &= \det(xI_{2k} - M_1) \left\{ 1 + \mathbb{1}_{2k}^T (xI_{2k} - M_1)^{-1} \mathbb{1}_{2k} \right\} \\ &= \det(xI_{2k} - M_1) \left\{ 1 + \Gamma_{M_1}(x) \right\} \\ &= (x - m + 2 - 2k)^k \cdot \frac{(x^2 - (2k + m)x + 4k)^k}{(x - 2)^k} \cdot \left\{ 1 + \frac{2k(x - 2)}{x^2 - (2k + m)x + 4k} \right\} \\ &\quad [\text{by (2.2.1)}] \\ &= x(x - m)(x - m + 2 - 2k)^k \frac{(x^2 - (2k + m)x + 4k)^{k-1}}{(x - 2)^k}. \quad (2.3.4) \end{aligned}$$

Using (2.3.4) in (2.3.3), and by Theorem 2.2.1, we have the result.  $\blacksquare$

The following result describes the structure of the adjacency eigenvalues of a cycle of order  $n$ , which will be useful to prove the next result of this section.

**Lemma 2.3.3.** [7] For  $n \geq 3$ , the eigenvalues of  $A(C_n)$  are  $2 \cos \frac{2\pi l}{n}$ , where  $l = 1, 2, \dots, n$ .

**Corollary 2.3.4.** *Let  $F = K_n$  and  $H_{uv}$  be a graph of order  $m$ , where  $n \geq 3$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  and  $S$  be a  $k$ -element subset of  $E(F)$ , such that  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$  and  $F_S = C_n$ . If  $\sigma^L(H_{uv}) = \{\mu_1(H_{uv}), \mu_2(H_{uv}), \dots, \mu_{m-1}(H_{uv}), \mu_m(H_{uv}) = 0\}$ , then  $\sigma^L(G[F_S, H_{uv}])$  consists of the eigenvalues*

- (a)  $0, 2m - 2$  with multiplicity 1;
- (b)  $\mu_j(H_{uv})$  with multiplicity  $n$ , for each  $j = 3, 4, \dots, m - 1$ ;
- (c) two roots of the equation  $x^2 - (2m - 2 + n)x + 2n + 2(m - 2)(1 - \cos \frac{2\pi l}{n}) = 0$ , for each  $l = 1, 2, \dots, n - 1$ .

**Proof.** By Theorem 2.3.1, we have

$$\phi(L(G[F_S, H_{uv}]); x) = (x - 2)^n \prod_{j=1}^{m-3} (x - 2 - \mu_j(H))^n \cdot \phi(M; x), \quad (2.3.5)$$

where  $H = H_{uv} - \{u, v\}$

$$\begin{aligned} \sigma^L(H) &= \{\mu_1(H), \mu_2(H), \dots, \mu_{m-3}(H), \mu_{m-2}(H) = 0\} \text{ and} \\ M &= 2((m - 2) + \Gamma_{L(H)}(x - 2))I_n + (nI_n - J_n) + \Gamma_{L(H)}(x - 2)A(C_n) \\ &= \left(2(m - 2) + \frac{2(m - 2)}{x - 2} + n\right) I_n - J_n + \frac{m - 2}{x - 2} A(C_n) \text{ [by (2.2.2)].} \end{aligned}$$

Let  $M_1 = \left(2(m - 2) + \frac{2(m-2)}{x-2} + n\right) I_n + \frac{m-2}{x-2} A(C_n)$  so that  $M = M_1 - J_n$ .

$$\begin{aligned} \text{Now } \phi(M; x) &= \det(xI_n - M) \\ &= \det(xI_n - M_1 + J_n) \\ &= \det(xI_n - M_1) + \mathbf{1}_n^T \text{adj}(xI_n - M_1) \mathbf{1}_n \\ &= \det(xI_n - M_1) \left\{ 1 + \mathbf{1}_n^T (xI_n - M_1)^{-1} \mathbf{1}_n \right\} \\ &= \det(xI_n - M_1) \left\{ 1 + \Gamma_{M_1}(x) \right\} \\ &= \frac{x^2 - (2m - 2 + n)x + 2n}{x - 2} \left\{ 1 + \frac{n(x - 2)}{x^2 - (2m - 2 + n)x + 2n} \right\}. \\ &\quad \prod_{l=1}^{n-1} \frac{x^2 - (2m - 2 + n)x + 2n + 2(m - 2)(1 - \cos \frac{2\pi l}{n})}{x - 2} \\ &\quad \text{[by (2.2.1) and Lemma 2.3.3]} \end{aligned}$$



$$\Rightarrow \phi(M; x) = \frac{x(x - 2m + 2)}{x - 2} \cdot \prod_{l=1}^{n-1} \frac{x^2 - (2m - 2 + n)x + 2n + 2(m - 2)(1 - \cos \frac{2\pi l}{n})}{x - 2}$$

(2.3.6)

Using (2.3.6) in (2.3.5), and by Theorem 2.2.1, we have the result.  $\blacksquare$

**Remark 2.3.5.** *If in Corollary 2.3.4,  $n$  is odd, then it can be seen as an analogue of Corollary 2.3.2 for odd complete graph and a 2-factor of it.*

Now, we consider a more general case. Let  $F$  and  $H_{uv}$  be two graphs of order  $n$  and  $m$ , respectively, where  $n \geq 2$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  and  $S$  be a  $k$ -element subset of  $E(F)$ , such that  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$ . If  $F_S$  is a regular graph, then except  $n + k$  Laplacian eigenvalues, we describe all other Laplacian eigenvalues of  $G[F_S, H_{uv}]$  using the Laplacian eigenvalues of  $H_{uv}$ . We also show that the remaining  $n + k$  Laplacian eigenvalues of  $G[F_S, H_{uv}]$  are independent of the graph  $H_{uv}$ . Let  $C_e^m$  be the graph of order  $m$  formed by  $m - 2$  triangles such that each pair of triangles have exactly one common edge  $e$  (See Fig. 2.2).

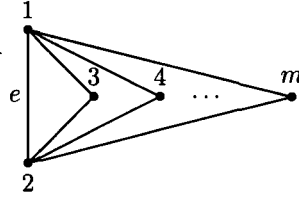


Figure 2.2: The graph  $C_e^m$ .

**Theorem 2.3.6.** *Let  $F$  and  $H_{uv}$  be two graphs of order  $n$  and  $m$ , respectively, where  $n \geq 2$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}$  and  $S$  be a  $k$ -element subset of  $E(F)$  such that  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$ . If  $F_S$  is a regular graph and  $\sigma^L(H_{uv}) = \{\mu_1(H_{uv}), \mu_2(H_{uv}), \dots, \mu_{m-1}(H_{uv}), \mu_m(H_{uv}) = 0\}$ , then  $\sigma^L(G[F_S, H_{uv}])$  consists of the eigenvalues*

- (a)  $\mu_j(H_{uv})$  with multiplicity  $k$ , for each  $j = 3, 4, \dots, m - 1$  and
- (b)  $\lambda \in \sigma^L(G[F_S, C_e^m]) - \underbrace{\{2, 2, \dots, 2\}}_{(m-3)k}$ , where  $e = uv$  of  $C_e^m$ .

**Proof.** Since  $d_{H_{uv}}(u) = d_{H_{uv}}(v) = m - 1$ , so  $H_{uv}$  can be written as  $H_{uv} = (\{u, v\}, \{uv\}) \vee H$ , where  $H = H_{uv} - \{u, v\}$ . Let  $F_S$  be a  $r$ -regular graph on the

first  $p$  vertices of  $F$ . Thus, with a permutation similarity operation we can write

$$L(G[F_S, H_{uv}]) = \begin{bmatrix} L(F) + r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} & \mathbb{1}_{m-2}^T \otimes \begin{bmatrix} -R(F_S) \\ \mathbf{0}_{n-p \times k} \end{bmatrix} \\ \hline \mathbb{1}_{m-2} \otimes \begin{bmatrix} -R(F_S)^T & \mathbf{0}_{k \times n-p} \end{bmatrix} & (L(H) + 2I_{m-2}) \otimes I_k \end{bmatrix}.$$

The Laplacian characteristic polynomial of  $G[F_S, H_{uv}]$  is given by

$$\begin{aligned} & \phi(L(G[F_S, H_{uv}]); x) \\ &= \det \begin{bmatrix} xI_n - L(F) - r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} & \mathbb{1}_{m-2}^T \otimes \begin{bmatrix} R(F_S) \\ \mathbf{0}_{n-p \times k} \end{bmatrix} \\ \hline \mathbb{1}_{m-2} \otimes \begin{bmatrix} R(F_S)^T & \mathbf{0}_{k \times n-p} \end{bmatrix} & ((x-2)I_{m-2} - L(H)) \otimes I_k \end{bmatrix} \\ &= \det \left( (x-2)I_{m-2} - L(H) \right)^k \cdot \det(S_1) \\ &= \phi(L(H); x-2)^k \cdot \det(S_1) \\ &= (x-2)^k \prod_{j=1}^{m-3} (x-2 - \mu_j(H))^k \cdot \det(S_1), \end{aligned} \tag{2.3.7}$$

where

$$\begin{aligned} S_1 &= xI_n - L(F) - r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\ &\quad - \Gamma_{L(H)}(x-2) \begin{bmatrix} R(F_S)R(F_S)^T & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\ &= xI_n - L(F) - (m-2) \begin{bmatrix} rI_p + \frac{1}{x-2}R(F_S)R(F_S)^T & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\ &\quad \text{[by (2.2.2)]} \end{aligned} \tag{2.3.8}$$

is the Schur complement of  $((x-2)I_{m-2} - L(H)) \otimes I_k$ .

Similarly, we have

$$L(G[F_S, C_e^m]) = \begin{bmatrix} L(F) + r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} & \mathbb{1}_{m-2}^T \otimes \begin{bmatrix} -R(F_S) \\ \mathbf{0}_{n-p \times k} \end{bmatrix} \\ \hline \mathbb{1}_{m-2} \otimes \begin{bmatrix} -R(F_S)^T & \mathbf{0}_{k \times n-p} \end{bmatrix} & 2I_{m-2} \otimes I_k \end{bmatrix}.$$

Thus, the Laplacian characteristic polynomial of  $G[F_S, C_e^m]$  is given by

$$\begin{aligned}
& \phi(L(G[F_S, C_e^m]); x) \\
&= \det \left[ \begin{array}{c|c} xI_n - L(F) - r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} & \mathbf{1}_{m-2}^T \otimes \begin{bmatrix} R(F_S) \\ \mathbf{0}_{n-p \times k} \end{bmatrix} \\ \hline \mathbf{1}_{m-2} \otimes \begin{bmatrix} R(F_S)^T & \mathbf{0}_{k \times n-p} \end{bmatrix} & (x-2)I_{m-2} \otimes I_k \end{array} \right] \\
&= \det \left( (x-2)I_{m-2} \right)^k \cdot \det(S_2) = (x-2)^{k(m-2)} \cdot \det(S_2), \tag{2.3.9}
\end{aligned}$$

where

$$\begin{aligned}
S_2 &= xI_n - L(F) - r(m-2) \begin{bmatrix} I_p & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\
&\quad - \Gamma_{2I_{m-2}}(x) \begin{bmatrix} R(F_S)R(F_S)^T & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\
&= xI_n - L(F) - (m-2) \begin{bmatrix} rI_p + \frac{1}{x-2}R(F_S)R(F_S)^T & \mathbf{0}_{p \times n-p} \\ \mathbf{0}_{n-p \times p} & \mathbf{0}_{n-p \times n-p} \end{bmatrix} \\
&\quad \text{[by (2.2.1)]} \tag{2.3.10}
\end{aligned}$$

is the Schur complement of  $(x-2)I_{m-2} \otimes I_k$ .

By (2.3.10) and (2.3.8), we have  $S_1 = S_2$ . Hence using (2.3.9) in (2.3.7) we get

$$\phi(L(G[F_S, H_{uv}]); x) = \prod_{j=1}^{m-3} (x-2 - \mu_j(H))^k \cdot \frac{\phi(L(G[F_S, C_e^m]); x)}{(x-2)^{k(m-3)}}. \tag{2.3.11}$$

For each  $j$ , let  $F_{1j}^l$  denote a column vector of order  $n + k(m-2)$  with only two non zero components 1 and -1 corresponding to the 1<sup>st</sup> vertex and the  $j^{\text{th}}$  vertex, respectively, in the  $l^{\text{th}}$  copy of  $C_e^m - \{u, v\}$ , where  $2 \leq j \leq m-2$  and  $1 \leq l \leq k$ . Then  $\{F_{1j}^l : j = 2, 3, \dots, m-2; l = 1, 2, \dots, k\}$  is a set of  $(m-3)k$  linearly independent eigenvectors of  $L(G[F_S, C_e^m])$  corresponding to the eigenvalue 2. Therefore, by (2.3.11) and Theorem 2.2.1, the result follows.  $\blacksquare$

The above theorem is illustrated by the following example.

**Example 2.3.7.** Consider the graphs  $F, H_{uv}$  of order 3 and 5, respectively, in Fig. 2.3. The vertices  $u$  and  $v$  of  $H_{uv}$  have degree 4. Let  $S = \{f\} \subseteq E(F)$ ,  $G[F_S, H_{uv}]$  is the graph obtained by taking one copy of  $H_{uv}$  and pasting the edge  $uv$  to the edge  $f$  of  $F$ , and  $G[F_S, C_e^5]$  is the graph obtained by taking one copy of  $C_e^5$  and pasting the edge  $e$  to the edge  $f$  of  $F$ .

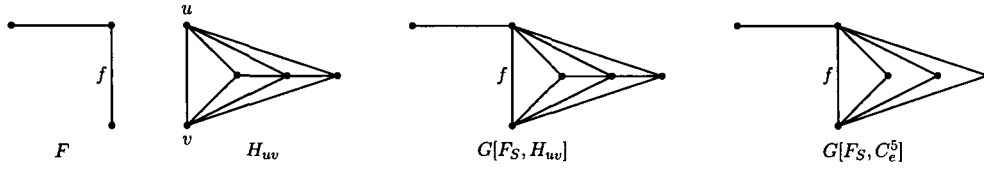


Figure 2.3: The graphs  $F$ ,  $H_{uv}$ ,  $G[F_S, H_{uv}]$  and  $G[F_S, C_e^5]$  in Example 2.3.7

It can be checked that  $\sigma^L(H_{uv}) = \{5, 5, 5, 3, 0\}$ ,  $\sigma^L(G[F_S, C_e^5]) = \{6, 5, 2, 2, 1, 0\}$  and  $\sigma^L(G[F_S, H_{uv}]) = \{6, 5, 5, 3, 1, 0\}$ . Notice that  $\sigma^L(G[F_S, H_{uv}])$  can be obtained from  $\sigma^L(G[F_S, C_e^5])$  and  $\sigma^L(H_{uv})$  as described in Theorem 2.3.6.

**Remark 2.3.8.** The largest Laplacian eigenvalue of a graph  $G$  is called the Laplacian spectral radius of  $G$  and is denoted by  $\rho^L(G)$ . Notice that  $G = G[F_S, H_{uv}]$  in Theorem 2.3.6 contains vertices of degree  $m$ . Thus by using Theorem 4.2 of [7],  $\rho^L(G) \geq m + 1 > \mu_1(H_{uv})$ . This implies that  $\rho^L(G)$  is one of the  $n + k$  eigenvalues of  $G$  that are independent of the graph  $H_{uv}$ .

**Remark 2.3.9.** In Theorem 2.3.6, if we take  $S = E(F)$ , then  $G[F_S, H_{uv}]$  is nothing but the edge corona  $F \diamond H$ , where  $H = H_{uv} - \{u, v\}$ . If  $F$  is a regular graph, then the complete  $L$ -spectrum of  $G[F_S, H_{uv}]$  is described using the  $L$ -spectra of  $F$  and  $H$  [35].

From Theorem 2.3.6 we have the following corollary, which enables us to construct infinitely many pairs of  $L$ -cospectral graphs.

**Corollary 2.3.10.** Let  $F$  be a graph of order  $n$ , and  $H_{uv}^1$ ,  $H_{xy}^2$  be two disjoint graphs of same order  $m$ , where  $n \geq 2$  and  $m \geq 3$ . Let  $uv$  be a specified edge of  $H_{uv}^1$  and  $xy$  be a specified edge of  $H_{xy}^2$  such that  $d_{H_{uv}^1}(u) = d_{H_{uv}^1}(v) = d_{H_{xy}^2}(x) = d_{H_{xy}^2}(y) = m - 1$  and  $S$  be a  $k$ -element subset of  $E(F)$ . If  $F_S$  is a regular graph and  $H_{uv}^1$  is  $L$ -cospectral to  $H_{xy}^2$ , then  $G[F_S, H_{uv}^1]$  is  $L$ -cospectral to  $G[F_S, H_{xy}^2]$ .

# Chapter 3

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## On the distance spectral radius of graphs with $r$ pendent vertices

### 3.1 Introduction

Let  $\mathcal{G}_n^r$  be the class of all connected graphs of order  $n$  with  $r$  pendent vertices, where  $r \geq 1$ . In Section 3.2, we introduce a graph transformation which affects the distance spectral radius and in Section 3.3, we use it to determine the unique graph with minimal distance spectral radius in  $\mathcal{G}_n^r$ .

Let  $\mathbb{T}_n^r$  be the class of all trees on  $n$  vertices with  $r$  pendent vertices and  $\mathcal{T}_n^m$  be the class of all trees on  $n$  vertices with matching number  $m$ . The *dumbbell*  $D(n, a, b)$  consists of the path  $P_{n-a-b}$  together with  $a$ -independent vertices adjacent to one pendent vertex of  $P$  and  $b$ -independent vertices adjacent to the other pendent vertex, where  $a, b \geq 1$ . Ilić in [36], has determined the unique graph that minimizes the distance spectral radius in  $\mathcal{T}_n^m$ . Furthermore, the author posed the following conjecture.

**Conjecture 3.1.1.** *Among trees on  $n$  vertices and matching number  $m$ , the dumbbell  $D(n, \lceil \frac{n+1}{2} \rceil - m, \lfloor \frac{n+1}{2} \rfloor - m)$  is the unique tree that maximizes the distance spectral radius.*

In Section 3.4, we give an ordering of the components of the Perron vector of a dumbbell. As applications of this result, we give an affirmative answer to the Conjecture 3.1.1, and find the unique tree that maximizes the distance spectral radius in  $\mathbb{T}_n^r$ .

In Section 3.5, we characterize the unique graph that maximizes the distance spectral radius in  $\mathcal{G}_n^r$  for each  $r \in \{2, 3, n-3, n-2, n-1\}$ . In [61], Yu et al. have found the graph with maximal distance spectral radius in  $\mathcal{G}_n^1$ . They have also posed the following conjecture.

**Conjecture 3.1.2.** *If  $G$  is a graph with the maximal distance spectral radius among all graphs on  $n$  vertices and  $r$  pendent vertices, then  $G \cong D(n, \lceil \frac{r}{2} \rceil, \lfloor \frac{r}{2} \rfloor)$ , where  $4 \leq r \leq n - 2$ .*

Using the results obtained in Section 3.4, we give an affirmative solution to the above conjecture. Hence the graph having the maximal distance spectral radius in  $\mathcal{G}_n^r$  is completely characterized.

## 3.2 A Transformation

Here we give a graph transformation which will be useful to derive one of our main results of this chapter.

**Lemma 3.2.1.** *Let  $G$  be a graph with a clique  $K_s$  of order  $s$  ( $s \geq 2$ ) and  $u, v$  be two vertices on the clique with  $p, q$  pendent vertices, respectively, where  $d_G(v) = q + s - 1$ . If  $p \geq q \geq 1$  and  $G' = G - vw + uw$ , where  $w$  is a pendent vertex adjacent to  $v$  in  $G$ , then  $\rho(G) > \rho(G')$ .*

**Proof.**

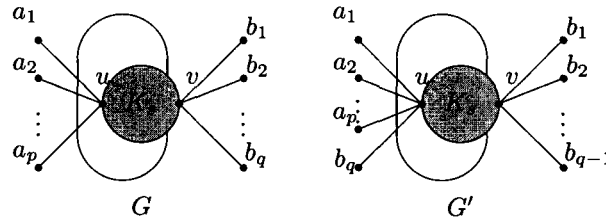


Figure 3.1: The graphs  $G$  and  $G'$  in Lemma 3.2.1

Let the vertices of  $G$  and  $G'$  be labelled as in Fig 3.1. We partition  $V(G) = V(G')$  into  $A_1 \cup A_2 \cup \{u\} \cup \{v\} \cup A \cup B \cup \{b_q\}$ , where  $A = \{a_1, a_2, \dots, a_p\}$ ,  $B = \{b_1, b_2, \dots, b_{q-1}\}$ ,  $A_1 = \{w \mid d(w, u) < d(w, v)\} - A - \{u, b_q\}$ ,  $A_2 = \{w \mid d(w, u) = d(w, v)\}$ . As we pass from  $G$  to  $G'$ , the distances within  $A \cup A_1 \cup A_2 \cup \{u\} \cup \{v\} \cup B$  are unchanged; the distance of  $b_q$  with  $A_2$  is also unchanged; the distance of  $b_q$  from a vertex in  $A \cup A_1 \cup \{u\}$  is decreased by 1, whereas the distance of  $b_q$  from a vertex in  $B \cup \{v\}$  is increased by 1. If the distance matrices are partitioned according to

$A_1, A_2, \{u\}, \{v\}, A, B,$  and  $\{b_q\}$ , then their difference is

$$D(G) - D(G') = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & e_{A_1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & e_A \\ 0 & 0 & 0 & 0 & 0 & 0 & -e_B \\ e_{A_1}^T & 0 & 1 & -1 & e_A^T & -e_B^T & 0 \end{bmatrix},$$

where  $e_i = \underbrace{(1, \dots, 1)^T}_{|i|} = \mathbf{1}_{|i|}$  and  $i = A_1, A, B$ . We denote  $\rho(G)$  by  $\rho$  and  $\rho(G')$  by  $\rho_1$ . Let  $X$  be an eigenvector of  $D(G')$  corresponding to  $\rho_1$ . By symmetry the components of  $X$  have the same value, say  $a$  for the vertices in  $A \cup \{b_q\}$  and  $b$  for the vertices in  $B$  whereas we take the components of  $X$  as  $y_1, y_2, \dots, y_t$ , for the vertices in  $A_1, z_1, z_2, \dots, z_l$ , for the vertices in  $A_2, x_1$  for  $u$  and  $x_2$  for  $v$ . Then  $X$  can be written as,

$$X = \left( y_1, y_2, \dots, y_t, z_1, z_2, \dots, z_l, x_1, x_2, \underbrace{a, \dots, a}_p, \underbrace{b, \dots, b}_{q-1}, a \right)^T.$$

We now have

$$\frac{1}{2}(\rho - \rho_1) \geq \frac{1}{2}X^T(D(G) - D(G'))X > a \left[ x_1 - x_2 + pa - b(q-1) + \sum_{i=1}^t y_i \right]. \quad (3.2.1)$$

From eigenequations we have

$$\begin{aligned} \rho_1 x_2 - \rho_1 x_1 &= x_1 + (p+1)a - x_2 - (q-1)b + \sum_{i=1}^t y_i \\ \Rightarrow (\rho_1 + 1)(x_2 - x_1) &= (p+1)a - (q-1)b + \sum_{i=1}^t y_i, \end{aligned} \quad (3.2.2)$$

$$\begin{aligned} \rho_1 b - \rho_1 a &= x_1 - x_2 - b - qb + pa + 3a + \sum_{i=1}^t y_i \\ \Rightarrow (\rho_1 + 1)(b - a) &= x_1 - x_2 - qb + pa + 2a + \sum_{i=1}^t y_i, \end{aligned} \quad (3.2.3)$$

$$\begin{aligned} \rho_1 a - \rho_1 x_2 &= \sum_{j=1}^l z_j + 2x_2 - 2a + 2(q-1)b \\ \Rightarrow (\rho_1 + 2)(a - x_2) &= \sum_{j=1}^l z_j + 2(q-1)b. \end{aligned} \quad (3.2.4)$$

From (3.2.4), we conclude that  $a > x_2$ . If we assume  $a \geq b$ , then the L.H.S. of (3.2.3) is non positive, whereas the R.H.S. of (3.2.3) is

$$x_1 + q(a - b) + (p - q)a + 2a - x_2 + \sum_{i=1}^t y_i,$$

which is positive as  $a > x_2$ , an absurdity. Thus we must have  $a < b$ .

Therefore by (3.2.3), we have

$$\begin{aligned} x_1 - x_2 - qb + pa + 2a + \sum_{i=1}^t y_i &> 0 \\ \Rightarrow q(a - b) &> x_2 - x_1 - (p - q)a - 2a - \sum_{i=1}^t y_i. \end{aligned}$$

Again by (3.2.2), we have

$$\begin{aligned} (\rho_1 + 1)(x_2 - x_1) &= q(a - b) + (p - q)a + a + b + \sum_{i=1}^t y_i \\ &> x_2 - x_1 + b - a, \text{ which gives } x_2 > x_1. \end{aligned}$$

Since distance matrix is nonnegative and irreducible, its spectral radius is bounded below by the minimum row sum and thus we have

$$s + 2q + p - 2 < \rho_1 \text{ i.e., } 2q + p < \rho_1. \quad (3.2.5)$$

If  $p = q + t$ , where  $t \geq 0$ , then

$$\begin{aligned} pa - (q - 1)b &= p(a - b) + (t + 1)b \\ &= \frac{p}{\rho_1 + 1} \left[ x_2 + (p - t)b - (p + 2)a - x_1 - \sum_{i=1}^t y_i \right] + (t + 1)b \\ &= \frac{1}{\rho_1 + 1} \left[ p(x_2 - x_1) + p^2(b - a) - ptb - 2pa - p \sum_{i=1}^t y_i \right. \\ &\quad \left. + (t + 1)b(\rho_1 + 1) \right] \end{aligned}$$

and

$$\begin{aligned} x_2 - x_1 &= \frac{1}{\rho_1 + 1} \left[ (p + 1)a - (p - t - 1)b + \sum_{i=1}^t y_i \right] \\ &= \frac{1}{\rho_1 + 1} \left[ p(a - b) + a + (t + 1)b + \sum_{i=1}^t y_i \right]. \end{aligned}$$



Therefore,  $pa - (q - 1)b - (x_2 - x_1) + \sum_{i=1}^t y_i$

$$= \frac{1}{\rho_1 + 1} [p(x_2 - x_1) + (p^2 + p)(b - a) + (t + 1)b\rho_1 - ptb - 2pa - a + (\rho_1 - p) \sum_{i=1}^t y_i]. \quad (3.2.6)$$

From (3.2.5), we have  $\rho_1 > 2q + p = 3p - 2t$ .

Therefore,

$$\begin{aligned} (t + 1)b\rho_1 &> (t + 1)b(3p - 2t) \\ &= ptb + 2bp + (2btp + bp - 2t^2b - 2tb) \\ &> ptb + 2ap + b(2tp + p - 2t^2 - 2t). \end{aligned} \quad (3.2.7)$$

Since  $t \geq 0$  and  $q \geq 1$ , so

$$\begin{aligned} 2tp + p - 2t^2 - 2t &= 2(p - q)p + p - 2(p - q)^2 - 2(p - q) \\ &= 2q(1 - q + p) - p \\ &= 2q(1 + t) - p \\ &= q + 2qt + q - p \\ &= q + 2qt - t \geq 1. \end{aligned}$$

Therefore, (3.2.7) gives

$$\begin{aligned} (t + 1)b\rho_1 &> ptb + 2ap + b > ptb + 2ap + a \\ \Rightarrow (t + 1)b\rho_1 - ptb - 2pa - a &> 0. \end{aligned} \quad (3.2.8)$$

Using (3.2.6) and (3.2.8) in (3.2.1) we get,  $\rho > \rho_1$ . ■

### 3.3 Graph with Minimal Distance Spectral Radius in $\mathcal{G}_n^r$

In this section, we determine the graph with minimal distance spectral radius in  $\mathcal{G}_n^r$ . Let  $K_n^k$  denote the graph obtained by joining  $k$  isolated vertices to one vertex of  $K_{n-k}$ . Further, we notice that  $\mathcal{G}_3^1 = \phi$ . However, when  $n \geq 4$ ,  $\mathcal{G}_n^r \neq \phi$  if and only if  $0 \leq r \leq n - 1$ ; furthermore,  $\mathcal{G}_n^{n-1}$  has only one graph, namely,  $K_{1,n-1}$ , and  $\mathcal{G}_n^{n-2}$  consists of precisely all dumbbells  $D(n, a, b)$ , where  $a + b = n - 2$ .

**Theorem 3.3.1.** *For  $n \geq 4$  and  $1 \leq r \leq n - 1$ , there is a unique graph in  $\mathcal{G}_n^r$  with minimal distance spectral radius, namely  $K_n^r$  for  $r \neq n - 2$  and the dumbbell  $D(n, n - 3, 1)$  for  $r = n - 2$ .*

**Proof.** Suppose that  $G^*$  is a graph with minimal distance spectral radius among all graphs in  $\mathcal{G}_n^r$ . If  $r = n - 1$ ,  $\mathcal{G}_n^r$  consists of only one graph, i.e., the star  $K_{1,n-1} = K_n^{n-1}$ , and the result follows in this case. Assume that  $1 \leq r \leq n - 3$ . Let  $P$  be the set of all pendent vertices of  $G^*$ , and let  $W$  be the set of all quasi-pendent vertices of  $G^*$ . We first claim that  $G^*[V - P]$  is a complete graph; otherwise by adding an edge between any two non adjacent vertices of  $V - P$ , the resulting graph still belongs to  $\mathcal{G}_n^r$  and by (1.4.2), it has a smaller distance spectral radius, which contradicts the minimality of  $G^*$ .

Thus, if  $r = 1$ , then clearly  $G^* \cong K_n^1$ . For  $2 \leq r \leq n - 3$ , we claim that  $W$  contains exactly one point. Otherwise, let  $w_1, w_2 \in W$  be two vertices such that there are  $p$  and  $q$  pendent vertices adjacent to  $w_1$  and  $w_2$  respectively where,  $p \geq q$ , say. But then by Lemma 3.2.1, if we delete one of the pendent edges incident on  $w_2$  and make the corresponding pendent vertex adjacent to  $w_1$ , the resulting graph still belongs to  $\mathcal{G}_n^r$  with a smaller distance spectral radius and that is a contradiction to the minimality of  $G^*$ . Therefore  $G^* \cong K_n^r$ , for  $1 \leq r \leq n - 3$ . Finally if  $r = n - 2$ , then  $G^*$  is a dumbbell  $D(n, p, q)$ , such that  $p + q = n - 2$ . Now by repeated application of Lemma 3.2.1, we conclude that  $G^* \cong D(n, n - 3, 1)$ .  $\blacksquare$

### 3.4 Components of the Perron vector of a dumbbell and some applications

In this section, we give an ordering of the components of the Perron vector of a dumbbell, which will be useful to obtain the main result of this section.

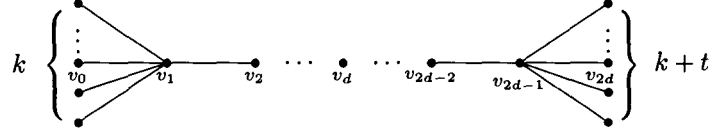
**Lemma 3.4.1.** *Let  $G = D(n, k + t, k)$  be a dumbbell of diameter  $2d$  and  $v_0 v_1 \dots v_{2d}$  be a diametrical path in it, where  $t \geq 0$ . If*

$$X = \left( \underbrace{x_0, \dots, x_0}_k, x_1, \dots, x_{2d-1}, \underbrace{x_{2d}, \dots, x_{2d}}_{k+t} \right)^T$$

*is the Perron vector of  $D(G)$ , then  $x_{d-i} \geq x_{d+i}$ , where  $1 \leq i \leq d$  and  $x_j$  corresponds to the vertex  $v_j$ , for each  $j = 0, 1, \dots, 2d$ ; equality holds only when  $t = 0$ .*

**Proof.** Let the vertices of  $G = D(n, k + t, k)$  be labeled as in Fig. 3.2. If  $t = 0$ , then by symmetry,  $x_{d-i} = x_{d+i}$  for  $1 \leq i \leq d$ . Assume  $t \geq 1$ .

We first claim that  $\sum_{j=d+1}^{2d-1} x_j + (k+t)x_{2d} > kx_0 + \sum_{j=1}^{d-1} x_j$ .


 Figure 3.2: The dumbbell  $D(n, k+t, k)$ 

Otherwise,

$$\sum_{j=d+1}^{2d-1} x_j + (k+t)x_{2d} \leq kx_0 + \sum_{j=1}^{d-1} x_j. \quad (3.4.1)$$

Then, from eigenequations we have

$$\begin{aligned} \rho(G)(x_{d-1} - x_{d+1}) &= 2 \left[ \sum_{j=d+1}^{2d-1} x_j + (k+t)x_{2d} - kx_0 - \sum_{j=1}^{d-1} x_j \right] \leq 0 \\ &\Rightarrow x_{d-1} \leq x_{d+1}. \end{aligned} \quad (3.4.2)$$

Similarly, for  $2 \leq i \leq d-1$ , using eigenequations we have

$$\begin{aligned} \rho(G)(x_{d-i} - x_{d+i}) &= -\sum_{j=1}^i 2jx_{d-j} - 2i \sum_{j=1}^{d-i-1} x_j - 2ikx_0 + \sum_{j=1}^i 2jx_{d+j} + 2i \sum_{j=d+i+1}^{2d-1} x_j \\ &\quad + 2i(k+t)x_{2d} \end{aligned} \quad (3.4.3)$$

and

$$\begin{aligned} \rho(G)(x_{d-i+1} - x_{d+i-1}) &= -\sum_{j=1}^{i-1} 2jx_{d-j} - 2(i-1) \sum_{j=1}^{d-i} x_j - 2(i-1)kx_0 + \sum_{j=1}^{i-1} 2jx_{d+j} \\ &\quad + 2(i-1) \sum_{j=d+i}^{2d-1} x_j + 2(i-1)(k+t)x_{2d}. \end{aligned} \quad (3.4.4)$$

By (3.4.3) and (3.4.4), we get

$$\begin{aligned} &\rho(G)(x_{d-i} - x_{d+i}) - \rho(G)(x_{d-i+1} - x_{d+i-1}) \\ &= 2 \left[ \sum_{j=d+i}^{2d-1} x_j + (k+t)x_{2d} - kx_0 - \sum_{j=1}^{d-i} x_j \right] \\ &= 2 \left[ \sum_{j=d+1}^{2d-1} x_j + (k+t)x_{2d} - kx_0 - \sum_{j=1}^{d-1} x_j \right] - 2 \sum_{j=1}^{i-1} [x_{d+j} - x_{d-j}]. \end{aligned} \quad (3.4.5)$$

We now prove  $x_{d-i} - x_{d+i} \leq 0$  by induction on  $i$ , where  $1 \leq i \leq d-1$ .

If  $i = 1$ , then by (3.4.2) we get,  $x_{d-1} \leq x_{d+1}$ .

For  $i \geq 2$ , by the induction hypothesis  $x_{d-j} - x_{d+j} \leq 0$ , where  $1 \leq j \leq i-1$ . Thus,

$$-2 \sum_{j=1}^{i-1} [x_{d+j} - x_{d-j}] \leq 0.$$

Hence, by (3.4.5) we have

$$\begin{aligned} \rho(G)(x_{d-i} - x_{d+i}) - \rho(G)(x_{d-i+1} - x_{d+i-1}) &\leq 0 \\ \Rightarrow \rho(G)(x_{d-i} - x_{d+i}) &\leq \rho(G)(x_{d-i+1} - x_{d+i-1}) \leq 0 \text{ [by the induction hypothesis]} \\ &\Rightarrow x_{d-i} \leq x_{d+i}. \end{aligned}$$

Therefore, we have proved that  $x_{d-i} - x_{d+i} \leq 0$ , where  $1 \leq i \leq d-1$ .

Again,

$$\begin{aligned} \rho(G)(x_0 - x_{2d}) - \rho(G)(x_1 - x_{2d-1}) &= 2(x_{2d} - x_0) \\ \Rightarrow (\rho(G) + 2)(x_0 - x_{2d}) &= \rho(G)(x_1 - x_{2d-1}) \leq 0 \\ \Rightarrow x_0 - x_{2d} &\leq 0, \end{aligned}$$

which in turn gives  $\sum_{j=d+1}^{2d-1} x_j + (k+t)x_{2d} > kx_0 + \sum_{j=1}^{d-1} x_j$ , a contradiction to (3.4.1).

Hence the claim is established.

Therefore, from (3.4.2) we get  $x_{d-1} > x_{d+1}$ . Proceeding as mentioned above and using induction, we get  $x_{d-i} > x_{d+i}$ , where  $1 \leq i \leq d$ .  $\blacksquare$

**Corollary 3.4.2.** *Let  $G = D(n, k+t, k)$  be a dumbbell of diameter  $2d$  and  $v_0v_1 \dots v_{2d}$  be a diametrical path in it, where  $t \geq 1$ . If*

$$X = \left( \underbrace{x_0, \dots, x_0}_k, x_1, \dots, x_{2d-1}, \underbrace{x_{2d}, \dots, x_{2d}}_{k+t} \right)^T$$

is the Perron vector of  $D(G)$ , where  $x_j$  corresponds to the vertex  $v_j$  for  $j = 0, 1, \dots, 2d$ , then

- (i)  $(x_{d-i} - x_{d+i}) > (x_{d-i+1} - x_{d+i-1})$ , where  $1 \leq i \leq d-1$ , and
- (ii)  $\left(1 + \frac{2}{\rho(G)}\right)(x_0 - x_{2d}) = (x_1 - x_{2d-1})$ .

Similar to the above lemma and the corollary, we have the following results.

**Lemma 3.4.3.** Let  $G = D(n, k+t, k)$  be a dumbbell of diameter  $2d+1$  and  $v_0v_1 \dots v_{2d+1}$  be a diametrical path in it, where  $t \geq 0$ . If

$$X = \left( \underbrace{x_0, \dots, x_0}_k, x_1, \dots, x_{2d}, \underbrace{x_{2d+1}, \dots, x_{2d+1}}_{k+t} \right)^T$$

is the Perron vector of  $D(G)$ , then  $x_{d-i} \geq x_{d+i+1}$ , where  $0 \leq i \leq d$  and  $x_j$  corresponds to the vertex  $v_j$ , for each  $j = 0, 1, \dots, 2d+1$ ; equality holds only when  $t = 0$ .

**Corollary 3.4.4.** Let  $G = D(n, k+t, k)$  be a dumbbell of diameter  $2d+1$  and  $v_0v_1 \dots v_{2d+1}$  be a diametrical path in it, where  $t \geq 1$ . If

$$X = \left( \underbrace{x_0, \dots, x_0}_k, x_1, \dots, x_{2d}, \underbrace{x_{2d+1}, \dots, x_{2d+1}}_{k+t} \right)^T$$

is the Perron vector of  $D(G)$ , where  $x_j$  corresponds to the vertex  $v_j$  for  $j = 0, 1, \dots, 2d+1$ , then

- (i)  $(x_{d-i} - x_{d+i+1}) > (x_{d-i+1} - x_{d+i})$ , where  $1 \leq i \leq d-1$ , and
- (ii)  $\left(1 + \frac{2}{\rho(G)}\right)(x_0 - x_{2d+1}) = (x_1 - x_{2d})$ .

The following lemma will be useful to prove our main result.

**Lemma 3.4.5.** If  $k \geq 2$ , then

$$\rho(D(n, k, k)) > \rho(D(n, k+1, k-1)) > \dots > \rho(D(n, 2k-1, 1)).$$

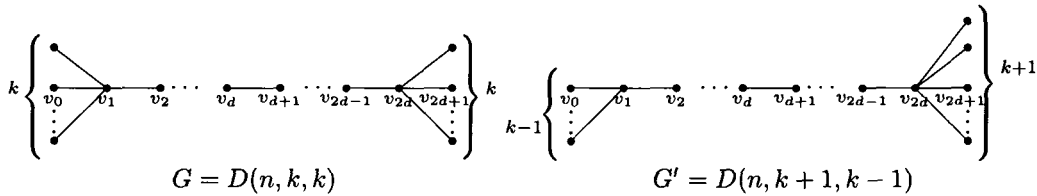


Figure 3.3: The graphs in Lemma 3.4.5

**Proof.** Let us denote  $D(n, k, k)$  and  $D(n, k+1, k-1)$  by  $G$  and  $G'$ , respectively.  
**Case 1:** Suppose the diameter of  $G$  is  $2d+1$ , and label the vertices as in Fig. 3.3.

If  $X = \left( \underbrace{x_0, \dots, x_0}_{k-1}, x_1, \dots, x_{2d}, \underbrace{x_{2d+1}, \dots, x_{2d+1}}_{k+1} \right)^T$  is the Perron vector of  $D(G')$ , then from  $G$  to  $G'$  we have,

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}X^T(D(G) - D(G'))X \\ &= x_{2d+1} \left[ (2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} \right. \\ &\quad \left. + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \right]. \end{aligned} \quad (3.4.6)$$

Claim:  $(2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) > 0$ .

Suppose to the contrary that

$$(2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \leq 0.$$

Then, from eigenequations we have

$$\begin{aligned} &\rho(G')(x_0 - x_{2d+1}) \\ &= (2d+1)(x_{2d+1} - x_0) + (2d-1)(k-2)(x_{2d+1} - x_0) + 2(2d-1)x_{2d+1} \\ &\quad + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \\ &= 2 \left[ (2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} + \right. \\ &\quad \left. \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \right] + \sum_{i=1}^d (2d-2i+1)(x_i - x_{2d-i+1}) \\ &\quad + \{(2d-1)(k-1) - 2\}(x_0 - x_{2d+1}) \\ &\leq 2 \left[ (2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \right] \\ &\quad + \left( 1 + \frac{2}{\rho(G')} \right) \left[ \sum_{i=1}^d (2d-2i+1)(x_0 - x_{2d+1}) \right] \\ &\quad + \{(2d-1)(k-1) - 2\}(x_0 - x_{2d+1}) \text{ [by Corollary 3.4.4]}, \end{aligned}$$

i.e.,

$$\left[ \rho(G') - \left[ \left( 1 + \frac{2}{\rho(G')} \right) \left\{ \sum_{i=1}^d (2d-2i+1) \right\} + \{(2d-1)(k-1) - 2\} \right] \right] (x_0 - x_{2d+1})$$

$$\begin{aligned}
 &= 2 \left[ (2d-1)(k-1)(x_{2d+1} - x_0) + (2d-1)x_{2d+1} + \sum_{i=1}^d (2d-2i+1)(x_{2d-i+1} - x_i) \right] \\
 &\leq 0
 \end{aligned}$$

or

$$\left[ \rho(G') - \left[ \left(1 + \frac{2}{\rho(G')}\right) d^2 + \{(2d-1)(k-1) - 2\} \right] \right] (x_0 - x_{2d+1}) \leq 0. \quad (3.4.7)$$

Since the spectral radius is bounded below by minimum row sum, we have

$$\rho(G') \geq \left[ d^2 + (k-1)(2d+1) + 2d \right] > \left[ \left(1 + \frac{2}{\rho(G')}\right) d^2 + \{(2d-1)(k-1) - 2\} \right].$$

Hence, (3.4.7) implies that  $x_0 - x_{2d+1} \leq 0$ , a contradiction to the fact  $x_0 > x_{2d+1}$ , as given by Lemma 3.4.3. Hence the claim, and therefore by (3.4.6) we get  $\rho(G) > \rho(G')$ .

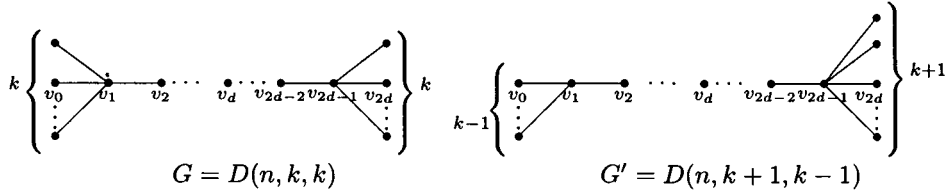


Figure 3.4: The graphs in Lemma 3.4.5

**Case 2:** Suppose the diameter of  $G$  is  $2d$ , and label the vertices as in Fig. 3.4. If  $X = \left( \underbrace{x_0, \dots, x_0}_{k-1}, x_1, \dots, x_{2d-1}, \underbrace{x_{2d}, \dots, x_{2d}}_{k+1} \right)^T$  is the Perron vector of  $D(G')$ , then from  $G$  to  $G'$  we have,

$$\begin{aligned}
 \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2} X^T (D(G) - D(G')) X \\
 &= x_{2d} \left[ (2d-2)(k-1)(x_{2d} - x_0) + (2d-2)x_{2d} \right. \\
 &\quad \left. + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) \right]. \quad (3.4.8)
 \end{aligned}$$

Claim:  $(2d-2)(k-1)(x_{2d} - x_0) + (2d-2)x_{2d} + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) > 0$ .

Suppose to the contrary that

$$(2d-2)(k-1)(x_{2d}-x_0) + (2d-2)x_{2d} + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i}-x_i) \leq 0.$$

Then, from eigenequations we have

$$\begin{aligned} & \rho(G')(x_0 - x_{2d}) \\ = & 2d(x_{2d} - x_0) + (2d-2)(k-2)(x_{2d} - x_0) + 2(2d-2)x_{2d} \\ & + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) \\ = & 2 \left[ (2d-2)(k-1)(x_{2d} - x_0) + (2d-2)x_{2d} + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) \right] \\ & + \sum_{i=1}^{d-1} (2d-2i)(x_i - x_{2d-i}) + \{(2d-2)k - 2d\}(x_0 - x_{2d}) \\ \leq & 2 \left[ (2d-2)(k-1)(x_{2d} - x_0) + (2d-2)x_{2d} + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) \right] \\ & + \left(1 + \frac{2}{\rho(G')}\right) \left[ \sum_{i=1}^{d-1} (2d-2i)(x_0 - x_{2d}) \right] + \{(2d-2)k - 2d\}(x_0 - x_{2d}) \\ & \text{[by Corollary 3.4.2],} \end{aligned}$$

i.e.,

$$\begin{aligned} & \left[ \rho(G') - \left[ \left(1 + \frac{2}{\rho(G')}\right) \left\{ \sum_{i=1}^{d-1} (2d-2i) \right\} + \{(2d-2)k - 2d\} \right] \right] (x_0 - x_{2d}) \\ = & 2 \left[ (2d-2)(k-1)(x_{2d} - x_0) + (2d-2)x_{2d} + \sum_{i=1}^{d-1} (2d-2i)(x_{2d-i} - x_i) \right] \leq 0 \end{aligned}$$

or

$$\left[ \rho(G') - \left[ \left(1 + \frac{2}{\rho(G')}\right)(d^2 - d) + \{(2d-2)k - 2d\} \right] \right] (x_0 - x_{2d}) \leq 0. \quad (3.4.9)$$

Since the spectral radius is bounded below by minimum row sum, we have

$$\rho(G') \geq [d^2 - d + 2kd - 1] > \left[ \left(1 + \frac{2}{\rho(G')}\right)(d^2 - d) + \{(2d-2)k - 2d\} \right].$$

Hence, (3.4.9) implies that  $x_0 - x_{2d} \leq 0$ , a contradiction to the fact  $x_0 > x_{2d}$ , as given by Lemma 3.4.1. Hence the claim, and therefore by (3.4.8) we get  $\rho(G) > \rho(G')$ .



The other inequalities can be proved in a similar way. ■

Similar to the above lemma, we have the following lemma.

**Lemma 3.4.6.** *If  $k \geq 2$ , then*

$$\rho(D(n, k + 1, k)) > \rho(D(n, k + 2, k - 1)) > \dots > \rho(D(n, 2k, 1)).$$

If  $v$  is a vertex of a tree  $T$ , then the components of  $T - v$  are called the *branches* of  $T$  at  $v$ . For  $u \in N_T(v)$ , we denote the branch of  $T$  resulting from deletion of  $v$  and containing  $u$  by  $T_u$ . If  $H$  is a subgraph of  $G$ , then the sum of the components of the Perron vector of  $D(G)$  corresponding to the vertices in  $H$  is denoted by  $S(H)$ . As applications of the results obtained in this section, we give an affirmative solution to the Conjecture 3.1.1. The following lemmas will be helpful in doing so.

**Lemma 3.4.7.** [61] *Let  $u$  be a cut vertex of a graph  $G$  such that  $G - \{u\}$  has at least three components  $G_1, G_2, G_3$  and  $S(G_1) \leq S(G_2)$ , where  $S(G_i)$  is the sum of the components of the Perron vector of  $D(G)$  corresponding to the vertices in  $G_i$ , for  $i = 1, 2$ . If  $G' = G - \sum_{v \in N_{G_3}(u)} uv + \sum_{v \in N_{G_3}(u)} vw$ , where  $w$  is any vertex in  $G_1$ , then  $\rho(G') > \rho(G)$ .*

**Lemma 3.4.8.** [62] *Suppose  $uv$  is a cut-edge of a connected graph  $G$ , but  $uv$  is not a pendent edge. If  $G'$  is the graph obtained from  $G$  by identifying  $u$  and  $v$ , and creating a new pendent vertex at the identified vertex, then  $\rho(G) > \rho(G')$ .*

**Theorem 3.4.9.** *The dumbbell  $D(n, \lceil \frac{n+1}{2} \rceil - m, \lfloor \frac{n+1}{2} \rfloor - m)$  is the unique tree that maximizes the distance spectral radius in  $\mathcal{T}_n^m$ .*

**Proof.** If  $m = 1$ , then the result is trivial. Suppose  $m \geq 2$ , and let  $T$  be a tree in  $\mathcal{T}_n^m$  with maximal distance spectral radius. Then  $T$  has two quasi-pendent vertices. Otherwise, there exists a vertex  $v$  in  $T$  such that  $T - v$  has at least three components, and at least two of which are nontrivial. Let  $T_x, T_y, T_z$  be three branches at the vertex  $v$  of  $T$ , and  $M$  be an  $m$ -matching of  $T$ . Then, at least two of  $vx, vy$  and  $vz$  are not in  $M$ .

Case 1: Suppose  $T_x$  and  $T_y$  are non-trivial and  $vz$  is not in  $M$ .

Without loss of generality assume that  $S(T_x) \geq S(T_y)$  and let  $v_1$  be a quasi-pendent vertex of  $T_y$ . Then the tree  $T' = T - vz + v_1z$  is in  $\mathcal{T}_n^m$ , and by Lemma 3.4.7,  $\rho(T') > \rho(T)$ , a contradiction to the maximality of  $T$ .

Case 2: Suppose  $vz$  is in  $M$  and  $T_z$  is non-trivial.

Then both  $vx$  and  $vy$  are not in  $M$ , and say  $T_x$  is non trivial. Reversing the roles of  $y$  and  $z$  in Case 1, we have a contradiction.

Case 3: Suppose  $vz$  is in  $M$  and  $T_z$  is trivial.

Then using Lemma 3.4.8 the tree  $T' = T - vx + zx$  still has matching number  $m$ , but has a larger distance spectral radius than  $T$ , a contradiction to the maximality of  $T$ .

Thus  $T \cong D(n, a, b)$ , for some  $a$  and  $b$ . If  $a = b = 1$ , then the result follows trivially.

Suppose  $a = \max(a, b) > 1$ , then any  $m$  matching of  $T$  can not be a perfect matching of a diametrical path. Otherwise, by Lemma 3.4.8, we get  $T' \cong D(n, a - 1, b) \in \mathcal{T}_n^m$ , and  $\rho(T') > \rho(T)$ , a contradiction. Thus, if  $\max(a, b) > 1$ , then  $P_{n-a-b}$  is of order  $2m - 1$ . By Lemmas 3.4.5 and 3.4.6, we get  $T \cong D(n, \lceil \frac{n+1}{2} \rceil - m, \lfloor \frac{n+1}{2} \rfloor - m)$ . ■

We now find the tree having maximal distance spectral radius in  $\mathbb{T}_n^r$ . Since  $\mathbb{T}_n^{n-1} = \{S_n\}$ , so there is nothing to do in this case. Let us now consider  $2 \leq r \leq n - 2$ .

**Theorem 3.4.10.** *The dumbbell  $D(n, \lceil \frac{r}{2} \rceil, \lfloor \frac{r}{2} \rfloor)$  uniquely maximizes the distance spectral radius in  $\mathbb{T}_n^r$ .*

**Proof.** Let  $T$  be a tree in  $\mathbb{T}_n^r$  with maximal distance spectral radius. Then  $T$  has two quasi-pendent vertices. Otherwise, there exists a vertex  $v$  in  $T$  such that  $T - v$  has at least three components, and at least two of which are nontrivial. Let  $T_x, T_y, T_z$  be three branches at the vertex  $v$  of  $T$ , and  $T_x, T_y$  are non-trivial. Without loss of generality assume that  $S(T_x) \geq S(T_y)$ . If  $v_1$  is a non-pendent vertex of  $T_y$ , then the tree  $T' = T - vz + v_1z$  is in  $\mathbb{T}_n^r$  and by Lemma 3.4.7,  $\rho(T') > \rho(T)$ , a contradiction to the maximality of  $T$ . Thus  $T \cong D(n, a, b)$ , where  $a + b = r$ . By Lemmas 3.4.5 and 3.4.6, we get  $T \cong D(n, \lceil \frac{r}{2} \rceil, \lfloor \frac{r}{2} \rfloor)$ . ■

### 3.5 Graph with Maximal Distance Spectral Radius in $\mathcal{G}_n^r$

In this section, we characterize the graph with maximal distance spectral radius in  $\mathcal{G}_n^r$ . Clearly  $\mathcal{G}_n^{n-1} = \{K_{1, n-1}\}$  and hence for  $r = n - 1$ , the discussion is trivial.

**Theorem 3.5.1.** *The dumbbell  $D(n, \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$  uniquely maximizes the distance spectral radius in  $\mathcal{G}_n^{n-2}$ , where  $n \geq 4$ .*

**Proof.** Clearly  $\mathcal{G}_n^{n-2}$  contains only dumbbells  $D(n, p, q)$ , where  $p + q = n - 2$ . Thus by Theorem 3.4.10, we have the result. ■

Let  $G$  be a simple graph and  $v$  be one of its vertices. A *pendent path* in  $G$  is a path having one end vertex of degree at least 3, the other is of degree 1 and the intermediate vertices are of degree 2. For  $k, l \geq 0$ ,  $G(v, k, l)$  denotes the graph obtained from  $G \cup P_k \cup P_l$  by adding edges between  $v$  and one of the end vertices in both  $P_k$  and  $P_l$ . The broom  $B_{n,s}$  is the tree consisting of a star  $S_{s+1}$  along with a path  $P_{n-s-1}$  attached to a pendent vertex of the star.

To prove our next results we need the following two lemmas.

**Lemma 3.5.2.** [57] *If  $k \geq l \geq 1$ , then  $\rho(G(v, k, l)) < \rho(G(v, k + 1, l - 1))$ .*

**Lemma 3.5.3.** [57] *Let  $T \neq B_{n,\Delta}$  be an arbitrary tree on  $n$  vertices with the maximum vertex degree  $\Delta$ , where  $3 \leq \Delta \leq n - 2$ , then  $\rho(B_{n,\Delta}) > \rho(T)$ .*

**Theorem 3.5.4.** *The dumbbell  $D(n, \lceil \frac{n-3}{2} \rceil, \lfloor \frac{n-3}{2} \rfloor)$  uniquely maximizes the distance spectral radius in  $\mathcal{G}_n^{n-3}$ , where  $n \geq 6$ .*

**Proof.** Let  $G_1 \in \mathcal{G}_n^{n-3}$  be a graph with maximum distance spectral radius. Since  $G_1$  has three non pendent vertices, so they induce either a path or a triangle. If they induce a path then by Theorem 3.4.10, the result follows.

If they induce a triangle then there will be two cases.

Case 1: At least two vertices of the triangle are quasi-pendent vertices. If we remove an edge joining two quasi-pendent vertices then the resulting graph belongs to  $\mathcal{G}_n^{n-3}$  and has larger spectral radius than  $G_1$ , which is a contradiction.

Case 2: Exactly one vertex of the triangle is a quasi-pendent vertex. Then removing an edge of the triangle incident on the quasi-pendent vertex we get  $D(n, n - 3, 1)$  and  $\rho(D(n, n - 3, 1)) > \rho(G_1)$ . Then by Lemma 3.5.2, we have  $\rho(D(n, n - 4, 1)) > \rho(D(n, n - 3, 1))$  and  $D(n, n - 4, 1)$  belongs to  $\mathcal{G}_n^{n-3}$ , a contradiction. ■

**Theorem 3.5.5.** *The broom  $B_{n,3}$  has the largest distance spectral radius in  $\mathcal{G}_n^3$ , where  $n \geq 4$ .*

**Proof.** Let  $\mathcal{G}_n^{(3)}$  be the class of all connected graphs on  $n$  vertices, having at least three pendent vertices. Clearly  $\mathcal{G}_n^3 \subset \mathcal{G}_n^{(3)}$ . Suppose  $G \in \mathcal{G}_n^{(3)}$  is a graph, having maximal distance spectral radius. We first observe that  $G$  is a tree, as otherwise, the deletion of an edge from a cycle in  $G$  results in a graph  $G' \in \mathcal{G}_n^{(3)}$  with  $\rho(G) < \rho(G')$ . We now claim that  $G \in \mathcal{G}_n^3$ . If not, then  $G$  has at least four pendent vertices. Then, we can find two pendent vertices  $u$  and  $v$  in  $G$ , which are the end points of two pendent paths  $uu_1 \dots u_p w$  and  $vv_1 \dots v_q w$ , where  $u_1, \dots, u_p, v_1, \dots, v_q$  are all distinct. Let  $L_1 = uu_1 \dots u_p$  and  $L_2 = vv_1 \dots v_q$ . Then  $G \cong H(w, p, q)$ , where  $H = G - (L_1 \cup L_2)$ .

Applying Lemma 3.5.2, on  $G \cong H(w, p, q)$  repeatedly we will end up in a graph  $G''$  having at least three pendent vertices with  $\rho(G) < \rho(G'')$ . This contradicts the maximality of  $G$  and so  $G \in \mathcal{G}_n^3$ . But then  $G$  is a tree with maximum degree 3. So by Lemma 3.5.3,  $G \cong B_{n,3}$  and the result follows. ■

**Theorem 3.5.6.** *The path  $P_n$  is the unique graph with maximal distance spectral radius in  $\mathcal{G}_n^2$ , where  $n \geq 3$ .*

**Proof.** It is obvious that  $P_n \in \mathcal{G}_n^2$ . Let  $G$  be any graph in  $\mathcal{G}_n^2$  and  $G \neq P_n$ . Then for any spanning tree  $T$  of  $G$ , using (1.4.1) we have  $\rho(G) \leq \rho(T)$ . Again from [55], we know that among trees on  $n$  vertices, the path  $P_n$  has the maximal distance spectral radius, where  $n \geq 3$ . So  $\rho(G) < \rho(P_n)$  and the result follows. ■

In [61], Yu et al. have proved that  $P'_n$  is the graph with maximal distance spectral radius in  $\mathcal{G}_n^1$ , where  $P'_n$  is obtained from a triangle  $C_3$  by attaching a path of length  $n - 3$  to one of its vertices. For  $2 \leq r \leq n - 2$ , they showed that the graph with maximal distance spectral radius in  $\mathcal{G}_n^r$  is a dumbbell and posed the Conjecture 3.1.2. Theorem 3.4.10 essentially proves the Conjecture 3.1.2 to be true for all values of  $r$ , where  $2 \leq r \leq n - 2$ . Hence, the graph having the maximal distance spectral radius in  $\mathcal{G}_n^r$  is completely determined.

# Chapter 4

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## On the distance spectral radius of graphs without a pendent vertex

### 4.1 Introduction

Let  $C_p$  and  $C_q$  be two vertex-disjoint cycles. Suppose  $v_0$  is a vertex of  $C_p$  and  $v_l$  is a vertex of  $C_q$ . The graph obtained by joining  $v_0$  and  $v_l$  by a path  $v_0v_1 \dots v_l$  of length  $l$  (where  $l \geq 0$ ;  $l = 0$  means identifying  $v_0$  with  $v_l$ ) is an *infinity* and is denoted by  $\infty(p; l; q)$ . A bicyclic graph containing an infinity  $\infty(p; l; q)$  as an induced subgraph is an  $\infty(p; l; q)$ -*graph*. Let  $P_{p+1} = x_1x_2 \dots x_{p+1}$ ,  $P_{t+1} = y_1y_2 \dots y_{t+1}$  and  $P_{q+1} = z_1z_2 \dots z_{q+1}$  be three vertex-disjoint paths. Identifying the initial vertices as  $u_0$  and the terminal vertices as  $v_0$  of these paths results in the graph  $\theta(p; t; q)$ , called a *theta*. A bicyclic graph containing a theta  $\theta(p; t; q)$  as an induced subgraph is a  $\theta(p; t; q)$ -*graph*. We call the vertices  $u_0$  and  $v_0$  of  $\theta(p; t; q)$ -graph as *distinguished vertices*.

A *cactus* is a connected graph, in which any two cycles have at most one vertex in common. Let  $\mathcal{C}(n, k)$  be the class of all cacti on  $n$  vertices and  $k$  cycles. A *saw-graph* of order  $n$  and *length*  $k$  is a cactus obtained from a path of length  $n - k$  by replacing  $k$  of its blocks with  $k$  triangles, where  $0 \leq k \leq \lfloor \frac{n-1}{2} \rfloor$ . A saw graph of length  $k$  and order  $2k + 1$  is a *proper saw-graph*. The saw-graph obtained by joining an end of a proper saw graph of length  $p$  with an end of another proper saw graph of length  $q$  by a path of length  $l$  is denoted by  $S(p, q; l)$ . If  $l = 0$ , then we have the proper saw-graph of length  $p + q$ . A *balanced saw-graph* of length  $k$  is obtained by joining two proper saw-graphs of lengths  $\lfloor \frac{k}{2} \rfloor$  and  $\lceil \frac{k}{2} \rceil$  by a path. An *unbalanced saw-graph* is obtained by joining two proper saw-graphs of lengths  $p$  and  $q$  by a path such that  $|p - q| \geq 2$ . We shall use the following result from [13].

**Lemma 4.1.1.** [13] If  $G$  is a graph with maximal distance spectral radius in  $\mathcal{C}(n, k)$ , then  $G \cong S(p, q; l)$ , where  $p + q = k$  and  $l = n - 2k - 1$ .

Let  $\mathcal{G}_n^r$  be the class of all graphs on  $n$  vertices with  $r$  pendent vertices. For  $1 \leq$

$r \leq n - 1$ , the graph having the maximal (minimal) distance spectral radius in  $\mathcal{G}_n^r$  is obtained in Chapter 3. In this Chapter, we consider the case  $r = 0$ , and hence the structure of the graph with maximal (minimal) distance spectral radius in  $\mathcal{G}_n^r$  is completely characterized. By (1.4.2), it is obvious that  $K_n$  is the graph having the minimal distance spectral radius in  $\mathcal{G}_n^0$ .

Clearly,  $C_3$  and  $C_4$  are spanning subgraphs of any graph in  $\mathcal{G}_3^0$  and  $\mathcal{G}_4^0$ , respectively, whereas  $C_5$  or  $\infty(3; 0; 3)$  is a spanning subgraph of any graph in  $\mathcal{G}_5^0$ . It can be verified that  $C_n$  is the graph with maximal distance spectral radius in  $\mathcal{G}_n^0$ , where  $3 \leq n \leq 5$ .

In this chapter, we prove that for  $n \geq 6$ ,  $\infty(3; n - 5; 3)$  is the unique graph with maximal distance spectral radius in  $\mathcal{G}_n^0$ .

## 4.2 Preliminary Lemmas

In this section we establish some preliminary lemmas, which will be useful to derive our main result.

**Lemma 4.2.1.** *If  $n \geq 7$ , then  $\rho(\infty(3; n - 5; 3)) > \rho(C_n)$ .*

**Proof.** Let us denote  $\infty(3; n - 5; 3)$  by  $\hat{G}$  and label the vertices in  $V(C_n) = V(\infty(3; n - 5; 3))$  as shown in Fig. 4.1. As we pass from  $C_n$  to  $\hat{G}$ , the following changes occur:

The distances of  $v_n$  are decreased by 1 from  $\{v_{\lfloor \frac{n}{2} \rfloor}, v_{\lfloor \frac{n}{2} \rfloor + 1}, \dots, v_{n-2}\}$  and is increased by  $n - 4$  from  $v_1$ ; the distances of  $v_1$  are decreased by 1 from  $\{v_3, v_4, \dots, v_{\lfloor \frac{n+1}{2} \rfloor}\}$  and is increased by  $n - 5$  from  $v_{n-1}$ ; distances among other vertices are increased or remain unchanged.

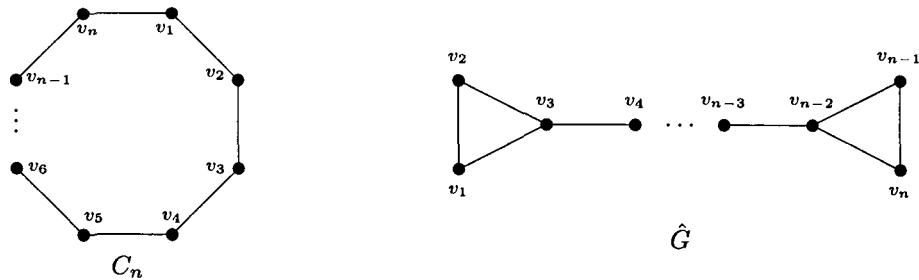


Figure 4.1: The graphs  $C_n$  and  $\hat{G}$  in Lemma 4.2.1.

If  $X$  is the Perron vector of  $D(C_n)$ , then by symmetry we have  $x_i = a$  (say), for all

$i = 1, 2, \dots, n$ . Therefore

$$\begin{aligned} \frac{1}{2}(\rho(\hat{G}) - \rho(C_n)) &\geq \frac{1}{2}X^T(D(\hat{G}) - D(C_n))X \\ &\geq \left[n - 4 - \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\right] a^2 + \left[n - 5 - \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\right] a^2 \\ &= \left(\left\lceil \frac{n}{2} \right\rceil - 3\right) a^2 + \left(\left\lceil \frac{n}{2} \right\rceil - 4\right) a^2 = \left(2 \left\lceil \frac{n}{2} \right\rceil - 7\right) a^2 > 0. \end{aligned}$$

Hence,  $\rho(\hat{G}) > \rho(C_n)$ . ■

Let  $G''$  be the  $\infty(3; 0; 3)$ -graph obtained by identifying an end vertex of a path of length  $n - 5$  with a vertex of degree 2 in  $\infty(3; 0; 3)$ . If the vertices of  $G''$  are labeled as in Fig. 4.2, then we have the following result.

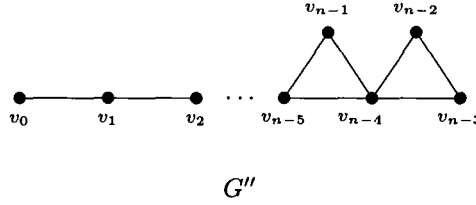


Figure 4.2: The graph  $G''$  in Lemma 4.2.2.

**Lemma 4.2.2.** *If  $n \geq 9$  and  $X = (x_0, x_1, \dots, x_{n-1})^T$  is the Perron vector of  $D(G'')$ , then*

$$x_{\lfloor \frac{n-3}{2} \rfloor - i} \geq x_{\lceil \frac{n-3}{2} \rceil + i},$$

where  $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$  and  $x_j$  corresponds to the vertex  $v_j$ , for each  $j = 0, 1, \dots, n - 1$ ; equality holds only at  $i = 0$ , if  $n$  is odd.

**Proof.** We first claim that

$$\sum_{j=\lfloor \frac{n-3}{2} \rfloor}^{n-1} x_j > \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j. \quad (4.2.1)$$

Otherwise

$$\sum_{j=\lfloor \frac{n-3}{2} \rfloor}^{n-1} x_j \leq \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j. \quad (4.2.2)$$

Then from eigenequations we have

$$\begin{aligned} & \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \right) \\ &= \begin{cases} 0 & , \text{ if } n \text{ is odd;} \\ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j & , \text{ if } n \text{ is even,} \end{cases} \end{aligned} \quad (4.2.3)$$

which gives  $x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \leq 0$ . Similarly for  $1 \leq i \leq \lfloor \frac{n-7}{2} \rfloor$ , using eigenequations we have

$$\begin{aligned} & \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) - \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \\ &= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil + i}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor - i} x_j \right] \\ &= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] - 2 \sum_{j=0}^{i-1} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right]. \end{aligned} \quad (4.2.4)$$

We now prove  $x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0$  by induction on  $i$ , where  $0 \leq i \leq \lfloor \frac{n-7}{2} \rfloor$ .

If  $i = 0$ , then by (4.2.3) we get  $x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \leq 0$ .

For  $i \geq 1$ , by induction hypothesis  $x_{\lfloor \frac{n-3}{2} \rfloor - j} - x_{\lceil \frac{n-3}{2} \rceil + j} \leq 0$ , where  $0 \leq j \leq i - 1$ .

Thus

$$-2 \sum_{j=0}^{i-1} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] \leq 0.$$

Hence by (4.2.2) and (4.2.4), we have

$$\begin{aligned} & \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) - \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \leq 0 \\ \Rightarrow & \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) \leq \rho(G'') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \leq 0 \\ & \text{[by induction hypothesis]} \\ \Rightarrow & x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0. \end{aligned}$$

Therefore if  $0 \leq i \leq \lfloor \frac{n-7}{2} \rfloor$ , then we have proved by induction on  $i$ , that

$$x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0. \quad (4.2.5)$$



Similarly from eigenequations, we have

$$\begin{aligned}
& \rho(G'')(x_1 - x_{n-4}) - \rho(G'')(x_2 - x_{n-5}) \\
&= 2(x_{n-4} + x_{n-3} + x_{n-2} - x_0 - x_1) + x_{n-1} \quad (4.2.6) \\
&= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] \\
&\quad - 2 \sum_{j=0}^{\lfloor \frac{n-7}{2} \rfloor} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] - x_{n-1} \\
&< 0 \text{ [by (4.2.2) and (4.2.5)]} \\
\Rightarrow \rho(G'')(x_1 - x_{n-4}) &< \rho(G'')(x_2 - x_{n-5}) \leq 0 \text{ [by (4.2.5)]} \\
\Rightarrow x_1 - x_{n-4} &< 0, \quad (4.2.7)
\end{aligned}$$

$$\begin{aligned}
\text{and } \rho(G'')(x_0 - x_{n-3}) - \rho(G'')(x_1 - x_{n-4}) \\
&= 2(x_{n-3} - x_0) + x_{n-2} \quad (4.2.8) \\
&= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] \\
&\quad - 2 \sum_{j=0}^{\lfloor \frac{n-5}{2} \rfloor} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] - x_{n-2} - 2x_{n-1} \\
&< 0 \text{ [by (4.2.2) and (4.2.5)]} \\
\Rightarrow \rho(G'')(x_0 - x_{n-3}) &< \rho(G'')(x_1 - x_{n-4}) < 0 \text{ [by (4.2.7)]} \\
\Rightarrow x_0 - x_{n-3} &< 0. \quad (4.2.9)
\end{aligned}$$

From (4.2.5), (4.2.7), and (4.2.9) we have

$$\sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j < \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-3} x_j < \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j.$$

This is a contradiction to (4.2.2) and hence the claim is established.

Therefore from (4.2.3) we get,  $x_{\lfloor \frac{n-3}{2} \rfloor} \geq x_{\lceil \frac{n-3}{2} \rceil}$ , where the equality holds only if  $n$  is odd. Proceeding as mentioned above and using induction we get

$$x_{\lfloor \frac{n-3}{2} \rfloor - i} > x_{\lceil \frac{n-3}{2} \rceil + i}, \text{ where } 1 \leq i \leq \left\lfloor \frac{n-7}{2} \right\rfloor. \quad (4.2.10)$$

Adding (4.2.6) and (4.2.8), we get

$$\begin{aligned}
& \rho(G'')(x_0 - x_{n-3}) - \rho(G'')(x_2 - x_{n-5}) \\
&= -4x_0 - 2x_1 + 2x_{n-4} + 4x_{n-3} + 3x_{n-2} + x_{n-1} \\
&= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] - 2 \sum_{j=0}^{\lfloor \frac{n-7}{2} \rfloor} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] \\
&\quad + 2(x_{n-3} - x_0) + (x_{n-2} - x_{n-1}) \\
&\Rightarrow \left( \rho(G'') + 2 \right) (x_0 - x_{n-3}) - \rho(G'')(x_2 - x_{n-5}) \\
&= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] + (x_{n-2} - x_{n-1}) \\
&\quad - 2 \sum_{j=0}^{\lfloor \frac{n-7}{2} \rfloor} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] \tag{4.2.11}
\end{aligned}$$

Again from eigenequations we have

$$\begin{aligned}
\rho(G'')(x_{n-2} - x_{n-1}) &= \sum_{j=0}^{n-5} x_j - x_{n-3} + 2(x_{n-1} - x_{n-2}) \\
\Rightarrow \left( \rho(G'') + 2 \right) (x_{n-2} - x_{n-1}) &= \sum_{j=0}^{n-5} x_j - x_{n-3} \\
&> x_2 + x_{n-6} + x_{n-5} - x_{n-3} \\
&> x_{n-6} + 2x_{n-5} - x_{n-3} \\
&\quad \text{[by (4.2.10), } x_2 > x_{n-5}\text{]}, \tag{4.2.12}
\end{aligned}$$

and

$$\begin{aligned}
\rho(G'')(x_{n-6} + 2x_{n-5} - x_{n-3}) &> -x_{n-6} - x_{n-5} + 7x_{n-3} \\
\Rightarrow \left( \rho(G'') + 1 \right) (x_{n-6} + 2x_{n-5} - x_{n-3}) &> x_{n-5} + 6x_{n-3} > 0 \\
\Rightarrow x_{n-6} + 2x_{n-5} - x_{n-3} &> 0. \tag{4.2.13}
\end{aligned}$$

Using (4.2.13) in (4.2.12) we have

$$x_{n-2} - x_{n-1} > 0. \tag{4.2.14}$$

Therefore, using (4.2.1), (4.2.10), and (4.2.14) in (4.2.11) we have

$$\begin{aligned}
\left( \rho(G'') + 2 \right) (x_0 - x_{n-3}) &> \rho(G'')(x_2 - x_{n-5}) > 0. \\
\Rightarrow x_0 - x_{n-3} &> 0. \tag{4.2.15}
\end{aligned}$$

Finally subtracting (4.2.8) from (4.2.6), we get

$$\begin{aligned}
& 2\rho(G'')(x_1 - x_{n-4}) - \rho(G'')(x_2 - x_{n-5}) - \rho(G'')(x_0 - x_{n-3}) \\
&= -2x_1 + 2x_{n-4} + x_{n-2} + x_{n-1} \\
&\Rightarrow \left(2\rho(G'') + 2\right)(x_1 - x_{n-4}) - \rho(G'')(x_2 - x_{n-5}) \\
&= \rho(G'')(x_0 - x_{n-3}) + x_{n-2} + x_{n-1} > 0 \text{ [by (4.2.15)]} \\
&\Rightarrow \left(2\rho(G'') + 2\right)(x_1 - x_{n-4}) > \rho(G'')(x_2 - x_{n-5}) > 0 \\
&\Rightarrow x_1 - x_{n-4} > 0. \tag{4.2.16}
\end{aligned}$$

Hence by (4.2.10), (4.2.15), and (4.2.16) we have  $x_{\lfloor \frac{n-3}{2} \rfloor - i} \geq x_{\lceil \frac{n-3}{2} \rceil + i}$ , where  $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$ . ■

From the proof of the above lemma we have the following corollary.

**Corollary 4.2.3.** *If  $n \geq 9$  and  $X = (x_0, x_1, \dots, x_{n-1})^T$  is the Perron vector of  $D(G'')$ , where  $x_j$  corresponds to the vertex  $v_j$  for  $j = 0, 1, \dots, n-1$ , then*

- (i)  $x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} > x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1}$ , where  $1 \leq i \leq \lfloor \frac{n-7}{2} \rfloor$
- (ii)  $\left(1 + \frac{2}{\rho(G'')}\right)(x_0 - x_{n-3}) > (x_1 - x_{n-4})$  and
- (iii)  $\left(1 + \frac{2}{\rho(G'')}\right)(x_0 - x_{n-3}) > (x_2 - x_{n-5})$ .

It was conjectured in [13], that  $S(\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil; n - 2k - 1)$  uniquely maximizes the distance spectral radius in  $\mathcal{C}(n, k)$ . The following lemma together with Lemma 4.1.1 prove the conjecture for  $k = 2$ .

**Lemma 4.2.4.** *If  $n \geq 6$ , then  $\rho(\infty(3; n - 5; 3)) > \rho(G'')$ .*

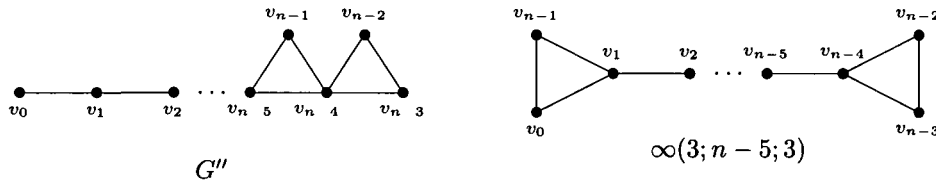


Figure 4.3: The graphs  $G''$  and  $\infty(3; n - 5; 3)$  in Lemma 4.2.4

**Proof.** For  $n \in \{6, 7, 8\}$  it can be easily verified that  $\rho(\infty(3; n - 5; 3)) > \rho(G'')$ . So let  $n \geq 9$  and denote  $\infty(3; n - 5; 3)$  by  $G$  and label the vertices in  $V(G) = V(G'')$  as

in Fig. 4.3. If  $X$  is the Perron vector of  $D(G'')$  and  $x_i$  denotes the component of  $X$  corresponding to vertex  $v_i$ , where  $0 \leq i \leq n-1$ , then from  $G''$  to  $G$  we have

$$\begin{aligned}
& \frac{1}{2}(\rho(G) - \rho(G'')) \\
& \geq \frac{1}{2}X^T(D(G) - D(G''))X \\
& \geq x_{n-1} \left[ (n-5)(x_{n-3} - x_0) + \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-4)(x_{n-k-3} - x_k) \right. \\
& \quad \left. + x_{n-4} + 2 \sum_{j=\lceil \frac{n-1}{2} \rceil}^{n-5} x_j + x_{\lceil \frac{n-3}{2} \rceil} + (n-5)x_{n-2} \right] \tag{4.2.17}
\end{aligned}$$

Claim:

$$\begin{aligned}
L & = (n-5)(x_{n-3} - x_0) + \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-4)(x_{n-k-3} - x_k) + x_{n-4} \\
& \quad + 2 \sum_{j=\lceil \frac{n-1}{2} \rceil}^{n-5} x_j + x_{\lceil \frac{n-3}{2} \rceil} + (n-5)x_{n-2} > 0.
\end{aligned}$$

To the contrary, if  $L \leq 0$ , then from eigenequations we have

$$\begin{aligned}
\rho(G'')(x_0 - x_{n-3}) & = \sum_{k=0}^{\lfloor \frac{n-3}{2} \rfloor} (n-2k-3)(x_{n-k-3} - x_k) + (n-4)x_{n-2} \\
& \quad + (n-6)x_{n-1}. \tag{4.2.18}
\end{aligned}$$

By (4.2.18), we have

$$\begin{aligned}
& \rho(G'')(x_0 - x_{n-3}) \\
& = 2L + (n-7)(x_0 - x_{n-3}) + \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-5)(x_k - x_{n-k-3}) - 2x_{n-4} \\
& \quad - 4 \sum_{j=\lceil \frac{n-1}{2} \rceil}^{n-5} x_j + \left( \left\lfloor \frac{n-3}{2} \right\rfloor - \left\lceil \frac{n-3}{2} \right\rceil \right) x_{\lfloor \frac{n-3}{2} \rfloor} \\
& \quad + \left( \left\lceil \frac{n-3}{2} \right\rceil - \left\lfloor \frac{n-3}{2} \right\rfloor - 2 \right) x_{\lceil \frac{n-3}{2} \rceil} + (n-6)(x_{n-1} - x_{n-2})
\end{aligned}$$

$$\begin{aligned}
&< 2L + (n-7)(x_0 - x_{n-3}) + \left(1 + \frac{2}{\rho(G'')}\right) \left[ \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-5)(x_0 - x_{n-3}) \right] \\
&+ \left[ \left( \left\lfloor \frac{n-3}{2} \right\rfloor - \left\lceil \frac{n-3}{2} \right\rceil \right) x_{\lfloor \frac{n-3}{2} \rfloor} + \left( \left\lceil \frac{n-3}{2} \right\rceil - \left\lfloor \frac{n-3}{2} \right\rfloor - 2 \right) x_{\lceil \frac{n-3}{2} \rceil} \right. \\
&\left. - 2x_{n-4} - 4 \sum_{j=\lceil \frac{n-1}{2} \rceil}^{n-5} x_j + (n-6)(x_{n-1} - x_{n-2}) \right] \text{ [by Corollary 4.2.3],}
\end{aligned}$$

i.e.,

$$\begin{aligned}
&\left[ \rho(G'') - \left\{ (n-7) + \left(1 + \frac{2}{\rho(G'')}\right) \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-5) \right\} \right] (x_0 - x_{n-3}) \\
&< \left[ \left( \left\lfloor \frac{n-3}{2} \right\rfloor - \left\lceil \frac{n-3}{2} \right\rceil \right) x_{\lfloor \frac{n-3}{2} \rfloor} + \left( \left\lceil \frac{n-3}{2} \right\rceil - \left\lfloor \frac{n-3}{2} \right\rfloor - 2 \right) x_{\lceil \frac{n-3}{2} \rceil} \right. \\
&\left. - 2x_{n-4} - 4 \sum_{j=\lceil \frac{n-1}{2} \rceil}^{n-5} x_j + (n-6)(x_{n-1} - x_{n-2}) \right] + 2L \\
&< 0 \text{ [by assumption and (4.2.14)].} \tag{4.2.19}
\end{aligned}$$

We have

$$\sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-5) = \begin{cases} \frac{(n-7)(n-5)}{4} & , \text{ if } n \text{ is odd;} \\ \frac{(n-6)^2}{4} & , \text{ if } n \text{ is even.} \end{cases} \tag{4.2.20}$$

If  $f(j)$  denotes the row sum in  $D(G'')$  corresponding to the vertex  $v_j$  of  $G''$ , then for  $0 \leq j \leq n-5$ , we have

$$f(j) = \frac{j(j+1)}{2} + \frac{(n-j-3)(n-j-2)}{2} + (n-j-4) + (n-j-3).$$

Since  $f'(j) = 2j - n + 1$ , therefore as a function over  $\mathbb{R}$ ,  $f$  will have minimum at  $j = \frac{n-1}{2}$ . Hence as a function over  $\mathbb{Z}$ ,  $f$  has a minimum at  $j = \lfloor \frac{n-1}{2} \rfloor$  or  $j = \lceil \frac{n-1}{2} \rceil$ , because  $f$  is a quadratic polynomial. Now

$$f\left(\left\lfloor \frac{n-1}{2} \right\rfloor\right) = f\left(\left\lceil \frac{n-1}{2} \right\rceil\right) = \begin{cases} \frac{n^2-17}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-16}{4}, & \text{if } n \text{ is even.} \end{cases} \tag{4.2.21}$$

Also, the row sum in  $D(G'')$  corresponding to the vertex  $v_{n-4}$  of  $G''$  is  $f(n-4) = \frac{n^2-7n+18}{2}$ , and

$$f(n-4) \leq \min\{f(n-1), f(n-2), f(n-3), f(n-4)\}. \tag{4.2.22}$$

From (4.2.21) and (4.2.22), the minimum row sum in  $D(G'')$  is

$$f\left(\left\lfloor \frac{n-1}{2} \right\rfloor\right) = \begin{cases} \frac{n^2-17}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-16}{4}, & \text{if } n \text{ is even.} \end{cases}$$

Since the spectral radius is bounded below by the minimum row sum, therefore

$$\rho(G'') > \begin{cases} \frac{n^2-17}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-16}{4}, & \text{if } n \text{ is even.} \end{cases} \quad (4.2.23)$$

If  $n$  is odd then by (4.2.20), we have

$$\begin{aligned} & (n-7) + \left(1 + \frac{2}{\rho(G'')}\right) \left[ \sum_{k=1}^{\lfloor \frac{n-5}{2} \rfloor} (n-2k-5) \right] \\ &= (n-7) + \left(1 + \frac{2}{\rho(G'')}\right) \frac{(n-7)(n-5)}{4} \\ &= (n-7) + \frac{n^2-12n+35}{4} + \frac{n^2-12n+35}{2} \left[ \frac{1}{\rho(G'')} \right] \\ &< (n-7) + \frac{n^2-12n+35}{4} + \frac{n^2-12n+35}{2} \left[ \frac{4}{n^2-17} \right] \quad [\text{by (4.2.23)}] \\ &= \frac{n^2-8n+7}{4} + \frac{2(n^2-12n+35)}{n^2-17} \\ &< \frac{n^2-8n+7}{4} + 2 \quad [\text{as } n^2-12n+35 < n^2-17 \Leftrightarrow 52 < 12n] \\ &= \frac{n^2-8n+15}{4} < \frac{n^2-17}{4} < \rho(G''). \end{aligned}$$

Hence by (4.2.19)  $x_0 - x_{n-3} < 0$ , a contradiction to the fact  $x_0 \geq x_{n-3}$ , as given by Lemma 4.2.2. Hence the claim and therefore by (4.2.17) we get,  $\rho(G) > \rho(G'')$ .

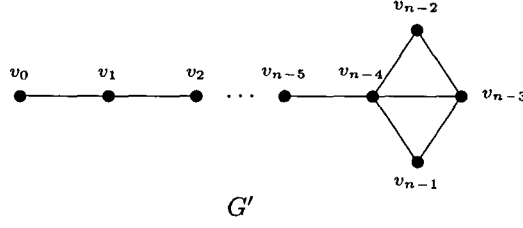
Similarly if  $n$  is even, then proceeding as above we obtain  $\rho(G) > \rho(G'')$ .  $\blacksquare$

Let  $G'$  be the  $\theta(2; 1; 2)$ -graph obtained by identifying an end vertex of a path of length  $n-4$  with a vertex of degree 3 in  $\theta(2; 1; 2)$ . If the vertices of  $G'$  are labeled as in Fig. 4.4, then we have the following result.

**Lemma 4.2.5.** *If  $n \geq 9$  and  $X = (x_0, x_1, \dots, x_{n-1})^T$  is the Perron vector of  $D(G')$ , then*

$$x_{\lfloor \frac{n-3}{2} \rfloor - i} \geq x_{\lceil \frac{n-3}{2} \rceil + i},$$

where  $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$  and  $x_j$  corresponds to the vertex  $v_j$ , for each  $j = 0, 1, \dots, n-1$ ; equality holds only at  $i = 0$ , if  $n$  is odd.

Figure 4.4: The graph  $G'$  in Lemma 4.2.5

**Proof.** We first claim that

$$\sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j > \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j.$$

Otherwise

$$\sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j \leq \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j. \quad (4.2.24)$$

From eigenequations we have

$$\rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \right) = \begin{cases} 0 & , \text{ if } n \text{ is odd;} \\ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j & , \text{ if } n \text{ is even,} \end{cases} \quad (4.2.25)$$

which gives  $x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \leq 0$ . Similarly for  $1 \leq i \leq \lfloor \frac{n-5}{2} \rfloor$ , using eigenequations we have

$$\begin{aligned} & \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) - \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \\ &= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil + i}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor - i} x_j \right] \\ &= 2 \left[ \sum_{j=\lceil \frac{n-3}{2} \rceil}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] - 2 \sum_{j=0}^{i-1} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right]. \end{aligned} \quad (4.2.26)$$

We now prove  $x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0$  by induction on  $i$ , where  $0 \leq i \leq \lfloor \frac{n-5}{2} \rfloor$ .

If  $i = 0$ , then by (4.2.25) we get  $x_{\lfloor \frac{n-3}{2} \rfloor} - x_{\lceil \frac{n-3}{2} \rceil} \leq 0$ .

For  $i \geq 1$ , by induction hypothesis  $x_{\lfloor \frac{n-3}{2} \rfloor - j} - x_{\lceil \frac{n-3}{2} \rceil + j} \leq 0$ , where  $0 \leq j \leq i - 1$ . Thus,

$$-2 \sum_{j=0}^{i-1} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] \leq 0.$$

Hence by (4.2.24) and (4.2.26) we have

$$\begin{aligned} & \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) - \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \leq 0 \\ \Rightarrow & \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \right) \leq \rho(G') \left( x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1} \right) \leq 0 \\ & \text{[by induction hypothesis]} \\ \Rightarrow & x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0. \end{aligned}$$

Therefore if  $0 \leq i \leq \lfloor \frac{n-5}{2} \rfloor$ , then we have proved by induction on  $i$ , that

$$x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} \leq 0. \quad (4.2.27)$$

Again

$$\begin{aligned} & \rho(G')(x_0 - x_{n-3}) - \rho(G')(x_1 - x_{n-4}) \\ = & 2(x_{n-3} - x_0) + x_{n-2} + x_{n-1} \quad (4.2.28) \\ = & 2 \left[ \sum_{j=\lfloor \frac{n-3}{2} \rfloor}^{n-1} x_j - \sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j \right] \\ & - 2 \sum_{j=0}^{\lfloor \frac{n-5}{2} \rfloor} \left[ x_{\lceil \frac{n-3}{2} \rceil + j} - x_{\lfloor \frac{n-3}{2} \rfloor - j} \right] - x_{n-2} - x_{n-1} \\ & < 0 \text{ [by (4.2.24) and (4.2.27)]} \\ \Rightarrow & \rho(G')(x_0 - x_{n-3}) < \rho(G')(x_1 - x_{n-4}) \leq 0 \text{ [by (4.2.27)]} \\ \Rightarrow & x_0 - x_{n-3} < 0. \quad (4.2.29) \end{aligned}$$

From (4.2.27) and (4.2.29), we have

$$\sum_{j=0}^{\lfloor \frac{n-3}{2} \rfloor} x_j < \sum_{j=\lfloor \frac{n-3}{2} \rfloor}^{n-3} x_j < \sum_{j=\lfloor \frac{n-3}{2} \rfloor}^{n-1} x_j.$$

This is a contradiction to (4.2.24) and hence the claim is established.



Therefore from (4.2.25) we get  $x_{\lfloor \frac{n-3}{2} \rfloor} \geq x_{\lceil \frac{n-3}{2} \rceil}$ , where equality holds only if  $n$  is odd. Proceeding as mentioned above and using induction we get  $x_{\lfloor \frac{n-3}{2} \rfloor - i} > x_{\lceil \frac{n-3}{2} \rceil + i}$ , where  $1 \leq i \leq \lfloor \frac{n-5}{2} \rfloor$ . Finally, from (4.2.28) we have

$$\begin{aligned} (\rho(G') + 2)(x_0 - x_{n-3}) - \rho(G')(x_1 - x_{n-4}) &= x_{n-2} + x_{n-1} > 0 \\ \Rightarrow (\rho(G') + 2)(x_0 - x_{n-3}) &> \rho(G')(x_1 - x_{n-4}) > 0 \\ \Rightarrow x_0 &> x_{n-3}. \end{aligned}$$

Hence  $x_{\lfloor \frac{n-3}{2} \rfloor - i} \geq x_{\lceil \frac{n-3}{2} \rceil + i}$ , where  $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$ . ■

From the proof of the above lemma we have the following corollary.

**Corollary 4.2.6.** *If  $n \geq 9$  and  $X = (x_0, x_1, \dots, x_{n-1})^T$  is the Perron vector of  $D(G')$ , where  $x_j$  corresponds to the vertex  $v_j$ , for  $j = 0, 1, \dots, n-1$ , then*

- (i)  $x_{\lfloor \frac{n-3}{2} \rfloor - i} - x_{\lceil \frac{n-3}{2} \rceil + i} > x_{\lfloor \frac{n-3}{2} \rfloor - i + 1} - x_{\lceil \frac{n-3}{2} \rceil + i - 1}$ , where  $1 \leq i \leq \lfloor \frac{n-5}{2} \rfloor$  and
- (ii)  $\left(1 + \frac{2}{\rho(G')}\right)(x_0 - x_{n-3}) > (x_1 - x_{n-4})$ .

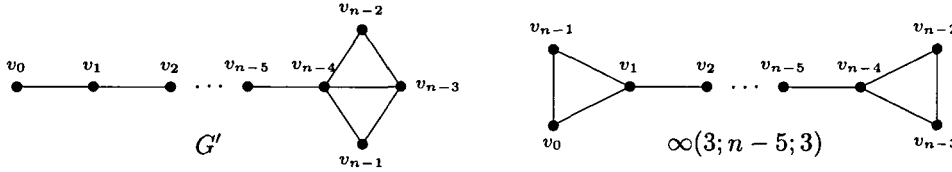


Figure 4.5: The graphs  $G'$  and  $\infty(3; n-5; 3)$  in Lemma 4.2.7

**Lemma 4.2.7.** *If  $n \geq 9$ , then  $\rho(\infty(3; n-5; 3)) > \rho(G')$ .*

**Proof.** Let us denote  $\infty(3; n-5; 3)$  by  $G$  and label the vertices in  $V(G) = V(G')$  as in Fig. 4.5. If  $X$  is the Perron vector of  $D(G')$  and  $x_i$  denotes the component of  $X$  corresponding to vertex  $v_i$  for  $0 \leq i \leq n-1$ , then by symmetry  $x_{n-1} = x_{n-2}$ . Therefore from  $G'$  to  $G$  we have

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}X^T(D(G) - D(G'))X \\ &= x_{n-1} \left[ (n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} \right. \\ &\quad \left. + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \right] \end{aligned} \quad (4.2.30)$$

Claim:  $(n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) > 0$ .

Suppose to the contrary, that

$$(n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \leq 0. \quad (4.2.31)$$

Then from eigenequations we have

$$\begin{aligned} & \rho(G')(x_0 - x_{n-3}) \\ &= (n-3)(x_{n-3} - x_0) + (n-4)x_{n-1} + (n-4)x_{n-2} \\ & \quad + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \\ &= (n-3)(x_{n-3} - x_0) + 2(n-4)x_{n-2} + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \\ &= \frac{2(n-4)}{(n-5)} \left[ (n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} \right. \\ & \quad \left. + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \right] + \frac{n^2 - 8n + 17}{n-5}(x_0 - x_{n-3}) \\ & \quad + \frac{(n-3)}{(n-5)} \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_i - x_{n-i-3}) \\ &< \frac{2(n-4)}{(n-5)} \left[ (n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} \right. \\ & \quad \left. + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \right] + \frac{n^2 - 8n + 17}{n-5}(x_0 - x_{n-3}) \\ & \quad + \frac{(n-3)}{(n-5)} \left( 1 + \frac{2}{\rho(G')} \right) \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_0 - x_{n-3}). \end{aligned}$$

[by Corollary 4.2.6],

i.e.,

$$\left[ \rho(G') - \left\{ \frac{n^2 - 8n + 17}{n-5} + \frac{(n-3)}{(n-5)} \left( 1 + \frac{2}{\rho(G')} \right) \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3) \right\} \right] (x_0 - x_{n-3})$$

$$\begin{aligned}
&< \frac{2(n-4)}{(n-5)} \left[ (n-4)(x_{n-3} - x_0) + (n-5)x_{n-2} + \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3)(x_{n-i-3} - x_i) \right] \\
&\leq 0 \text{ [by (4.2.31)].} \tag{4.2.32}
\end{aligned}$$

We have

$$\sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n-2i-3) = \begin{cases} \frac{(n-5)(n-3)}{4}, & \text{if } n \text{ is odd;} \\ \frac{(n-4)^2}{4}, & \text{if } n \text{ is even.} \end{cases} \tag{4.2.33}$$

If  $f(j)$  denotes the row sum in  $D(G')$  corresponding to the vertex  $v_j$  of  $G'$ , then for  $0 \leq j \leq n-4$ , we have

$$f(j) = \frac{j(j+1)}{2} + \frac{(n-j-4)(n-j-3)}{2} + 3(n-j-3).$$

Since  $f'(j) = 2j - n + 1$ , therefore as a function over  $\mathbb{R}$ ,  $f$  will have minimum at  $j = \frac{n-1}{2}$ . Hence as a function over  $\mathbb{Z}$ ,  $f$  has a minimum at  $j = \lfloor \frac{n-1}{2} \rfloor$  or  $j = \lceil \frac{n-1}{2} \rceil$ , because  $f$  is a quadratic polynomial. Now

$$f\left(\left\lfloor \frac{n-1}{2} \right\rfloor\right) = f\left(\left\lceil \frac{n-1}{2} \right\rceil\right) = \begin{cases} \frac{n^2-13}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-12}{4}, & \text{if } n \text{ is even.} \end{cases} \tag{4.2.34}$$

Also the row sum in  $D(G')$  corresponding to the vertex  $v_{n-4}$  is  $f(n-4) = \frac{n^2-7n+18}{2}$  and

$$f(n-4) \leq \min\{f(n-1), f(n-2), f(n-3), f(n-4)\}. \tag{4.2.35}$$

From (4.2.34) and (4.2.35), the minimum row sum in  $D(G')$  is

$$f\left(\left\lfloor \frac{n-1}{2} \right\rfloor\right) = \begin{cases} \frac{n^2-13}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-12}{4}, & \text{if } n \text{ is even.} \end{cases}$$

Since the spectral radius is bounded below by the minimum row sum, therefore

$$\rho(G') > \begin{cases} \frac{n^2-13}{4}, & \text{if } n \text{ is odd;} \\ \frac{n^2-12}{4}, & \text{if } n \text{ is even.} \end{cases} \tag{4.2.36}$$

If  $n$  is odd then by (4.2.33), we have

$$\begin{aligned}
& \frac{n^2 - 8n + 17}{n - 5} + \frac{(n - 3)}{(n - 5)} \left( 1 + \frac{2}{\rho(G')} \right) \left[ \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n - 2i - 3) \right] \\
&= \frac{n^2 - 8n + 17}{n - 5} + \frac{(n - 3)}{(n - 5)} \left( 1 + \frac{2}{\rho(G')} \right) \frac{(n - 5)(n - 3)}{4} \\
&= \frac{n^2 - 8n + 17}{n - 5} + \frac{(n^2 - 6n + 9)}{4} + \frac{(n^2 - 6n + 9)}{2} \left[ \frac{1}{\rho(G')} \right] \\
&< \frac{n^2 - 8n + 17}{n - 5} + \frac{(n^2 - 6n + 9)}{4} + \frac{(n^2 - 6n + 9)}{2} \left[ \frac{4}{n^2 - 13} \right] \quad [\text{by (4.2.36)}] \\
&= \frac{n^5 - 7n^4 + 2n^3 + 26n^2 + 221n - 659}{4n^3 - 20n^2 - 52n + 260} \quad (4.2.37)
\end{aligned}$$

If possible, let

$$\begin{aligned}
& \frac{n^5 - 7n^4 + 2n^3 + 26n^2 + 221n - 659}{4n^3 - 20n^2 - 52n + 260} \geq \frac{n^2 - 13}{4} \\
&\Leftrightarrow -8n^4 + 112n^3 - 416n^2 + 208n + 744 \geq 0 \\
&\Leftrightarrow (-8)(n^4 - 14n^3 + 52n^2 - 26n - 93) \geq 0 \\
&\Leftrightarrow n^4 - 14n^3 + 52n^2 - 26n - 93 \leq 0.
\end{aligned}$$

But if  $n$  is odd and  $n \geq 9$ , then  $n^4 - 14n^3 + 52n^2 - 26n - 93 > 0$ , which is a contradiction. Hence

$$\frac{n^5 - 7n^4 + 2n^3 + 26n^2 + 221n - 659}{4n^3 - 20n^2 - 52n + 260} < \frac{n^2 - 13}{4}. \quad (4.2.38)$$

Thus by (4.2.37) and (4.2.38), we have

$$\frac{n^2 - 8n + 17}{n - 5} + \frac{(n - 3)}{(n - 5)} \left( 1 + \frac{2}{\rho(G')} \right) \left[ \sum_{i=1}^{\lfloor \frac{n-3}{2} \rfloor} (n - 2i - 3) \right] < \frac{n^2 - 13}{4} < \rho(G').$$

Therefore if  $n$  is odd and  $n \geq 9$ , then from (4.2.32) we have,  $x_0 - x_{n-3} < 0$ , a contradiction to the fact  $x_0 \geq x_{n-3}$  as given by Lemma 4.2.5. Hence the claim and so by (4.2.30) we get  $\rho(G) > \rho(G')$ .

Similarly, if  $n$  is even, then proceeding as mentioned above we can obtain  $\rho(G) > \rho(G')$ . ■

To prove our next results we need the following lemma and the corollary after that.

**Lemma 4.2.8.** [65] Let  $u$  and  $v$  be two adjacent vertices of a connected graph  $G$  and for positive integers  $k$  and  $l$ , let  $G_{k,l}$  denote the graph obtained from  $G$  by adding paths of length  $k$  at  $u$  and length  $l$  at  $v$ . If  $k > l \geq 1$ , then  $\rho(G_{k,l}) < \rho(G_{k+1,l-1})$ ; if  $k = l \geq 1$ , then  $\rho(G_{k,l}) < \rho(G_{k+1,l-1})$  or  $\rho(G_{k,l}) < \rho(G_{k-1,l+1})$ .

**Corollary 4.2.9.** [65] Let  $v_l$  and  $v_m$  be two adjacent vertices of a connected graph  $G$ . Let  $P_l$  and  $P_m$  be two pendent paths with roots  $v_l$  and  $v_m$ , respectively. If  $l > m$  and  $X$  is the Perron vector of  $D(G)$ , then  $\sum_{v_j \in V(P_l)} x_{v_j} > \sum_{v_j \in V(P_m)} x_{v_j}$ .

**Lemma 4.2.10.** Let  $\theta(2; 1; 2)$  be formed from three vertex-disjoint paths  $P_3 = x_1x_2x_3$ ,  $P_2 = y_1y_2$  and  $P_3 = z_1z_2z_3$  by identifying the initial vertices as  $u_0$  and the terminal vertices as  $v_0$ . Let  $G$  be a graph obtained by attaching the ends  $v_1, u_1$  and  $w_1$  of the paths  $P_{l_1} = v_1v_2 \dots v_{l_1}$ ,  $P_{l_2} = u_1u_2 \dots u_{l_2}$  and  $P_{l_3} = w_1w_2 \dots w_{l_3}$  at  $v_0, x_2$  and  $z_2$  of  $\theta(2; 1; 2)$ , respectively. If  $l_2 \geq l_3 > l_1 \geq 1$  and  $G_0 = G - x_2u_0 + u_0v_1$ , then  $\rho(G') > \rho(G_0) > \rho(G)$ .

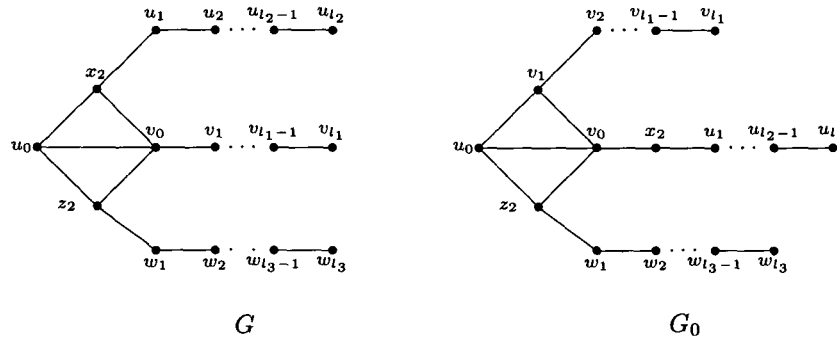


Figure 4.6: The graphs  $G$  and  $G_0$  in Lemma 4.2.10.

**Proof.** If  $X$  is the Perron vector of  $G$ , then we identify its components with the labels of the vertices of  $G$ . Since  $l_2 \geq l_3 > l_1$ , so by Corollary 4.2.9 we have

$$x_2 + \sum_{j=1}^{l_2} u_j > v_0 + \sum_{j=1}^{l_1} v_j. \quad (4.2.39)$$

As we pass from  $G$  to  $G_0$ , the distances of  $u_0$  are increased by 1 from  $\{x_2, u_1, u_2, \dots, u_{l_2}\}$  and are decreased by 1 from  $\{v_1, v_2, \dots, v_{l_1}\}$ ; distances among other vertices remain unchanged [Fig.4.6]. Therefore, we have

$$\begin{aligned} \frac{1}{2}(\rho(G_0) - \rho(G)) &\geq \frac{1}{2}X^T(D(G_0) - D(G))X \\ &= u_0 \left[ x_2 + \sum_{j=1}^{l_2} u_j - \sum_{j=1}^{l_1} v_j \right]. \end{aligned} \quad (4.2.40)$$

Using (4.2.39) in (4.2.40) we have  $\rho(G_0) > \rho(G)$ . Now using Lemma 4.2.8 repeatedly for the adjacent vertices  $v_0, v_1$  and  $v_0, v_2$ , we finally have  $\rho(G') > \rho(G_0) > \rho(G)$ . ■

**Lemma 4.2.11.** *Let  $\theta(2; 1; 2)$  be formed from three vertex-disjoint paths  $P_3 = x_1x_2x_3$ ,  $P_2 = y_1y_2$  and  $P_3 = z_1z_2z_3$  by identifying the initial vertices as  $u_0$  and the terminal vertices as  $v_0$ . For  $1 \leq i \leq 4$  and  $l_i \geq 0$ , suppose  $G$  is a graph obtained by attaching paths of lengths  $l_1, l_2, l_3$  and  $l_4$  at  $v_0, x_2, u_0$  and  $z_2$  of  $\theta(2; 1; 2)$ , respectively. If  $l_1 + l_3 \geq 1$ , then  $\rho(G') > \rho(G)$ .*

**Proof.** Here we have the following cases.

**Case 1.** If  $\min\{l_1, l_3\} \geq \max\{l_2, l_4\}$ , then by repeated applications of Lemma 4.2.8 we have  $\rho(G') > \rho(G)$ .

**Case 2.** Suppose  $\min\{l_1, l_3\} < \max\{l_2, l_4\}$ . If  $\min\{l_1, l_3\} > 0$ , then applying Lemma 4.2.10 we have  $\rho(G') > \rho(G)$ . If  $\min\{l_1, l_3\} = 0$  and  $\max\{l_1, l_3\} < \max\{l_2, l_4\}$ , then again applying Lemma 4.2.10 we have  $\rho(G') > \rho(G)$ . So let  $\max\{l_2, l_4\} \leq \max\{l_1, l_3\}$ , but then by Lemmas 4.2.8 and 4.2.10, we have  $\rho(G') > \rho(G)$ . ■

**Lemma 4.2.12.** *If  $G$  is a  $\theta(p; q; t)$ -graph, where  $\min\{p, q, t\} \geq 2$ , then there exists a  $\theta(2; 1; 2)$ -graph  $G^*$  such that one of the distinguished vertices of  $\theta(2; 1; 2)$ -graph is of degree at least 4 and  $\rho(G^*) > \rho(G)$ .*

**Proof.** Let  $G$  be a  $\theta(p; q; t)$ -graph formed by three vertex-disjoint paths  $P_{p+1} = x_1x_2 \dots x_{p+1}$ ,  $P_{t+1} = y_1y_2 \dots y_{t+1}$  and  $P_{q+1} = z_1z_2 \dots z_{q+1}$ , where  $\min\{p, t, q\} \geq 2$ . We identify the initial vertices as  $u_0$  and the terminal vertices as  $v_0$ . Let  $X$  be the Perron vector of  $D(G)$ ,  $T_v$  be the attached tree rooted at a vertex  $v$  and  $S'(v)$  be the sum of the components of  $X$  corresponding to the vertices in  $T_v$  (including  $v$  also). Then we have the following cases.

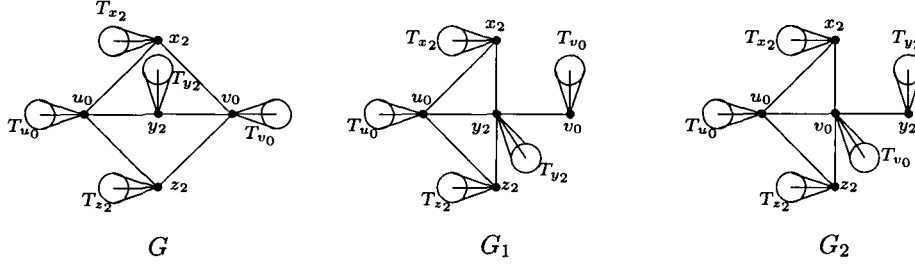
**Case 1.**  $p \geq q \geq t = 2$ .    **Case 2.**  $p \geq q \geq t \geq 3$ .

**Case 1.**

**Subcase (a).**  $p = q = t = 2$ . If  $S'(v_0) \geq S'(y_2)$  and  $G_1 = G - x_2v_0 - z_2v_0 + x_2y_2 + z_2y_2$ , [Fig. 4.7] then from  $G$  to  $G_1$  the distances of  $T_{x_2} \cup T_{z_2}$  are increased by 1 from  $T_{v_0}$  and decreased by 1 from  $T_{y_2}$ ; distances between any other vertices remain unchanged.

Thus,

$$\begin{aligned} \frac{1}{2}(\rho(G_1) - \rho(G)) &\geq \frac{1}{2}X^T(D(G_1) - D(G))X \\ &= \left[ S'(x_2) + S'(z_2) \right] \left( S'(v_0) - S'(y_2) \right) \geq 0 \\ \Rightarrow \rho(G_1) &\geq \rho(G). \end{aligned}$$

Figure 4.7: The graphs  $G$ ,  $G_1$  and  $G_2$  in Lemma 4.2.12 Case 1(a)

If  $\rho(G_1) = \rho(G)$ , then from  $\rho(G_1) \geq X^T D(G_1)X \geq X^T D(G)X = \rho(G)$ ,  $X$  must be a Perron vector of  $D(G_1)$ . But if  $D(G)_0$  (resp.  $D(G_1)_0$ ) denotes the row corresponding to  $v_0$  in  $D(G)$  (resp.  $D(G_1)$ ), then  $\rho(G_1)x_{v_0} = (D(G_1)_0)X > (D(G)_0)X = \rho(G)x_{v_0}$ , a contradiction. So  $\rho(G_1) > \rho(G)$ .

And if  $S'(v_0) < S'(y_2)$  and  $G_2 = G - y_2u_0 + v_0u_0$ , [Fig. 4.7] then from  $G$  to  $G_2$  the distances of  $T_{u_0}$  are increased by 1 from  $T_{y_2}$  and are decreased by 1 from  $T_{v_0}$ ; distances between any other vertices remain unchanged. Thus,

$$\begin{aligned} \frac{1}{2}(\rho(G_2) - \rho(G)) &\geq \frac{1}{2}X^T(D(G_2) - D(G))X \\ &= S'(u_0)(S'(y_2) - S'(v_0)) > 0 \\ \Rightarrow \rho(G_2) &> \rho(G). \end{aligned}$$

Thus, the lemma is proved in this case by taking  $G^* = G_1$  or  $G^* = G_2$ .

**Subcase (b).**  $p > q = t = 2$ . If  $\sum_{i=\lceil \frac{p+3}{2} \rceil}^p S'(x_i) + S'(v_0) \geq \sum_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} S'(x_i)$ , then let  $G_1 = G - y_2v_0 - z_2v_0 + y_2x_2 + z_2x_2$  [Fig. 4.8]. If  $p$  is even, then from  $G$  to  $G_1$  the distances of  $T_{y_2} \cup T_{z_2}$  are increased by at least 1 from  $\cup_{i=\lceil \frac{p+3}{2} \rceil}^p T_{x_i}$ , are increased by at least 3 from  $T_{v_0}$ , and are decreased by 1 from  $\cup_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} T_{x_i}$ ; the distances between any other vertices are increased or remain unchanged. And if  $p$  is odd, then from  $G$  to  $G_1$  the distances of  $T_{y_2} \cup T_{z_2}$  are increased by at least 2 from  $\cup_{i=\lceil \frac{p+3}{2} \rceil+1}^p T_{x_i}$ , are increased by at least 2 from  $T_{v_0}$ , and are decreased by 1 from  $\cup_{i=2}^{\lfloor \frac{p+3}{2} \rfloor-1} T_{x_i}$ ; the distances between

any other vertices are increased or remain unchanged. Thus for any  $p$ , we have

$$\begin{aligned}
\frac{1}{2}(\rho(G_1) - \rho(G)) &\geq \frac{1}{2}X^T(D(G_1) - D(G))X \\
&\geq (S'(y_2) + S'(z_2)) \left[ \sum_{i=\lceil \frac{p+3}{2} \rceil}^p S'(x_i) + 2S'(v_0) - \sum_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} S'(x_i) \right] \\
&> 0 \\
\Rightarrow \rho(G_1) &> \rho(G).
\end{aligned}$$

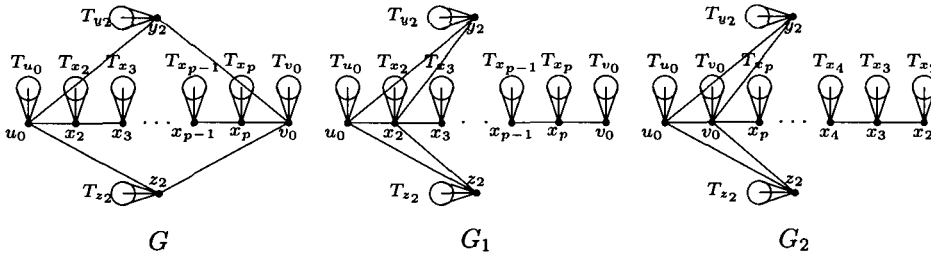


Figure 4.8: The graphs  $G$ ,  $G_1$  and  $G_2$  in Lemma 4.2.12 Case 1(b)

And if  $\sum_{i=\lceil \frac{p+3}{2} \rceil}^p S'(x_i) + S'(v_0) < \sum_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} S'(x_i)$ , then let  $G_2 = G - u_0x_2 + v_0u_0$  [Fig. 4.8].

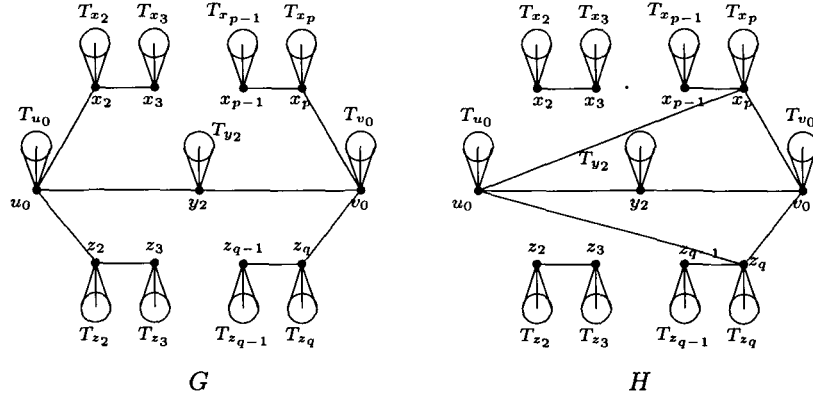
If  $p$  is even, then from  $G$  to  $G_2$  the distances of  $T_{u_0}$  are increased by at least 1 from  $\cup_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} T_{x_i}$ , and are decreased by 1 from  $\cup_{i=\lceil \frac{p+3}{2} \rceil}^p T_{x_i} \cup T_{v_0}$ ; the distances between any other vertices are increased or remain unchanged. And if  $p$  is odd, then from  $G$  to  $G_2$  the distances of  $T_{u_0}$  are increased by at least 1 from  $\cup_{i=2}^{\lfloor \frac{p+3}{2} \rfloor - 1} T_{x_i}$ , and are decreased by 1 from  $\cup_{i=\lceil \frac{p+3}{2} \rceil + 1}^p T_{x_i} \cup T_{v_0}$ ; the distances between any other vertices are increased or remain unchanged. Thus for any  $p$ , we have

$$\begin{aligned}
\frac{1}{2}(\rho(G_2) - \rho(G)) &\geq \frac{1}{2}X^T(D(G_2) - D(G))X \\
&\geq S'(u_0) \left[ \sum_{i=2}^{\lfloor \frac{p+3}{2} \rfloor} S'(x_i) - \sum_{i=\lceil \frac{p+3}{2} \rceil}^p S'(x_i) - S'(v_0) \right] > 0 \\
\Rightarrow \rho(G_2) &> \rho(G).
\end{aligned}$$

Thus, in this case also the lemma is proved by taking  $G^* = G_1$  or  $G^* = G_2$ .

**Subcase (c).**  $p \geq q > t = 2$ .



Figure 4.9: The graphs  $G$ ,  $H$  in Lemma 4.2.12 Case 1(c)

Without loss of generality assume that

$$\begin{aligned}
& 2 \left[ \sum_{i=2}^{\lfloor \frac{p}{2} \rfloor} S'(x_i) + \sum_{i=2}^{\lfloor \frac{q}{2} \rfloor} S'(z_i) \right] + S'(x_{\lfloor \frac{p}{2} + 1 \rfloor}) + S'(z_{\lfloor \frac{q}{2} + 1 \rfloor}) \\
& \geq S'(x_{\lceil \frac{p}{2} + 1 \rceil}) + S'(z_{\lceil \frac{q}{2} + 1 \rceil}) + 2 \left[ \sum_{i=\lceil \frac{p}{2} + 2 \rceil}^p S'(x_i) + \sum_{i=\lceil \frac{q}{2} + 2 \rceil}^q S'(z_i) \right],
\end{aligned}$$

and let  $H = G - x_2u_0 - z_2u_0 + x_pu_0 + z_pu_0$  [Fig. 4.9].

As we move from  $G$  to  $H$  the distances of  $T_{u_0}$  are increased by at least 2 from  $\left[ \bigcup_{i=2}^{\lfloor \frac{p}{2} \rfloor} T_{x_i} \right] \cup \left[ \bigcup_{i=2}^{\lfloor \frac{q}{2} \rfloor} T_{z_i} \right]$ , and are decreased by 2 from  $\left[ \bigcup_{i=\lceil \frac{p}{2} + 2 \rceil}^p T_{x_i} \right] \cup \left[ \bigcup_{i=\lceil \frac{q}{2} + 2 \rceil}^q T_{z_i} \right]$ ; the distances between  $T_{x_2}$  and  $T_{z_2}$  are increased by at least 2. Moreover,

(i) If  $p$  is even and  $q$  is odd, then the distances of  $T_{u_0}$  are increased by at least 1 from  $T_{z_{\lfloor \frac{q}{2} + 1 \rfloor}}$ , and are decreased by 1 from  $T_{x_{\lceil \frac{p}{2} + 1 \rceil}}$ .

(ii) If both  $p$  and  $q$  are odd, then the distances of  $T_{u_0}$  are increased by at least 1 from  $T_{x_{\lfloor \frac{p}{2} + 1 \rfloor}} \cup T_{z_{\lfloor \frac{q}{2} + 1 \rfloor}}$ , and are decreased by 1 from  $T_{x_{\lceil \frac{p}{2} + 1 \rceil}} \cup T_{z_{\lceil \frac{q}{2} + 1 \rceil}}$ .

(iii) If  $p$  is odd and  $q$  is even, then the distances of  $T_{u_0}$  are increased by at least 1 from  $T_{x_{\lfloor \frac{p}{2} + 1 \rfloor}}$ , and are decreased by 1 from  $T_{z_{\lceil \frac{q}{2} + 1 \rceil}}$ .

The distances between any other vertices are increased or remain unchanged. Thus

for any  $p$  and  $q$ , we have

$$\begin{aligned}
 & \frac{1}{2}(\rho(H) - \rho(G)) \\
 & \geq \frac{1}{2}X^T(D(H) - D(G))X \\
 & \geq S'(u_0) \left[ 2 \left\{ \sum_{i=2}^{\lfloor \frac{p}{2} \rfloor} S'(x_i) + \sum_{i=2}^{\lfloor \frac{q}{2} \rfloor} S'(z_i) \right\} + \left[ S'(x_{\lfloor \frac{p}{2} + 1 \rfloor}) + S'(z_{\lfloor \frac{q}{2} + 1 \rfloor}) \right] \right. \\
 & \quad \left. - \left[ S'(x_{\lceil \frac{p}{2} + 1 \rceil}) + S'(z_{\lceil \frac{q}{2} + 1 \rceil}) \right] - 2 \left\{ \sum_{i=\lfloor \frac{p}{2} + 2 \rfloor}^p S'(x_i) + \sum_{i=\lfloor \frac{q}{2} + 2 \rfloor}^q S'(z_i) \right\} \right] \\
 & \quad + 2S'(x_2)S'(z_2) \\
 & > 0 \\
 & \Rightarrow \rho(H) > \rho(G).
 \end{aligned}$$

In any case,  $H$  is a  $\theta(2; 2; 2)$ -graph. Now using Subcase (a), we can obtain the required graph  $G^*$ , such that  $\rho(G^*) \geq \rho(H) > \rho(G)$ .

**Case 2.**  $p \geq q \geq t \geq 3$ .

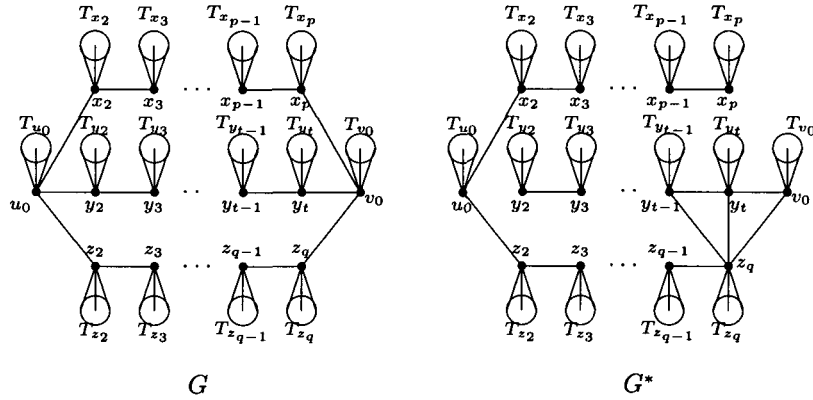


Figure 4.10: The graphs  $G$  and  $G^*$  in Lemma 4.2.12 Case 2

Without loss of generality assume that  $\sum_{i=2}^p S'(x_i) \geq \sum_{i=2}^q S'(z_i)$ , and let  $G^* = G - x_p v_0 - u_0 y_2 + z_q y_t + z_q y_{t-1}$  [Fig. 4.10]. Then from  $G$  to  $G^*$  the distances of  $\cup_{i=2}^p T_{x_i}$  are increased by at least 2 from  $\cup_{i=2}^{t-1} T_{y_i}$ , and are increased by at least 1 from  $T_{y_t}$ ; the distances between  $T_{y_j}$  and  $\cup_{i=\lfloor \frac{t+j}{2} \rfloor + 2 - j}^q T_{z_i}$  are decreased by at most 2, where  $j = 2, 3, \dots, t - 1$ ; the distances between  $T_{y_t}$  and  $\cup_{i=\lfloor \frac{t+q}{2} \rfloor + 2 - t}^q T_{z_i}$  are decreased by at most

1; the distances between any other vertices are increased or remain unchanged. Thus,

$$\begin{aligned}
\frac{1}{2}(\rho(G^*) - \rho(G)) &\geq \frac{1}{2}X^T(D(G^*) - D(G))X \\
&\geq 2 \sum_{j=2}^{t-1} \left( S'(y_j) \left[ \sum_{i=2}^p S'(x_i) - \sum_{i=\lfloor \frac{t+j}{2} \rfloor + 2 - j}^q S'(z_i) \right] \right) \\
&\quad + S'(y_t) \left[ \sum_{i=2}^p S'(x_i) - \sum_{i=\lfloor \frac{t+j}{2} \rfloor + 2 - t}^q S'(z_i) \right] > 0 \\
&\Rightarrow \rho(G^*) > \rho(G).
\end{aligned}$$

Therefore, combining all the above cases, we have the result.  $\blacksquare$

### 4.3 Graph with maximal distance spectral radius in $\mathcal{G}_n^0$

**Theorem 4.3.1.** *If  $n \geq 6$ , then  $\infty(3; n-5; 3)$  is the unique graph with maximal distance spectral radius in  $\mathcal{G}_n^0$ .*

**Proof.** If  $G \in \mathcal{G}_n^0$ , then we must have one of the following three cases.

**Case 1.**  $C_n$  is a spanning subgraph of  $G$ .

If  $n = 6$ , then it can be verified that  $\rho(\infty(3; 1; 3)) = 9.19615 > \rho(C_6) = 9 \geq \rho(G)$ ; whereas if  $n \geq 7$ , then by Lemma 4.2.1 we have  $\rho(\infty(3; n-5; 3)) > \rho(C_n) \geq \rho(G)$ .

**Case 2.** An  $\infty(p; q; r)$ -graph  $G_1$  is a spanning subgraph of  $G$ .

We have  $\rho(G_1) \geq \rho(G)$ . By Lemmas 4.1.1 and 4.2.4,  $\infty(3; n-5; 3)$  is the unique graph with maximal distance spectral radius in  $\mathcal{C}(n, 2)$ . Since  $G_1 \in \mathcal{C}(n, 2)$ , so  $\rho(\infty(3; n-5; 3)) \geq \rho(G_1)$ , which implies  $\rho(\infty(3; n-5; 3)) \geq \rho(G)$ .

**Case 3.** A  $\theta(p; q; r)$ -graph  $G_2$  is a spanning subgraph of  $G$ , where  $\min\{p, q, r\} \geq 2$ .

We have  $\rho(G_2) \geq \rho(G)$ . Applying Lemma 4.2.12 we get a  $\theta(2; 1; 2)$ -graph  $G^*$  with  $\rho(G^*) > \rho(G_2)$ . Now, by Lemmas 3.5.2, 4.2.8, 4.2.10 and 4.2.11, we have  $\rho(G') > \rho(G^*)$ . If  $6 \leq n \leq 8$ , then it can be verified that  $\rho(\infty(3; n-5; 3)) > \rho(G')$  and if  $n \geq 9$ , then by Lemma 4.2.7 we get  $\rho(\infty(3; n-5; 3)) > \rho(G')$ . Thus  $\rho(\infty(3; n-5; 3)) > \rho(G)$ .  $\blacksquare$

# Chapter 5

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## On the distance spectral radius of bipartite graphs

### 5.1 Introduction

Let  $\mathcal{B}_n^m$  be the class of all bipartite graphs of order  $n$  with matching number  $m$ , and  $\mathbf{B}_n^s$  be the class of all bipartite graphs of order  $n$  with vertex connectivity  $s$ . In Section 5.2, we determine the unique graph with minimum distance spectral radius in  $\mathcal{B}_n^m$ . In Section 5.3, we characterize the graphs with minimal distance spectral radius in  $\mathbf{B}_n^s$ .

### 5.2 Graph with minimum distance spectral radius in $\mathcal{B}_n^m$

Here we find the unique graph with minimum distance spectral radius in  $\mathcal{B}_n^m$ .

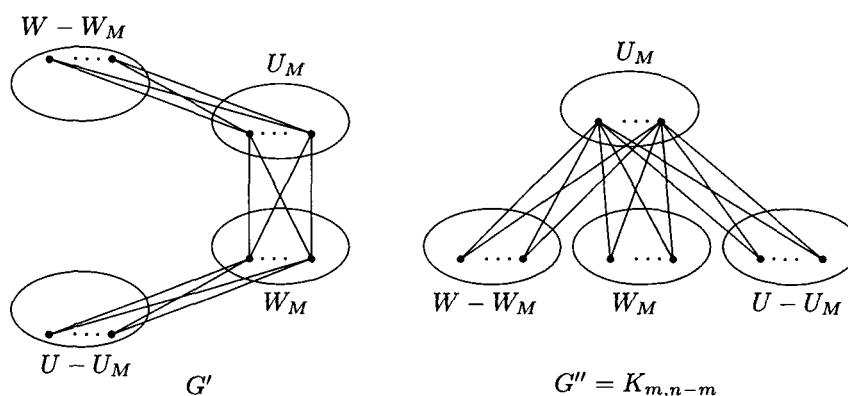


Figure 5.1: The graphs  $G'$  and  $G''$  in Theorem 5.2.1

**Theorem 5.2.1.**  $K_{m, n-m}$  is the unique graph that minimizes the distance spectral radius in  $\mathcal{B}_n^m$ .

**Proof.** Let  $G$  be a graph in  $\mathcal{B}_n^m$  with minimum distance spectral radius. For  $m = \lfloor \frac{n}{2} \rfloor$  the discussion is trivial.

Let  $(U, W)$  be the bipartition of the vertex set of  $G$  such that  $|W| \geq |U| \geq m$ , and let  $M$  be a maximal matching of  $G$ . Since the distance spectral radius of a graph decreases with addition of edges so for  $|U| = m$ ,  $G = K_{m, n-m}$ .

Let us assume that  $|U| > m$  and  $U_M, W_M$  be the sets of vertices of  $U, W$  which are incident to the edges of  $M$ , respectively. Therefore,  $|U_M| = |W_M| = m$ . Note that  $G$  contains no edges between the vertices of  $U - U_M$  and the vertices of  $W - W_M$ , otherwise any such edge may be united with  $M$  to produce a matching of cardinality greater than that of  $M$ , violating the maximality of  $M$ .

Adding all possible edges between the vertices of  $U_M$  and  $W_M, U_M$  and  $W - W_M, U - U_M$  and  $W_M$  we get a graph  $G'$  with  $\rho(G) > \rho(G')$ . We now form a complete bipartite graph  $G'' = K_{m, n-m}$  from  $G'$  with the bipartition  $(U_M, W \cup (U - U_M))$ .

Let  $|U - U_M| = n_1, |W - W_M| = n_2$ . So  $n_2 \geq n_1$ . We partition  $V(G') = V(G'')$  into  $U_M \cup W_M \cup (U - U_M) \cup (W - W_M)$  as shown in Fig. 5.1. If the distance matrices  $D(G')$  and  $D(G'')$  are partitioned according to  $U_M, W_M, (U - U_M)$ , and  $(W - W_M)$ , then their difference is

$$D(G') - D(G'') = \begin{bmatrix} 0 & 0 & J_{m \times n_1} & 0 \\ 0 & 0 & -J_{m \times n_1} & 0 \\ J_{n_1 \times m} & -J_{n_1 \times m} & 0 & J_{n_1 \times n_2} \\ 0 & 0 & J_{n_2 \times n_1} & 0 \end{bmatrix}.$$

We denote  $\rho(G')$  by  $\rho$  and  $\rho(G'')$  by  $\rho_1$ . Let  $X$  be the Perron vector of  $D(G'')$ . Then by symmetry, components of  $X$  have the same value, say  $x_1$  for the vertices in  $U_M$  and  $x_2$  for the vertices in  $W \cup (U - U_M)$ . Then,  $X$  can be written as

$$X = \left( \underbrace{x_1, \dots, x_1}_m, \underbrace{x_2, \dots, x_2}_{n-m} \right)^T.$$

We have

$$\frac{1}{2}(\rho - \rho_1) \geq \frac{1}{2}X^T(D(G') - D(G''))X = n_1x_2[mx_1 + n_2x_2 - mx_2]. \quad (5.2.1)$$

From eigenequations we have

$$\begin{aligned} \rho_1 x_1 &= 2(m-1)x_1 + (n-m)x_2, \\ \rho_1 x_2 &= mx_1 + 2(n-m-1)x_2. \end{aligned}$$

Thus,

$$(\rho_1 + 2 - m)(x_1 - x_2) = (2m - n)x_2 = -(n_1 + n_2)x_2. \quad (5.2.2)$$

Following [21], the distance spectral radius of the complete bipartite graph  $K_{p,q}$  is  $p + q - 2 + \sqrt{p^2 - pq + q^2}$ , so  $\rho_1 > n + m - 1$ .

Again,

$$\begin{aligned} m(x_1 - x_2) + n_2x_2 &= -\frac{(n_1 + n_2)mx_2}{\rho_1 + 2 - m} + n_2x_2 \quad [\text{by (5.2.2)}] \\ &> \frac{[-(n_1 + n_2)m + n_2(n + 1)]x_2}{\rho_1 + 2 - m} \\ &\quad [\text{since } \rho_1 > n + m - 1] \\ &= \frac{[-(n_1 + n_2)m + n_2(n_1 + n_2 + 2m + 1)]x_2}{\rho_1 + 2 - m} \\ &> \frac{[n_2^2 + n_2n_1 + n_2]x_2}{\rho_1 + 2 - m} > 0. \end{aligned}$$

Thus from (5.2.1) we get  $\rho > \rho_1$ , and so  $\rho(G) > \rho(G'')$ , a contradiction. Therefore  $|U| = m$ .  $\blacksquare$

### 5.3 Graphs in $\mathbf{B}_n^s$ with minimal distance spectral radius

In this section, we characterize the graphs with minimal distance spectral radius in  $\mathbf{B}_n^s$ . It is shown in [67] that  $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$  has minimum distance spectral radius among all connected bipartite graphs. This result also says that for vertex connectivity  $s = \lfloor \frac{n}{2} \rfloor$ ,  $K_{s, n-s}$  is the unique graph with minimum distance spectral radius in  $\mathbf{B}_n^s$ .

Clearly  $\mathbf{B}_4^1 = \{P_4, S_4\}$  and  $\mathbf{B}_5^1 = \{P_5, S_5, C_4^1\}$ , where  $C_4^1$  is the graph with a single pendent attached to a vertex of  $C_4$ . It can be easily verified that  $S_4$  and  $C_4^1$  are the graphs with minimal distance spectral radius in  $\mathbf{B}_4^1$  and  $\mathbf{B}_5^1$ , respectively. Thus for  $3 \leq n \leq 5$ , the discussion is over. From now onwards we will assume that  $n \geq 6$ .

To prove the main result in this section, we need to define some notations and prove some lemmas.

In  $K_{p,q}$ , we assume that  $p \geq q \geq 1$ . By  $K_1$ , we mean  $K_{1,0}$  or  $K_{0,1}$ , which will be clear from the context. By  $O_s \vee_1(K_{n_1, n_2} \cup K_{m_1, m_2})$ , we mean the graph obtained by joining all the vertices in  $O_s$  to the vertices belonging to the partitions of cardinality  $n_1$  in  $K_{n_1, n_2}$  and  $m_1$  in  $K_{m_1, m_2}$ , respectively, where  $n_1, m_1 > 0$ . Similarly, by  $O_s \vee_2(K_{n_1, n_2} \cup K_{m_1, m_2})$ ,

we mean the graph obtained by joining all the vertices in  $O_s$  to the vertices belonging to the partitions of cardinality  $n_2$  in  $K_{n_1, n_2}$  and  $m_2$  in  $K_{m_1, m_2}$ , respectively, where  $n_2, m_2 > 0$ .

**Lemma 5.3.1.** *If  $s + q \geq p + 1$  and  $p \geq s$ , then*

$$\rho(O_s \vee_1 (K_1 \cup K_{p,q})) > \rho(O_s \vee_1 (K_1 \cup K_{p+1, q-1})).$$

**Proof.** Let us denote  $O_s \vee_1 (K_1 \cup K_{p,q})$  by  $G$  and  $O_s \vee_1 (K_1 \cup K_{p+1, q-1})$  by  $G'$ . We partition  $V(G) = V(G')$  into  $\{v\} \cup C \cup A \cup B \cup \{b_q\}$ , where  $C = \{c_1, c_2, \dots, c_s\}$ ,  $A = \{a_1, a_2, \dots, a_p\}$  and  $B = \{b_1, b_2, \dots, b_{q-1}\}$  as in Fig. 5.2.

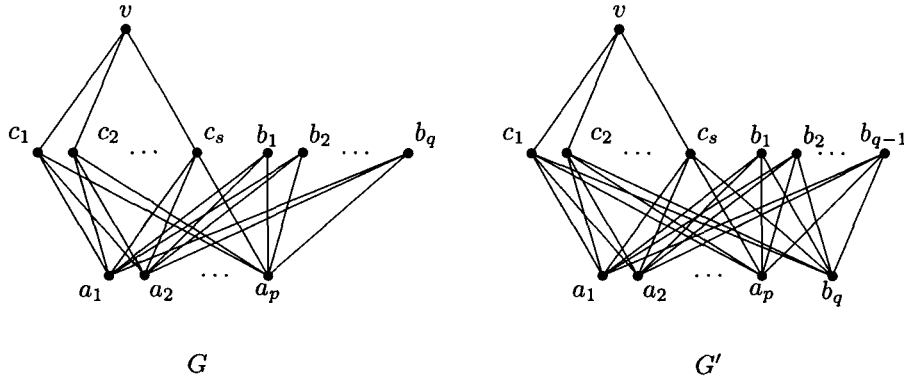


Figure 5.2: The graphs  $G$  and  $G'$  in Lemma 5.3.1

As we pass from  $G$  to  $G'$ , the distance of  $b_q$  is decreased by 1 with  $\{v\} \cup C \cup B$  and the distance of  $b_q$  is increased by 1 with  $A$ ; the distances within any other pairs of vertices remain unaltered. If the distance matrices are partitioned according to  $\{v\}, C, A, B$  and  $\{b_q\}$ , then their difference is

$$D(G) - D(G') = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & e_C \\ 0 & 0 & 0 & 0 & -e_A \\ 0 & 0 & 0 & 0 & e_B \\ 1 & e_C^T & -e_A^T & e_B^T & 0 \end{bmatrix}$$

where  $e_i = \underbrace{(1, \dots, 1)^T}_{|i|} = \mathbf{1}_{|i|}$  and  $i = A, B, C$ . We denote  $\rho(G)$  by  $\rho$  and  $\rho(G')$  by  $\rho_1$ .

Let  $X$  be the Perron vector of  $D(G')$ . Then by symmetry, components of  $X$  have the same value, say  $a$  for the vertices in  $A \cup \{b_q\}$ ,  $b$  for the vertices in  $B$ ,  $c$  for the vertices

in  $C$ , and  $x_1$  for  $v$ . Then,  $X$  can be written as

$$X = \left( x_1, \underbrace{c, \dots, c}_s, \underbrace{a, \dots, a}_p, \underbrace{b, \dots, b}_{q-1}, a \right)^T.$$

We now have

$$\frac{1}{2}(\rho - \rho_1) \geq \frac{1}{2}X^T(D(G) - D(G'))X = a[x_1 + cs - pa + b(q-1)]. \quad (5.3.1)$$

From eigenequations we have

$$\begin{aligned} \rho_1 x_1 &= sc + 3(q-1)b + 2(p+1)a, \\ \rho_1 c &= x_1 + 2(s-1)c + 2(q-1)b + (p+1)a, \\ \rho_1 a &= 2x_1 + sc + (q-1)b + 2pa, \\ \rho_1 b &= 3x_1 + 2sc + 2(q-2)b + (p+1)a. \end{aligned}$$

From which we get,

$$(\rho_1 + 2)(b - c) = 2x_1 > 0 \Rightarrow b > c, \quad (5.3.2)$$

$$(\rho_1 + 1)(x_1 - c) = c + (p+1)a + (q-1)b - sc, \quad (5.3.3)$$

$$(\rho_1 + 1)(c - a) = -x_1 + (s-1)c - pa + (q-1)b, \quad (5.3.4)$$

$$(\rho_1 + 2)(x_1 - a) = 2(q-1)b \geq 0 \Rightarrow x_1 \geq a. \quad (5.3.5)$$

Since distance matrix is nonnegative and irreducible, its spectral radius is bounded below by the minimum row sum and thus we have  $\rho_1 > 3p \geq 3s$ .

Again by the given condition  $q-1 \geq p-s = k$  (say). Therefore from (5.3.4), we get

$$\begin{aligned} (\rho_1 + 1)(c - a) &\geq -x_1 + pc - pa + (s-1-p)c + (p-s)b \\ \Rightarrow (\rho_1 + 1 - p)(c - a) &\geq -x_1 + (-k-1)c + kb \\ \Rightarrow (\rho_1 + 1 - p)(c - a) &\geq -c - x_1 + k(b - c) \\ \Rightarrow (c - a) &\geq \frac{1}{(\rho_1 + 1 - p)}[-c - x_1 + k(b - c)]. \end{aligned} \quad (5.3.6)$$



Using (5.3.5) in (5.3.3), we get

$$\begin{aligned}
(\rho_1 + 1)(x_1 - c) &= c + (p + 1)a - sc + \frac{(\rho_1 + 2)(x_1 - a)}{2} \\
\Rightarrow (\rho_1 + 1)(x_1 - c) &= \frac{1}{2}[2c + 2(p + 1)a - 2sc + (\rho_1 + 2)(x_1 - a)] \\
\Rightarrow (\rho_1 + 1)(x_1 - c) &\geq \frac{1}{2}[2c + 2(p + 1)a - 2sc + 2s(x_1 - a)] \text{ [since } \rho_1 \geq 3s\text{]} \\
\Rightarrow (\rho_1 + 1 - s)(x_1 - c) &\geq \frac{1}{2}[2c + 2(p + 1 - s)a] > 0 \\
&\Rightarrow x_1 > c.
\end{aligned}$$

$$\begin{aligned}
\text{Again, } x_1 + cs - pa + b(q - 1) &\geq x_1 + cs - pa + b(p - s) \\
&= x_1 + (p - k)c - pa + kb \\
&= x_1 + p(c - a) + k(b - c) \\
&\geq x_1 + \frac{p}{\rho_1 + 1 - p}[-c - x_1 + k(b - c)] + \frac{2kx_1}{\rho_1 + 2} \\
&\quad \text{[by (5.3.2) and (5.3.6)]} \\
&= \frac{\rho_1 + 2 + 2k}{\rho_1 + 2}x_1 + \frac{p}{\rho_1 + 1 - p}[-c - x_1 + \frac{2kx_1}{\rho_1 + 2}] \\
&= \frac{(\rho_1 + 1)2kx_1 + (\rho_1 + 2)[(\rho_1 + 1 - 2p)x_1 - pc]}{(\rho_1 + 1 - p)(\rho_1 + 2)} \\
&> \frac{(\rho_1 + 1)2kx_1 + (\rho_1 + 2)p(x_1 - c)}{(\rho_1 + 1 - p)(\rho_1 + 2)} \text{ [since } \rho_1 + 1 - 2p > p\text{]} \\
&> 0.
\end{aligned}$$

Thus by (5.3.1),  $\rho > \rho_1$ . ■

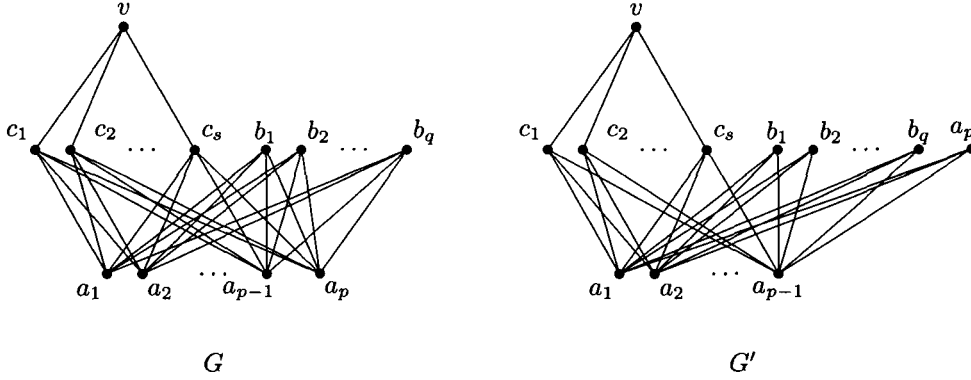
By the above lemma we have the following corollary.

**Corollary 5.3.2.** *If  $q \geq 1$ , then  $\rho(O_s \vee_2 (K_1 \cup K_{p,q})) \geq \rho(O_s \vee_1 (K_1 \cup K_{p,q}))$ ; equality holds only when  $p = q$ .*

**Lemma 5.3.3.** *If  $s + q + 4 \leq p$ , then*

$$\rho(O_s \vee_1 (K_1 \cup K_{p,q})) > \rho(O_s \vee_1 (K_1 \cup K_{p-1,q+1})).$$

**Proof.** Let  $p = s + q + k$ ,  $k \geq 4$ . Let us denote  $O_s \vee_1 (K_1 \cup K_{p,q})$  by  $G$  and  $O_s \vee_1 (K_1 \cup K_{p-1,q+1})$  by  $G'$ . We partition  $V(G) = V(G')$  into  $\{v\} \cup C \cup A \cup B \cup \{a_p\}$ , where  $C = \{c_1, c_2, \dots, c_s\}$ ,  $A = \{a_1, a_2, \dots, a_{p-1}\}$  and  $B = \{b_1, b_2, \dots, b_q\}$  as in Fig. 5.3.

Figure 5.3: The graphs  $G$  and  $G'$  in Lemma 5.3.3

As we pass from  $G$  to  $G'$ , the distance of  $a_p$  is increased by 1 with  $\{v\} \cup C \cup B$  and the distance of  $a_p$  is decreased by 1 with  $A$ ; the distances within any other pair of vertices remain unaltered. If the distance matrices are partitioned according to  $\{v\}$ ,  $C$ ,  $A$ ,  $B$ , and  $\{a_p\}$ , then their difference is

$$D(G) - D(G') = \begin{bmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -e_C \\ 0 & 0 & 0 & 0 & e_A \\ 0 & 0 & 0 & 0 & -e_B \\ -1 & -e_C^T & e_A^T & -e_B^T & 0 \end{bmatrix}$$

where  $e_i = \underbrace{(1, \dots, 1)}_{|i|}^T = \mathbb{1}_{|i|}$  and  $i = A, B, C$ . We denote  $\rho(G)$  by  $\rho$  and  $\rho(G')$  by  $\rho_1$ . Let  $X$  be the Perron vector of  $D(G')$ . Then by symmetry, components of  $X$  have the same value, say  $a$  for the vertices in  $A$ ,  $b$  for the vertices in  $B \cup \{a_p\}$ ,  $c$  for the vertices in  $C$ , and  $x_1$  for  $v$ . Then  $X$  can be written as,

$$X = \left( x_1, \underbrace{c, \dots, c}_s, \underbrace{a, \dots, a}_{p-1}, \underbrace{b, \dots, b}_{q+1} \right)^T.$$

We now have

$$\frac{1}{2}(\rho - \rho_1) \geq \frac{1}{2}X^T(D(G) - D(G'))X = b[-x_1 - sc - bq + a(p-1)]. \quad (5.3.7)$$

From eigenequations we have

$$\begin{aligned} (\rho_1 + 2)(x_1 - a) &= 2(q+1)b > 0, \\ (\rho_1 + 2)(b - c) &= 2x_1 > 0. \end{aligned}$$

Thus  $x_1 > a$  and  $b > c$ . We also have,

$$(\rho_1 + 2)(2a - b) = x_1 + 3(p - 1)a > 0 \Rightarrow 2a > b, \quad (5.3.8)$$

and

$$\begin{aligned} (\rho_1 + 4)(2a - x_1) &= sc + 2(p + 1)a - (q + 1)b > 0 \quad [\text{by (5.3.8)}] \\ &\Rightarrow 2a > x_1. \end{aligned} \quad (5.3.9)$$

Again,

$$(\rho_1 + 1)(a - b) = -x_1 - sc + (p - 1)a - a - qb. \quad (5.3.10)$$

If  $a \geq b$ , then from (5.3.10), we have  $-x_1 - sc + (p - 1)a - qb \geq a$ ; and by (5.3.7), we get  $\rho > \rho_1$ .

Let us assume that  $a < b$ . Since distance matrix is nonnegative and irreducible, its spectral radius is bounded below by the minimum row sum and thus we have

$$\rho_1 > p + 2q + 2s.$$

Therefore,

$$\begin{aligned} (q + 1)a - qb &= q(a - b) + a \\ \Rightarrow (\rho_1 + 1)[(q + 1)a - qb] &= [-qx_1 - sqc + (p - 2)qa - q^2b] + (\rho_1 + 1)a \\ &\quad [\text{by (5.3.10)}] \\ &> [-qx_1 - sqc + (p - 2)qa - q^2b] \\ &\quad + (p + 2q + 2s + 1)a \\ &= q(2a - x_1) + p(q + 1)a + 2(s - q)a + a \\ &\quad - qsc - q^2b \\ &> q(2a - x_1) + p(q + 1)a + 2(s - q)a + a \\ &\quad - qsb - q^2b \quad [\text{since } b > c] \\ &= q(2a - x_1) + p(q + 1)a + 2(s - q)a + a \\ &\quad - qb(s + q) \\ &= q(2a - x_1) + p(q + 1)a + 2(s - q)a + a \\ &\quad - qb(p - k) \\ \Rightarrow (\rho_1 + 1 - p)[(q + 1)a - qb] &> q(2a - x_1) + 2(s - q)a + a + qbk. \end{aligned} \quad (5.3.11)$$

If  $s \geq q$ , then by (5.3.9) and (5.3.11),  $(q + 1)a > qb$ .

Otherwise, let  $t = q - s$ . Then again by (5.3.11),

$$\begin{aligned}
(\rho_1 + 1 - p)[(q + 1)a - qb] &> q(2a - x_1) + a + (kqb - 2ta) \\
&> q(2a - x_1) + (4qb - 2ta) \\
&> q(2a - x_1) + (4tb - 2ta) \quad [\text{since } q > t] \\
&> 0 \quad [\text{since } 2a > x_1 \text{ and } b > a].
\end{aligned}$$

Thus we can conclude that  $(q + 1)a > qb$ .

Finally,

$$\begin{aligned}
(\rho_1 + 2)(a - c) &= x_1 - sc + (p - 1)a - (q + 1)b \\
&= (x_1 - a) - sc + (q + s + k)a - (q + 1)b \\
&= (x_1 - a) + s(a - c) + \{(q + 1)a - qb\} \\
&\quad + \{(k - 1)a - b\} \\
\Rightarrow (\rho_1 + 2 - s)(a - c) &= (x_1 - a) + \{(q + 1)a - qb\} + \{(k - 1)a - b\} \\
&\geq (x_1 - a) + \{(q + 1)a - qb\} + (3a - b) \\
&> 0 \quad [\text{since } x_1 > a, (q + 1)a > qb \text{ and } 2a > b] \\
&\Rightarrow a > c.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&-x_1 - sc - bq + a(p - 1) \\
&= -x_1 - sc - bq + a(q + s + k - 1) \\
&= \{(q + 1)a - qb\} + s(a - c) + \{(k - 2)a - x_1\} \\
&\geq \{(q + 1)a - qb\} + s(a - c) + (2a - x_1) \\
&> 0 \quad [\text{since } (q + 1)a > qb, a > c \text{ and } 2a > x_1].
\end{aligned}$$

Therefore from (5.3.7), we get  $\rho > \rho_1$ . ■

Similar to the above lemma we have the following lemma.

**Lemma 5.3.4.** *If  $n \geq 6$  and  $1 \leq s < \lfloor \frac{n-1}{2} \rfloor$ , then*

$$\rho(K_{s,n-s}) > \rho(O_s \vee_1 (K_1 \cup K_{n-s-2,1})).$$

**Lemma 5.3.5.** *If  $G \in \mathbf{B}_n^s$  and  $U$  is a vertex cut-set of order  $s$  in  $G$  such that  $G - U$  has two nontrivial components, then  $G$  cannot be a graph with minimal distance spectral radius in  $\mathbf{B}_n^s$ .*

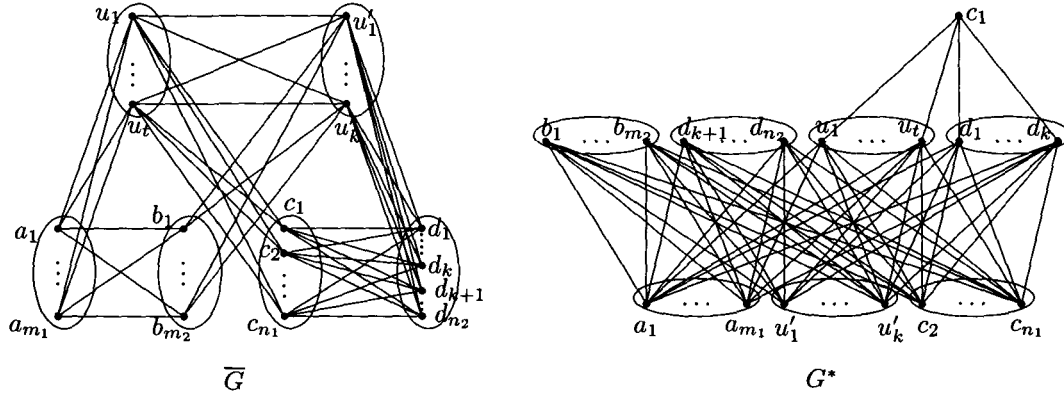


Figure 5.4: The graphs in Lemma 5.3.5

**Proof.** Let  $G_1$  and  $G_2$  be the nontrivial components of  $G - U$  with bipartitions  $(A, B)$  and  $(C, D)$  respectively. Let  $U = U_1 \cup U_2$  be the bipartition of  $U$  induced by the bipartition of  $G$ . Now joining all possible edges between the vertices of  $A$  and  $B$ ,  $C$  and  $D$ ,  $U_1$  and  $U_2$  we get a graph  $\bar{G}$  in  $\mathbf{B}_n^s$  such that  $\rho(G) \geq \rho(\bar{G})$ . Therefore we suppose that  $G = \bar{G}$ .

If there exists some vertex  $w$  in  $G - U$  such that  $d_G(w) = s$ , then forming a complete bipartite graph within the vertices of  $G - \{w\}$  we would get a graph in  $\mathbf{B}_n^s$  with smaller distance spectral radius. Thus we may assume that each vertex in  $G - U$  has degree greater than  $s$ .

$$\text{Let } |A| = m_1, |B| = m_2, |C| = n_1, |D| = n_2, |U_1| = t, |U_2| = k.$$

We choose a vertex  $c_1$  from  $C$  and observe that  $d_G(c_1) = t + |D| > s$ , where  $t(0 \leq t \leq s)$  is the total number of edges joining  $c_1$  and the vertices of  $U_1$ . Since  $U_1 \cup U_2$  is the vertex cut-set of order  $s$  so  $m_1, n_1 > t$ ,  $m_2, n_2 > k$ . Without loss of generality we may assume that  $m_1 = \max\{m_1, m_2, n_1, n_2\}$  and since  $s \geq 1$  so  $m_1 \geq 2$ . We now pick a subset  $D_2$  of  $D$  with  $|D_2| = |D| - k > 0$ . Deleting all the edges between  $c_1$  and the vertices of  $D_2$ , and then forming a complete bipartite graph within the vertices of  $G - \{c_1\}$  we get a new graph  $G^* \in \mathbf{B}_n^s$ .

We partition  $V(G) = V(G^*)$  into  $U_1 \cup U_2 \cup A \cup B \cup C' \cup D_1 \cup D_2 \cup \{c_1\}$ , where  $U_1 = \{u_1, u_2, \dots, u_t\}$ ,  $U_2 = \{u'_1, u'_2, \dots, u'_k\}$ ,  $A = \{a_1, a_2, \dots, a_{m_1}\}$ ,  $B = \{b_1, b_2, \dots, b_{m_2}\}$ ,  $C' = \{c_2, \dots, c_{n_1}\}$ ,  $D_1 = \{d_1, d_2, \dots, d_k\}$ , and  $D_2 = \{d_{k+1}, d_{k+2}, \dots, d_{n_2}\}$  as in Fig. 5.4.

If the distance matrices are partitioned according to  $U_1, U_2, A, B, C', D_1, D_2$  and

$\{c_1\}$ , then their difference is  $D(G) - D(G^*) =$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2J_{m_1 \times k} & 2J_{m_1 \times (n_2 - k)} & 0 \\ 0 & 0 & 0 & 0 & 2J_{m_2 \times (n_1 - 1)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2J_{(n_1 - 1) \times m_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 2J_{k \times m_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2J_{(n_2 - k) \times m_1} & 0 & 0 & 0 & 0 & -2e_{D_2} \\ 0 & 0 & 0 & 0 & 0 & 0 & -2e_{D_2}^T & 0 \end{bmatrix}$$

where  $e_{D_2} = \underbrace{(1, \dots, 1)^T}_{|D_2|} = \mathbb{1}_{|D_2|}$ . We denote  $\rho(G)$  by  $\rho$  and  $\rho(G^*)$  by  $\rho_1$ . Let  $X$  be the Perron vector of  $D(G^*)$ . Then by symmetry, components of  $X$  have the same value, say  $u$  for the vertices in  $U_1 \cup D_1$ ,  $b$  for the vertices in  $B \cup D_2$ ,  $a$  for the vertices in  $A \cup U_2 \cup C'$ , and  $c$  for  $c_1$ . Then  $X$  can be written as,

$$X = \left( \underbrace{u, \dots, u}_t, \underbrace{a, \dots, a}_k, \underbrace{a, \dots, a}_{m_1}, \underbrace{b, \dots, b}_{m_2}, \underbrace{a, \dots, a}_{n_1 - 1}, \underbrace{u, \dots, u}_k, \underbrace{b, \dots, b}_{n_2 - k}, c \right)^T.$$

We now have

$$\frac{1}{2}(\rho - \rho_1) \geq \frac{1}{2}X^T(D(G) - D(G^*))X = 2km_1au + 2abm_2(n_1 - 1) + 2(n_2 - k)b(m_1a - c). \quad (5.3.12)$$

From eigenequations we have

$$(\rho_1 + 6)(3a - c) = 2su + 4(m_1 + n_1 + k + 2)a > 0 \Rightarrow 3a > c, \quad (5.3.13)$$

$$(\rho_1 + 2)(2a - b) = c + 3(m_1 + n_1 + k - 1)a > 0 \Rightarrow 2a > b. \quad (5.3.14)$$

From (5.3.13) and (5.3.12), we have  $\rho > \rho_1$  if  $m_1 \geq 3$ .

Again if  $m_1 = 2$ , then

$$\begin{aligned} (\rho_1 + 4)(2a - c) &= su + 2(m_1 + n_1 + k + 1)a - (m_2 + n_2 - k)b \\ &\geq su + 8a - 4b \\ &> 0 \quad [\text{by (5.3.14)}]. \end{aligned}$$

Thus  $2a > c$  and therefore by (5.3.12), we have  $\rho > \rho_1$ . ■

Let  $G_1^*, G_2^*, G_3^*$ , and  $G_4^*$  be the graphs described in Fig. 5.5. The following is the main result in this section.

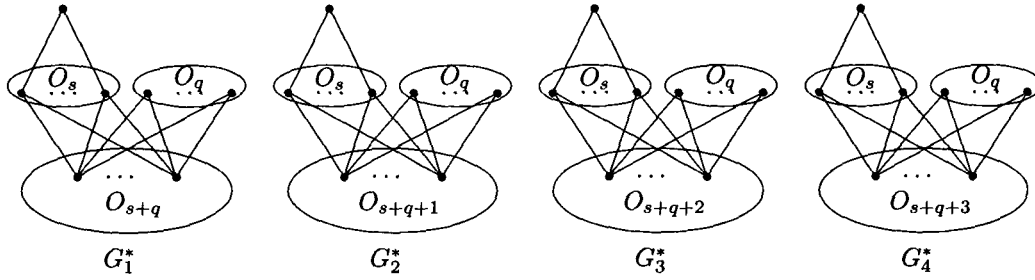


Figure 5.5: The graphs in Theorem 5.3.6

**Theorem 5.3.6.** *Let  $G$  be a graph in  $\mathbf{B}_n^s$  with minimal distance spectral radius, where  $1 \leq s \leq \lfloor \frac{n-1}{2} \rfloor$ . Then  $G \in \{G_1^*, G_3^*\}$ , if  $n$  is odd and  $G \in \{G_2^*, G_4^*\}$ , if  $n$  is even.*

**Proof.** Let  $G$  be a graph with minimal distance spectral radius in  $\mathbf{B}_n^s$ . Let  $U$  be a vertex cut-set of  $G$  containing  $s$  vertices, whose deletion yields the components  $G_1, G_2, \dots, G_t$  of  $G - U$ , where  $t \geq 2$ . If some component  $G_i$  of  $G - U$  has at least two vertices, then it must be complete bipartite. Again if some component  $G_i$  of  $G - U$  is a singleton, say  $G_i = \{u\}$ , then  $u$  is adjacent to all the vertices of  $U$  otherwise  $\kappa(G) < s$ ; hence the subgraph  $G[U]$  induced by  $U$  contains no edges, and belongs to the same partition of  $G$ . We now have the following cases.

**Case 1:** All the components of  $G - U$  are singletons. Then  $G = K_{s, n-s}$ . For  $s = \lfloor \frac{n-1}{2} \rfloor$  we have  $K_{s, n-s} \cong G_1^*$ , if  $n$  is odd and  $K_{s, n-s} \cong G_2^*$ , if  $n$  is even; and thus the result.

Let us assume that  $1 \leq s < \lfloor \frac{n-1}{2} \rfloor$ . Then by Lemma 5.3.4,  $\rho(K_{s, n-s}) > \rho(O_s \vee_1 (K_1 \cup K_{n-s-2, 1}))$ , which contradicts the minimality of  $G$ . Therefore not all the components of  $G - U$  can be singletons.

**Case 2:** One component of  $G - U$ , say  $G_1$ , contains at least two vertices. Then  $G - U$  contains exactly two components; otherwise, forming a complete bipartite graph within the vertices of  $G_1 \cup G_2 \cup \dots \cup G_{t-1}$  we obtain a new graph  $\hat{G}$  from  $G$  with smaller distance spectral radius such that  $\hat{G} \in \mathbf{B}_n^s$ , a contradiction. Let  $G_1, G_2$  be the components of  $G - U$ . By Lemma 5.3.5, either  $G_1 = K_1$  or  $G_2 = K_1$ . Without loss of generality assume that  $G_2 = K_1 = \{u\}$ . Then  $u$  joins all vertices of  $U$ , and each vertex of  $U$  joins every vertex of  $G_1$  which are in the same partition as  $u$ . Since  $G$  is a graph with minimal distance spectral radius then by Corollary 5.3.2,  $G = O_s \vee_1 (K_1 \cup K_{p, q})$  for some  $p$  and  $q$ . We note that  $p \geq s$ , otherwise  $s$  cannot be the vertex connectivity of  $G$ . If  $q + s \leq p \leq q + s + 3$ , then the result follows. Again if  $q + s > p$ , then by

repeated application of Lemma 5.3.1,  $G = G_1^*$ , if  $n$  is odd and  $G = G_2^*$ , if  $n$  is even. Finally if  $p \geq q + s + 4$ , then by using Lemma 5.3.3 repeatedly, we have  $G$  is either  $G_3^*$  or  $G_4^*$  according as  $n$  is odd or even. ■



# Chapter 6

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## On the distance Laplacian eigenvalues of graphs

### 6.1 Introduction

The second smallest Laplacian eigenvalue (known as the *algebraic connectivity* of a graph) is studied extensively in literature (see [24, 38–40, 47] and the references therein). Aouchiche and Hansen have introduced the distance Laplacian matrix and proved that for a connected graph  $G$  of order  $n$ , the second smallest distance Laplacian eigenvalue is at least  $n$ , where the equality holds if and only if  $\overline{G}$  is disconnected [2]. In that case, the multiplicity of  $n$  as a distance Laplacian eigenvalue of  $G$  is one less than the number of components of  $\overline{G}$ . In Section 6.3, we study the second smallest distance Laplacian eigenvalue for some class of graphs whose complement is connected (precisely a tree or a unicyclic graph, respectively). In Section 6.4, we study the distance Laplacian spectrum of path and prove that the largest distance Laplacian eigenvalue (called the *distance Laplacian spectral radius*) is simple. We also describe the structure of the corresponding eigenvector.

### 6.2 Preliminary Lemmas

Here we mention some preliminary lemmas which will be useful to obtain our main results of this chapter. Let  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} \geq \mu_n = 0$  (resp.  $\delta_1 \geq \delta_2 \geq \dots \geq \delta_{n-1} > \delta_n = 0$ ) denote the Laplacian (resp. distance Laplacian) eigenvalues of a graph.

**Lemma 6.2.1.** [38] *Let  $G$  be a connected graph with a cut vertex  $v$ . Then*

$$\mu_{n-1}(G) \leq 1;$$

*equality holds if and only if  $v$  is adjacent to every vertex of  $G$ .*

It is known that ([31, Corollary 4.2]) if  $G$  is a graph and a new pendent vertex is added at some vertex of  $G$  to obtain  $H$ , then

$$\mu_i(H) \leq \mu_i(G), \quad (6.2.1)$$

where  $\mu_i(H), \mu_i(G)$  are the  $i$ -th smallest Laplacian eigenvalues of  $H$  and  $G$ , respectively.

Let  $K_n^k$  be the graph obtained by joining  $k$  isolated vertices to a single vertex of  $K_{n-k}$  and  $\mathcal{U}_n$  be the class of all unicyclic graphs of order  $n$ , where  $n \geq 3$ .

**Lemma 6.2.2.** [40] *The maximum algebraic connectivity over  $\mathcal{U}_n$  is uniquely attained by  $C_n$  if  $n \leq 5$  and uniquely attained by  $K_n^{n-3}$  if  $n > 6$ . When  $n = 6$ ,  $C_6$  and  $K_6^3$  are the only two graphs, up to isomorphism, having the maximum algebraic connectivity over  $\mathcal{U}_6$ .*

The following result gives a relation between the Laplacian eigenvalues and the distance Laplacian eigenvalues, for graphs of diameter at most 2.

**Lemma 6.2.3.** [2] *Let  $G$  be a connected graph on  $n$  vertices with diameter  $d(G) \leq 2$ . Let  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$  be the Laplacian eigenvalues of  $G$ . Then the distance Laplacian eigenvalues of  $G$  are  $2n - \mu_{n-1} \geq 2n - \mu_{n-2} \geq \dots \geq 2n - \mu_1 > \delta_n = 0$ . Moreover, for every  $i = 1, 2, \dots, n-1$ , the eigenspaces corresponding to  $\mu_i$  and to  $2n - \mu_i$  are the same.*

Two vertices are *co-neighbours* if they share the same neighbours. Clearly, if  $S$  is a set of pairwise co-neighbour vertices of a graph  $G$ , then  $S$  is an independent set. A *cluster of order  $k$*  of  $G$  is a set  $S$  of  $k$  pairwise co-neighbour vertices [47]. Clearly, each vertex of a cluster have the same transmission, which we call the *transmission of a cluster*. Following is an important observation for graphs with a cluster.

**Lemma 6.2.4.** *Let  $G$  be a graph with a cluster  $S$  of order  $k$  and transmission  $t$ , where  $k > 1$ . Then  $t + 2$  is a distance Laplacian eigenvalue of  $G$  with multiplicity at least  $k - 1$ .*

**Proof.** Let  $S = \{v_1, v_2, \dots, v_k\}$  be the cluster. Assuming  $N_G(v_1) = \{v_{k+1}, v_{k+2}, \dots, v_{k+l}\}$ , we have

$$D^L(G) = \left[ \begin{array}{ccc|cc} lI_k + 2L(K_k) + (t - l - 2k + 2)I_k & -\mathbb{1}_k \mathbb{1}_l^T & -P & & \\ & -\mathbb{1}_l \mathbb{1}_k^T & & * & \\ & -P^T & & & \end{array} \right],$$

where  $P$  is a  $k \times (n-k-l)$  matrix with all identical rows. It can be verified that the first  $k$  rows of the matrix  $D^L(G) - (t+2)I$  are equal. Therefore,  $\text{rank}(D^L(G) - (t+2)I) \leq n - (k-1)$ , i.e., the null space of  $D^L(G) - (t+2)I$  has dimension not less than  $k-1$ . Hence,  $t+2$  is an eigenvalue of  $D^L(G)$  with multiplicity at least  $k-1$ . ■

Suppose  $i$  and  $j$  are fixed but arbitrary nonadjacent vertices of a graph  $G$ . Let  $G+e$  be the graph obtained from  $G$  by joining the edge  $e = ij$ . Then with a suitable ordering, we have  $L(G+e) = L(G) + S$ , where

$$S = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \oplus 0_{n-2}.$$

The situation when the Laplacian spectra of  $G$  and  $G+e$  differ just at one place with one eigenvalue of  $G$  increasing by 2 while the others remaining the same, is called *spectral integral variation occurring at one place* [10, 25]. So [56] has proved that the spectral integral variation at one place occurs from  $G$  to  $G+e$  if and only if  $i$  and  $j$  are co-neighbours. Fan [25] has given some equivalent conditions for the occurrence of spectral integral variation at one place. Note that if  $i$  and  $j$  are two nonadjacent co-neighbour vertices of  $G$ , then  $D^L(G) = D^L(G+e) + S$ . Therefore, we can obtain similar results given in [25], when the distance Laplacian spectra of  $G$  and  $G+e$  differ just at one place with one eigenvalue of  $G$  decreasing by 2 while the others remaining the same. Among those results, the following will be important for us. We omit the proof, as it is similar to the proof given in [25].

**Lemma 6.2.5.** *Let  $i$  and  $j$  be two nonadjacent co-neighbour vertices of  $G$ , and  $G+e$  be the graph obtained from  $G$  by adding the edge  $e = ij$ . If the distance Laplacian spectra of  $G$  and  $G+e$  differ just at one place with one eigenvalue of  $G$  decreasing by 2 while the others remaining the same, then the changed eigenvalue is  $\text{Tr}(i) + 2$ .*

Note that in the above lemma, the fact that  $\text{Tr}(i) + 2$  is a distance Laplacian eigenvalue of  $G$ , is assured by Lemma 6.2.4.

### 6.3 Second smallest distance Laplacian eigenvalue

Here we study the second smallest distance Laplacian eigenvalue  $\delta_{n-1}$ . The following lemma, which gives a lower bound for  $\delta_{n-1}$  can be found in [2].

**Lemma 6.3.1.** [2] *Let  $G$  be a connected graph on  $n$  vertices. Then  $\delta_{n-1}(G) \geq n$  with equality holding if and only if  $\overline{G}$  is disconnected. Furthermore, the multiplicity of  $n$  as an eigenvalue of  $D^L(G)$  is one less than the number of components of  $\overline{G}$ .*

Thus, if  $\overline{G}$  is connected, then  $\delta_{n-1}(G) > n$ . In the following two subsections, we consider the graphs whose complement is connected (precisely a tree or a unicyclic graph, respectively) and characterize the graphs among them having  $n + 1$  as the second smallest distance Laplacian eigenvalue.

### 6.3.1 Second smallest distance Laplacian eigenvalue of a graph whose complement is a tree

For positive integers  $k, l$ , the following lemma determines the distance Laplacian eigenvalues of a graph whose complement is the dumbbell  $D(n, k, l)$ , where  $k + l = n - 2$ .

**Lemma 6.3.2.** *Let  $G$  be a graph of order  $n$  such that  $\overline{G} = D(n, k, l)$ , where  $k + l = n - 2$ . Then the distance Laplacian spectrum of  $G$  consists of the eigenvalues*

- (a) 0 with multiplicity 1;
- (b)  $n + 1$  with multiplicity  $n - 4$ ;
- (c)  $n + t_i$  with multiplicity 1, where  $t_i$  is a root of the equation

$$x^3 - (n + 4)x^2 + (3n + kl + 3)x - 2n = 0,$$

for each  $i = 1, 2, 3$ .

**Proof.** Let us label the vertices of  $D(n, k, l)$  as  $v_1, v_2, \dots, v_n$  such that  $v_1, v_2, \dots, v_k$  are the pendent vertices at  $v_n$  and  $v_{k+1}, v_{k+2}, \dots, v_{k+l}$  are the pendent vertices at  $v_{n-1}$ . Then, we have

$$\begin{aligned} D^L(G) &= \begin{bmatrix} (n+1)I_{n-2} - J_{n-2} & \begin{bmatrix} -\mathbf{1}_k & -2\mathbf{1}_k \\ -2\mathbf{1}_l & -\mathbf{1}_l \end{bmatrix} \\ \begin{bmatrix} -\mathbf{1}_k^T & -2\mathbf{1}_l^T \\ -2\mathbf{1}_k^T & -\mathbf{1}_l^T \end{bmatrix} & \begin{bmatrix} k+2l+3 & -3 \\ -3 & l+2k+3 \end{bmatrix} \end{bmatrix} \\ &= L(G) + 2L(\overline{G}) + \begin{bmatrix} \mathbf{0}_{n-2 \times n-2} & \mathbf{0}_{n-2 \times 2} \\ \mathbf{0}_{2 \times n-2} & \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \end{bmatrix} \end{aligned}$$

$$\begin{aligned}
\Rightarrow D^L(G) &= nI_n - J_n + \left[ \begin{array}{c|c} I_{n-2} & \begin{bmatrix} \mathbf{0}_k & -\mathbf{1}_k \\ -\mathbf{1}_l & \mathbf{0}_l \end{bmatrix} \\ \hline \begin{bmatrix} \mathbf{0}_k^T & -\mathbf{1}_l^T \\ -\mathbf{1}_k^T & \mathbf{0}_l^T \end{bmatrix} & \begin{bmatrix} l+2 & -2 \\ -2 & k+2 \end{bmatrix} \end{array} \right] \\
&= nI_n - J_n + P, \tag{6.3.1} \\
\text{where } P &= \left[ \begin{array}{c|c} I_{n-2} & \begin{bmatrix} \mathbf{0}_k & -\mathbf{1}_k \\ -\mathbf{1}_l & \mathbf{0}_l \end{bmatrix} \\ \hline \begin{bmatrix} \mathbf{0}_k^T & -\mathbf{1}_l^T \\ -\mathbf{1}_k^T & \mathbf{0}_l^T \end{bmatrix} & \begin{bmatrix} l+2 & -2 \\ -2 & k+2 \end{bmatrix} \end{array} \right]
\end{aligned}$$

The characteristic polynomial of  $P$  is given by

$$\begin{aligned}
\phi(P; x) &= \det \left[ \begin{array}{c|c} (x-1)I_{n-2} & \begin{bmatrix} \mathbf{0}_k & \mathbf{1}_k \\ \mathbf{1}_l & \mathbf{0}_l \end{bmatrix} \\ \hline \begin{bmatrix} \mathbf{0}_k^T & \mathbf{1}_l^T \\ \mathbf{1}_k^T & \mathbf{0}_l^T \end{bmatrix} & \begin{bmatrix} x-l-2 & 2 \\ 2 & x-k-2 \end{bmatrix} \end{array} \right] \\
&= (x-1)^{n-2} \cdot \det(S_1), \tag{6.3.2}
\end{aligned}$$

$$\begin{aligned}
\text{where } S_1 &= \begin{bmatrix} x-l-2 & 2 \\ 2 & x-k-2 \end{bmatrix} - \begin{bmatrix} \mathbf{1}_l^T \frac{1}{x-1} I_l \mathbf{1}_l & 0 \\ 0 & \mathbf{1}_k^T \frac{1}{x-1} I_k \mathbf{1}_k \end{bmatrix} \\
&= \begin{bmatrix} x-l-2 - \frac{l}{x-1} & 2 \\ 2 & x-k-2 - \frac{k}{x-1} \end{bmatrix} \tag{6.3.3}
\end{aligned}$$

is the Schur complement of  $(x-1)I_{n-2}$ . Using (6.3.3) in (6.3.2) we have

$$\phi(P; x) = x(x-1)^{n-4} \left( x^3 - (n+4)x^2 + (3n+kl+3)x - 2n \right) \tag{6.3.4}$$

It is known that the spectrum of  $nI_n - J_n$  consists of eigenvalue  $n$  with multiplicity  $n-1$  and  $0$  with multiplicity  $1$ . Clearly,  $\mathbf{1}_n$  is an eigenvector of both  $nI_n - J_n$  and  $P$  corresponding to eigenvalue  $0$ . Thus,  $0$  is an eigenvalue of  $D^L(G)$  with eigenvector  $\mathbf{1}_n$ .

Since 0 is a simple eigenvalue of  $D^L(G)$  and  $P$  is a positive semidefinite matrix that commutes with  $nI_n - J_n$ , so from (6.3.4) and (6.3.1) we have the result. ■

Following is the main result of this section.

**Theorem 6.3.3.** *There exist no graph  $G$  such that  $\overline{G}$  is a tree and  $\delta_{n-1}(G) = n + 1$ .*

**Proof.** If  $\overline{G}$  is a tree such that  $G$  is connected, then  $d(\overline{G}) \geq 3$ . If  $d(\overline{G}) \geq 4$ , then  $d(G) \leq 2$ . Thus, by Lemmas 6.2.1 and 6.2.3,  $\delta_{n-1}(G) = 2n - \mu_1(G) = n + \mu_{n-1}(\overline{G}) < n + 1$ . If  $d(\overline{G}) = 3$ , then  $\overline{G} \cong D(n, k, l)$ , where  $k + l = n - 2$  and  $k, l \geq 1$ . Let  $f(x) = x^3 - (n + 4)x^2 + (3n + kl + 3)x - 2n$ . Since  $f(0) < 0$  and  $f(1) > 0$ , so there is a root  $t$  of  $f(x) = 0$  in  $(0, 1)$ . Therefore, by Lemma 6.3.2,  $\delta_{n-1}(G) = n + t < n + 1$ . This completes the proof. ■

From the proof of the above theorem, we have the following.

**Corollary 6.3.4.** *If  $G$  is a graph such that  $\overline{G}$  is a tree, then  $n < \delta_{n-1}(G) < n + 1$ .*

### 6.3.2 Second smallest distance Laplacian eigenvalue of a graph whose complement is a unicyclic graph

Let  $C_g(k, l)$  be the graph obtained by joining  $k, l$  isolated vertices to two adjacent vertices of a cycle  $C_g$ , where  $k, l \geq 0$ . Then, similar to Lemma 6.3.2 we have the following three lemmas.

**Lemma 6.3.5.** *Let  $G$  be a graph of order  $n$  such that  $\overline{G} = C_3(k, l)$ , where  $k, l \geq 1$ . Then the distance Laplacian spectrum of  $G$  consists of the eigenvalues*

- (a) 0 with multiplicity 1;
- (b)  $n + 1$  with multiplicity  $n - 5$ ;
- (c)  $n + t_i$  with multiplicity 1, where  $t_i$  is a root of the equation

$$x^4 - (n + 7)x^3 + (6n + kl + 14)x^2 - 2(5n + kl + 4)x + 5n = 0,$$

for each  $i = 1, 2, 3, 4$ .

**Lemma 6.3.6.** *Let  $G$  be a graph of order  $n$  such that  $\overline{G} = C_4(k, l)$ , where  $k, l \geq 1$ . Then the distance Laplacian spectrum of  $G$  consists of the eigenvalues*

- (a) 0 with multiplicity 1;

- (b)  $n + 1$  with multiplicity  $n - 5$ ;  
(c)  $n + t_i$  with multiplicity 1, where  $t_i$  is a root of the equation

$$x^4 - (n + 7)x^3 + (7n + kl + 12)x^2 - (14n + 3kl + 2)x + 7n = 0,$$

for each  $i = 1, 2, 3, 4$ .

**Lemma 6.3.7.** *Let  $G$  be a graph of order  $n$  such that  $\overline{G} = C_4(k, 0)$ , where  $k \geq 1$ . Then the distance Laplacian spectrum of  $G$  consists of the eigenvalues*

- (a)  $0, n + 3$  with multiplicity 1;  
(b)  $n + 1$  with multiplicity  $n - 4$ ;  
(c)  $n + \frac{n+5 \pm \sqrt{n^2 - 6n + 25}}{2}$  with multiplicity 1.

We now discuss the case, when  $\delta_{n-1}(G) = n + 1$  and  $\overline{G}$  is a unicyclic graph.

**Lemma 6.3.8.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph of girth 3. Then  $\delta_{n-1}(G) < n + 1$ .*

**Proof.** Since  $G$  is connected and  $\overline{G}$  is of girth 3, so  $d(\overline{G}) \geq 3$ . If  $d(\overline{G}) = 3$ , then we have the following three cases:

**Case 1:**  $\overline{G}$  is obtained by joining two co-neighbour pendent vertices of  $D(n, k, l)$ , where  $k + l = n - 2$  and  $k, l \geq 1$ . Then by Lemmas 6.2.5 and 6.3.2, the distance Laplacian spectrum of  $G$  consists of the eigenvalues

- (a)  $0, n + 3$  with multiplicity 1;  
(b)  $n + 1$  with multiplicity  $n - 5$ ;  
(c)  $n + t_i$  with multiplicity 1, where  $t_i$  is a root of the equation

$$x^3 - (n + 4)x^2 + (3n + kl + 3)x - 2n = 0,$$

for each  $i = 1, 2, 3$ .

Since at least one  $t_i \in (0, 1)$ , so  $\delta_{n-1}(G) < n + 1$ .

**Case 2:**  $\overline{G} \cong C_3(k, l)$ , where  $k, l \geq 1$ . Then by Lemma 6.3.5, we have  $\delta_{n-1}(G) < n + 1$ , since a root of the equation  $x^4 - (n + 7)x^3 + (6n + kl + 14)x^2 - 2(5n + kl + 4)x + 5n = 0$  lies in  $(0, 1)$ .

**Case 3:**  $\overline{G} \cong C_3(k, l, m)$ , where  $C_3(k, l, m)$  is the graph obtained by joining  $k, l, m$  isolated vertices, respectively to each vertex of  $C_3$ , where  $k, l, m \geq 1$ . Then  $\overline{G}$  contains a cut vertex, and hence by Lemma 6.2.1,  $\mu_{n-1}(\overline{G}) < 1$ . Since  $d(G) = 2$ , by Lemma 6.2.3 we have,  $\delta_{n-1}(G) < n + 1$ .

Thus, if  $d(\overline{G}) = 3$ , then  $\delta_{n-1}(G) < n + 1$ .

Now, let us consider  $d(\overline{G}) \geq 4$ . Since  $\overline{G}$  have a cut vertex, by Lemma 6.2.1,  $\mu_{n-1}(\overline{G}) < 1$ . Thus, by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ , since  $d(G) = 2$ . ■

**Lemma 6.3.9.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph of girth 4. Then  $\delta_{n-1}(G) = n + 1$  if and only if  $\overline{G} \cong C_4(k, 0)$ , where  $k \geq 1$ .*

**Proof.** Since  $G$  is connected and  $\overline{G}$  is of girth 4, so  $d(\overline{G}) \geq 3$ . If  $d(\overline{G}) = 3$ , then either  $\overline{G} \cong C_4(k, 0)$ , where  $k \geq 1$  or  $\overline{G} \cong C_4(k, l)$ , where  $k, l \geq 1$ . In the first case by Lemma 6.3.7,  $\delta_{n-1}(G) = n + 1$ , since  $\frac{n+5 \pm \sqrt{n^2-6n+25}}{2} > 1$ .

In the second case by Lemma 6.3.6, we have  $\delta_{n-1}(G) < n + 1$ , since a root of the equation  $x^4 - (n + 7)x^3 + (7n + kl + 12)x^2 - (14n + 3kl + 2)x + 7n = 0$  lies in  $(0, 1)$ .

By Lemma 6.2.1, we have  $\mu_{n-1}(C_4(1, 0)) < 1$ . Since any other unicyclic graph  $\overline{G}$  contains  $C_4(1, 0)$  as an induced subgraph, so by (6.2.1),  $\mu_{n-1}(\overline{G}) < 1$ . Therefore if  $d(\overline{G}) \geq 4$ , then by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ , since  $d(G) = 2$ . ■

**Lemma 6.3.10.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph of girth 5. Then  $\delta_{n-1}(G) \neq n + 1$ .*

**Proof.** If  $\overline{G} \cong C_5$ , then  $d(\overline{G}) = d(G) = 2$ . Since  $\mu_{n-1}(C_5) \neq 1$ , so by Lemma 6.2.3,  $\delta_{n-1}(G) \neq n + 1$ .

By Lemma 6.2.1, we have  $\mu_{n-1}(C_5(1, 0)) < 1$ . Since any other unicyclic graph  $\overline{G}$  contains  $C_5(1, 0)$  as an induced subgraph, so by (6.2.1),  $\mu_{n-1}(\overline{G}) < 1$ . Therefore if  $d(\overline{G}) \geq 3$ , then by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ , since  $d(G) = 2$ . ■

**Lemma 6.3.11.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph of girth 6. Then  $\delta_{n-1}(G) = n + 1$  if and only if  $\overline{G} \cong C_6$ .*

**Proof.** If  $\overline{G} \cong C_6$ , then  $d(G) = 2$ . Since  $\mu_{n-1}(C_6) = 1$ , so by Lemma 6.2.3,  $\delta_{n-1}(G) = n + 1$ .

Suppose  $\overline{G} \not\cong C_6$ , then  $d(\overline{G}) \geq 4$  and  $\overline{G}$  contains a cut vertex. Hence by Lemma 6.2.1,  $\mu_{n-1}(\overline{G}) < 1$ . Thus by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ , since  $d(G) = 2$ . ■

**Lemma 6.3.12.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph of girth at least 7. Then  $\delta_{n-1}(G) < n + 1$ .*



**Proof.** If  $\overline{G} \cong C_n$ , then  $d(G) = 2$ . Since  $n \geq 7$ , by Lemma 6.2.2 we have,  $\mu_{n-1}(C_n) < 1$ . Hence by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ .

Suppose  $\overline{G} \not\cong C_n$ , then  $\overline{G}$  contains a cut vertex, and hence by Lemma 6.2.1,  $\mu_{n-1}(\overline{G}) < 1$ . Thus by Lemma 6.2.3,  $\delta_{n-1}(G) < n + 1$ , since  $d(G) = 2$ . ■

We summarize our discussions to state the main result of this subsection.

**Theorem 6.3.13.** *Let  $G$  be a graph such that  $\overline{G}$  is a unicyclic graph. Then  $\delta_{n-1}(G) = n + 1$  if and only if  $\overline{G} \cong C_6$  or  $\overline{G} \cong C_4(k, 0)$ , where  $k \geq 1$ .*

## 6.4 Distance Laplacian spectrum of path

In this section, we study the distance Laplacian spectrum of a path, specially the distance Laplacian spectral radius  $\delta_1$  and the corresponding eigenvectors. The following lemma will be useful in doing so.

**Lemma 6.4.1.** *Let  $P = \begin{bmatrix} A & B \\ B & A \end{bmatrix}$  be a partitioned matrix. Then  $\lambda$  is an eigenvalue of  $P$  if and only if  $\lambda$  is an eigenvalue of  $A + B$  or  $A - B$ .*

**Proof.** If  $\lambda$  is an eigenvalue of  $A + B$  (resp.  $A - B$ ) with corresponding eigenvector  $X$ , then it can be seen that  $\lambda$  is an eigenvalue of  $P$  with  $\begin{bmatrix} X \\ X \end{bmatrix}$  (resp.  $\begin{bmatrix} X \\ -X \end{bmatrix}$ ) as the corresponding eigenvector.

Conversely, let  $\lambda$  be an eigenvalue of  $P$  with  $\begin{bmatrix} X \\ Y \end{bmatrix}$  as the corresponding eigenvector. Then from eigenequation, we have  $(A - B)(X - Y) = \lambda(X - Y)$ . Therefore, if  $X \neq Y$ , then  $\lambda$  is an eigenvalue of  $A - B$ . And if  $X = Y$ , then  $(A + B)X = \lambda X$ , i.e.,  $\lambda$  is an eigenvalue of  $A + B$ . ■

Let the vertices of the path  $P_{2k}$  be labelled as in Fig. 6.1.

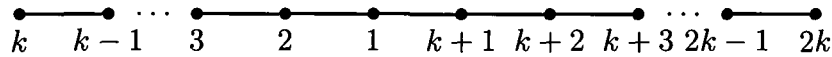


Figure 6.1: The path  $P_{2k}$ .

Then, for  $i = 1, 2, \dots, k$ , we have

$$Tr(i) = Tr(k + i) = k^2 + i^2 - i. \quad (6.4.1)$$

Therefore,

$$D^L(P_{2k}) = \left[ \begin{array}{c|c} A & B \\ \hline B & A \end{array} \right],$$

$$\text{where } A = \begin{bmatrix} Tr(1) & -1 & -2 & \cdots & -(k-1) \\ -1 & Tr(2) & -1 & \cdots & -(k-2) \\ -2 & -1 & Tr(3) & \cdots & -(k-3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -(k-1) & -(k-2) & -(k-3) & \cdots & Tr(k) \end{bmatrix} \quad (6.4.2)$$

$$\text{and } B = \begin{bmatrix} -1 & -2 & -3 & \cdots & -k \\ -2 & -3 & -4 & \cdots & -(k+1) \\ -3 & -4 & -5 & \cdots & -(k+2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -k & -(k+1) & -(k+2) & \cdots & -(2k-1) \end{bmatrix}. \quad (6.4.3)$$

Thus by Lemma 6.4.1, the eigenvalues of  $D^L(P_{2k})$  are those of  $A + B$  and  $A - B$ . But in this case we can say even more, as given in the following lemma.

**Lemma 6.4.2.** *If  $A$  and  $B$  are the matrices given by (6.4.2) and (6.4.3), respectively, then the spectrum of  $A + B = \{0, Tr(2), Tr(3), \dots, Tr(k)\}$ .*

**Proof.** Using (6.4.1), we have  $(A + B)\mathbb{1}_k = \mathbf{0}_k$ . Also by (6.4.1), it can be verified that  $X_i = \begin{bmatrix} -\mathbb{1}_{i-1} \\ i-1 \\ \mathbf{0}_{k-i} \end{bmatrix}$  is an eigenvector of  $(A + B)$  corresponding to  $Tr(i)$ , where  $i = 2, 3, \dots, k$ . Since order of  $A + B$  is  $k$  so the result follows.  $\blacksquare$

Thus from Lemmas 6.4.1 and 6.4.2, we have the following theorem.

**Theorem 6.4.3.** *If  $A$  and  $B$  are the matrices given by (6.4.2) and (6.4.3), respectively, then the distance Laplacian spectrum of  $P_{2k}$  is*

$$\{0, \lambda_1, \lambda_2, \dots, \lambda_k, Tr(2), Tr(3), \dots, Tr(k)\},$$

where  $\lambda_j$  is an eigenvalue of  $A - B$  for  $j = 1, 2, \dots, k$ .

If  $\Delta$  denotes the maximum vertex degree, then  $\mu_1 \geq \Delta + 1$  (see [7]). Let  $\Gamma$  be the maximum vertex transmission of a graph. Then, in a similar way (hence the proof is omitted) we can prove that  $\delta_1 > \Gamma + 1$ . Following is one of the main results of this section.

**Theorem 6.4.4.** *The distance Laplacian spectral radius of  $P_{2k}$  is simple with  $\begin{bmatrix} X \\ \cdots \\ -X \end{bmatrix}$  as the corresponding eigenvector, where  $X$  is positive. Moreover,  $X(i + 1) > X(i)$ , where  $i = 1, 2, \dots, k - 1$ , and  $X(i)$  is the component of  $X$  corresponding to vertex  $i$ .*

**Proof.** Since  $\delta_1 > \Gamma + 1$ , so by Theorem 6.4.3, the distance Laplacian spectral radius of  $P_{2k}$  is the largest eigenvalue of  $A - B$ , where  $A$  and  $B$  are given by (6.4.2) and (6.4.3), respectively. Since  $A - B$  is a positive matrix so by the Perron-Frobenius Theorem, the largest eigenvalue of  $A - B$  is simple and is afforded by a positive eigenvector  $X$ . From the proof of Lemma 6.4.1, it follows that  $\begin{bmatrix} X \\ \cdots \\ -X \end{bmatrix}$  is the eigenvector of  $D^L(P_{2k})$  corresponding to  $\delta_1$ .

For  $i = 1, 2, \dots, k - 1$ , from the eigenequation we have

$$\begin{aligned} (\delta_1(P_{2k}) - Tr(i + 1))X(i + 1) &= (\delta_1(P_{2k}) - Tr(i))X(i) + 2 \sum_{j=i+1}^k X(j), \\ &= (\delta_1(P_{2k}) - Tr(i + 1))X(i) + 2iX(i) \\ &\quad + 2 \sum_{j=i+1}^k X(j) \text{ [by (6.4.1)]} \end{aligned} \tag{6.4.4}$$

Since  $\delta_1(P_{2k}) > Tr(i + 1)$  and  $X$  is positive, so by (6.4.4) we get,  $X(i + 1) > X(i)$ . ■

We now consider the path of odd order. Let the vertices of the path  $P_{2k+1}$  be labelled as in Fig. 6.2.

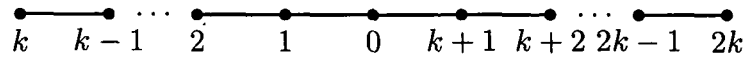


Figure 6.2: The path  $P_{2k+1}$ .

Then, for  $i = 0, 1, 2, \dots, k$ , we have

$$Tr(i) = k^2 + i^2 + k. \tag{6.4.5}$$

Also for  $i = 1, 2, \dots, k$ ,

$$Tr(i) = Tr(k + i). \tag{6.4.6}$$

Thus,

$$D^L(P_{2k+1}) = \begin{bmatrix} Tr(0) & Z^T & Z^T \\ \hline Z & A & C \\ \hline Z & C & A \end{bmatrix},$$

$$\text{where } Z = \begin{bmatrix} -1 \\ -2 \\ -3 \\ \vdots \\ -k \end{bmatrix}, \quad (6.4.7)$$

$$C = B - J_k, \quad (6.4.8)$$

and  $A, B$  are the matrices given by (6.4.2), (6.4.3), respectively.

**Theorem 6.4.5.** *If  $A$  and  $C$  are the matrices given by (6.4.2) and (6.4.8), respectively, then the distance Laplacian spectrum of  $P_{2k+1}$  is*

$$\{0, \lambda_1, \lambda_2, \dots, \lambda_k, Tr(1), Tr(2), \dots, Tr(k)\},$$

where  $\lambda_j$  is an eigenvalue of  $A - C$ , for  $j = 1, 2, \dots, k$ .

**Proof.** Clearly,  $\mathbb{1}_{2k+1}$  is the eigenvector of  $D^L(P_{2k+1})$  corresponding to 0. If  $\lambda_j$  is an eigenvalue of  $A - C$  with corresponding eigenvector  $X_j$ , then it can be seen that  $\lambda_j$  is also an eigenvalue of  $D^L(P_{2k+1})$  with  $\begin{bmatrix} 0 \\ \hline X_j \\ \hline -X_j \end{bmatrix}$  as the corresponding eigenvector, where  $j = 1, 2, \dots, k$ .

It is obvious that if  $\gamma$  is an eigenvalue of  $A + C + \frac{2}{\gamma - Tr(0)}ZZ^T$  with eigenvector  $Y$ , then  $\gamma$  is an eigenvalue of  $D^L(P_{2k+1})$  with eigenvector  $\begin{bmatrix} \frac{2}{\gamma - Tr(0)}Z^TY \\ \hline Y \\ \hline Y \end{bmatrix}$ , where  $Z$  is given by (6.4.7). Using (6.4.5) and (6.4.6), it can be verified that  $(A + C + \frac{2}{Tr(i) - Tr(0)}ZZ^T)Y_i = Tr(i)Y_i$ , where  $Y_i = \begin{bmatrix} -\frac{2}{2i-1}\mathbb{1}_{i-1} \\ \hline 1 \\ \hline \mathbf{0}_{k-i} \end{bmatrix}$  and  $i = 1, 2, \dots, k$ . Thus,  $Tr(i)$  is an eigenvalue of  $D^L(P_{2k+1})$  with  $\begin{bmatrix} \frac{2}{Tr(i) - Tr(0)}Z^TY_i \\ \hline Y_i \\ \hline Y_i \end{bmatrix}$  as the corresponding eigenvector, where  $i = 1, 2, \dots, k$ . It can be seen that

$$\left\{ \begin{bmatrix} 0 \\ \hline X_j \\ \hline -X_j \end{bmatrix} : j = 1, 2, \dots, k \right\} \cup \left\{ \begin{bmatrix} \frac{2}{Tr(i) - Tr(0)}Z^TY_i \\ \hline Y_i \\ \hline Y_i \end{bmatrix} : i = 1, 2, \dots, k \right\} \cup \{\mathbb{1}_{2k+1}\}$$

is a set of mutually orthogonal vectors. Since the order of  $D^L(P_{2k+1})$  is  $2k + 1$ , the result follows. ■

**Theorem 6.4.6.** *The distance Laplacian spectral radius of  $P_{2k+1}$  is simple with  $\begin{bmatrix} 0 \\ \cdots \\ X \\ \cdots \\ -X \end{bmatrix}$  as the corresponding eigenvector, where  $X$  is positive. Moreover,  $X(i+1) > X(i)$ , where  $i = 1, 2, \dots, k - 1$ , and  $X(i)$  is the component of  $X$  corresponding to vertex  $i$ .*

**Proof.** Similar to the proof of Theorem 6.4.4 ■

**Remark 6.4.7.** *Theorem 6.4.4 and Theorem 6.4.6 are similar in spirit to the work done by Fiedler (see [26], Theorem 3.11) and Merris (see [45], Section II, Theorem B), where the authors dealt with the eigenvector of the Laplacian matrix corresponding to the smallest positive eigenvalue.*

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