

T.R.
GEBZE TECHNICAL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

DISTANCE SPECTRA OF GRAPHS

AHMET TUGAY KUZU
A THESIS SUBMITTED FOR THE DEGREE OF
MASTER OF SCIENCE
DEPARTMENT OF MATHEMATICS

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ASSOC. PROF. DR. AYSEL EREY

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T.R.
GEBZE TEKNİK ÜNİVERSİTESİ
FEN BİLİMLERİ ENSTİTÜSÜ

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YÜKSEK LİSANS TEZİ
MATEMATİK ANABİLİM DALI

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SUMMARY

In this thesis, maximizing or minimizing the distance spectral radius of graphs in a given class or graphs with some given properties are investigated. Some important studies about maximizing or minimizing problems in the literature are given. The unique bicyclic graph that maximizes the distance spectral radius is investigated and given by being motivated by the studies in the literature. Moreover, the distance spectral radius of connected complements of bicyclic graphs are studied, but this study has not been completed. Yet, a path to find the unique graph that maximizes the distance spectral radius among connected complements of bicyclic graphs is given, and this problem is left as an open problem. In these studies, Perron-Frobenius Theorem and Rayleigh's Principle are used.

Keywords : Distance Matrix, Distance Spectral Radius, Graph, Bicyclic Graphs, Connected Complements of Bicyclic Graphs.

ÖZET

Bu tez çalışmasında, belirli bir çizge sınıfındaki veya belirli özelliklere sahip çizgelerin mesafe spektral yarıçaplarını maksimuma çıkarma veya minimuma indirme problemleri incelenmiştir. Bu problemler ile ilgili literatürde bulunan bazı çalışmalar paylaşılmıştır. Literatürdeki bu çalışmalardan esinlenilerek çift döngülü çizgeler incelenmiş ve mesafe spektral yarıçapı en büyük olan eşsiz çift döngülü çizge bulunmuştur. Ayrıca bağlı çift döngülü çizgelerin tümleyenleri incelenmiştir. Çift döngülü çizgelerin bağlı tümleyenleri arasında mesafe spektral yarıçapı en büyük olan çizge bulunmaya çalışılmıştır. Bu çalışma tamamlanamamasına rağmen sonuca götürecek ipuçları verilmiştir. Bu çalışmalar esnasında Perron-Frobenius teoremi ve Rayleigh prensibi kullanılmıştır.

Anahtar Kelimeler : Mesafe Martrisleri, Mesafe Spektral Yarıçap, Çift Döngülü Çizgeler, Çift Döngülü Çizgelerin Bağlı Tümleyenleri.

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LIST OF ABBREVIATIONS AND ACRONYMS

<u>Abbreviations</u>	<u>Explanations</u>
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<u>and Acronyms</u>

G	: Graph.
$D(G)$	: Distance matrix of G .
I	: $n \times n$ identity matrix.
$\rho(G)$	: Distance spectral radius of G .
P_n	: Path graph with n vertices.
C_n	: Cycle graph with n vertices.
S_n	: Star graph with n vertices.
$S(a, b, c)$	: Saw graph with given parameters.
$\theta(p; t; q)$	: Theta graph with given parameters.
$P(n; a, b)$	: The tree with given parameters.
$D(n; a, b)$	: The dumbbell graph with given parameters.
$T(n, i, j)$	: The tree with given parameters.
$T(p, q)$	: The tree with given parameters.
$U_{a,b}$	: The unicyclic graph with given parameters.
$U_{a,b,c}$	: The unicyclic graph with given parameters.

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1. INTRODUCTION

1.1. Overview of the Thesis

The main purpose of this thesis is to investigate the graph whose “distance spectral radius” is the largest amongst bicyclic graphs. Researchers have already investigated the unique graphs whose “distance spectral radius” is the largest among trees, trees with some given properties, complements of trees, unicyclic graphs, unicyclic graphs with some given properties, complements of unicyclic graphs, and some graphs with given properties. In addition to these maximization studies, minimization problems are begun to be studied recently. Some of these studies in the literature are given in the next chapters. These studies on “distance spectral radius” gives a motivation to find the unique bicyclic graph with the maximal “distance spectral radius” amongst bicyclic graphs. In order to do that, the class of bicyclic graphs are separated in two subclasses. It is proven that if a graph is a bicyclic graph, then either it is a cactus with two cycles or it includes a theta graph. The unique graphs with the largest “distance spectral radius” amongst cacti and amongst graphs which include a theta graph have already been investigated by some researchers. This gives a path to compare these two graphs that maximizes the “distance spectral radius” in each class. After solving the maximization problem in bicyclic graphs, the graph whose “distance spectral radius” is the largest amongst complements of bicyclic graphs is investigated. There is an open problem for complements of bicyclic graphs, and it is given as a conjecture with the studies which are done in the Conclusion chapter. In these problems, an equation that comes up from Perron-Frobenius Theorem and Rayleigh’s Principle is used with distance matrices and perron vectors. In the following sections, a general information about some definitions, useful theorems and lemmas that are used in the next chapters about in the field of graph theory and in the field of linear algebra are given separately, and also, it is explained that why these concepts are useful and how they are used to solve the maximization and minimization problems on “distance spectral radius”.

1.2. General Graph Theory

A *graph* G consists of a vertex set $V(G)$, and an edge set $E(G)$, and a relation where each edge is associated with two vertices. If a graph has finite number of vertices, then the graph is called *finite*. Let S be a graph. S is called a *subgraph* if $V(S) \subset V(G)$ and $E(S) \subset E(G)$. A subgraph S which is obtained from deleting some of the vertices of G is called an *induced subgraph* of G . If the vertices u and v are connected by an edge e , then these vertices are called the *endvertices*, and e is denoted by uv . If the endvertices of an edge are the same, then it is called a *loop*. If there is an edge e between the vertices u and v , then the vertices u and v are called *adjacent*. If there is no edge that connects the vertices u and v , then they are called *non – adjacent vertices*. A similar definition is used for edges, too. If any two edges have one common endvertex, then these two edges are called *adjacent*. Otherwise, they are called *non – adjacent*. The adjacent vertices are also called the *neighbors*. For example, assume that v_i is adjacent to v_j, v_k and v_l . Then, v_j, v_k and v_l are called the neighbors of v_i . The number of adjacent vertices of a vertex v is called the *degree* of the vertex v and denoted by $\deg(v)$. Neighbors of v are denoted by $N(v)$. The vertices which have the same neighbors are called *twin vertices*. If the twin vertices are adjacent, then they are called *true twins*. If the twin vertices are not adjacent, then they are called *false twins*. If v is not adjacent to any other vertices, then v is called *isolated*. A *pendant vertex* is a vertex whose degree is 1. The connected graphs with n vertices and k vertices of odd degree are denoted by $G(n, k)$. G_n^m denotes the class of graphs with n vertices and m pendant vertices. If all of the edges of a graph G

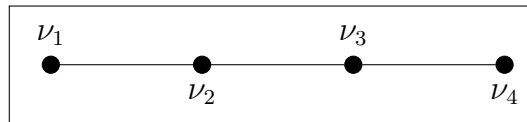


Figure 1.1: Sample graph.

are directed, then G is called a *directed graph*. A graph that is not directed is called *undirected*. A directed graph is also called a *digraph*. For example, a uv edge in a directed graph shows that the edge starts from the vertex u and moves to the vertex v . The direction is shown by arrows. If a graph has no loops, no edges more than one between any two vertices, then the graph is called a *simple graph*. All graphs in this

thesis are simple, finite, and undirected unless otherwise is stated. The following is a sample of a directed graph.

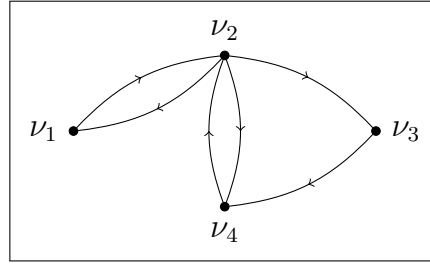


Figure 1.2: Directed Graph.

Example 1.1: The graph in the following figure is a simple graph. Let $v_1v_6 = e_1$,

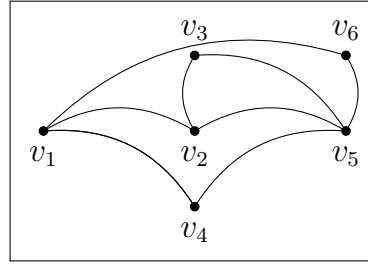


Figure 1.3: An example of a simple graph.

$v_1v_2 = e_2$, $v_1v_4 = e_3$, $v_2v_3 = e_4$, $v_2v_5 = e_5$, $v_3v_5 = e_6$, $v_4v_5 = e_7$, $v_5v_6 = e_8$ be the edges on the graph G .

A *path* is a graph where the vertices of the graph can be listed in a way that any two vertices which are consecutive in the list are adjacent, and denoted by P_n where n is the number of the vertices. For example, let P_n be a path graph and $v_i \in V(P_n)$ where $i = 1, \dots, n$. Then, P_n can be denoted by $v_1v_2v_3 \dots v_n$. Also, if a path starts with the vertex u and ends with the vertex v , then it is called a $u - v$ path.

If any vertex of a graph G can be connected by a path, then the graph G is called connected. If a graph is not connected then it is called *disconnected*. If between every pair of distinct vertices v_i, v_j of a directed graph G , there is a directed path with finite length that begins at v_i and ends at v_j , then the directed graph G is called *strongly connected*.

The *distance* between the vertices v_i and v_j of the graph G is the number of

edges of the shortest path between the vertices v_i and v_j , and it is denoted by $d(v_i, v_j)$. The *diameter* of a graph G is $\max_{v_i, v_j \in V(G)} d(v_i, v_j)$.

If each vertex is adjacent with each other in a graph, then it is called a *complete graph*, and denoted by K_n where n is the order. Complete graph with n vertices has $\binom{n}{2}$ edges. Let $\overline{G}$ be a graph with the same vertices as G where $u, v \in G$. $\overline{G}$ is called the *complement* of G if for any edge $uv \in G$, then $uv \notin \overline{G}$, and if for any edge $uv \notin G$, then $uv \in \overline{G}$ (see Figures 1.4, 1.5). A set of pairwise nonadjacent vertices

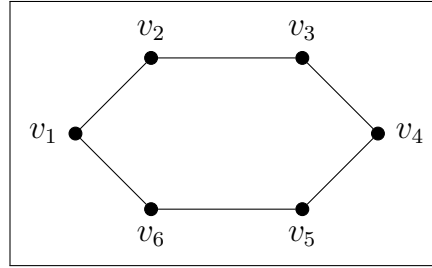


Figure 1.4: An example of a graph G

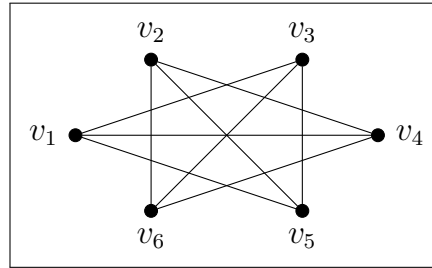


Figure 1.5: The complement $\overline{G}$ of the graph G in Figure 1.4.

in a graph G is called an *independent set*. If the vertex set of a graph G consists of 2 independent sets, then G is a *bipartite graph*. A *complete bipartite graph* with the order $m + n$ is a bipartite graph where each vertex in an independent set is adjacent to every vertex in the other independent set, and denoted by $K_{m,n}$ where m and n are the orders of the independent sets.

If a path is a *closed path i.e.*, starts and ends with the same vertex, then it is called a *cycle*. A cycle with n vertices is denoted by C_n . A cycle has the same number of edges and vertices.

A graph that has no cycle in it is called an *acyclic graph*. If a graph is connected and has no cycles, then it is called a *tree*. Removing an edge from a tree gives us a disconnected graph, so trees are called *minimally connected*. If a tree is a graph which

transforms into P_n after deleting all pendant vertices, then it is called a *caterpillar*. $P(n; a, b)$ denotes the tree by attaching a pendant vertex to v_a and a path $v_n v_{n-1}$ at the terminal vertex v_{n-1} to v_b where $2 \leq a < b \leq n - 5$ and $8 \leq n$. A *dumbbell graph* with order n is a tree which is transformed by adding a pendant vertices to a vertex with degree 1 and b pendant vertices to the other vertex with degree 1 of P_{n-a-b} , and it is denoted by $D(n; a, b)$. $T(n, k, l)$ denotes the tree which is formed from P_{n-k-l}

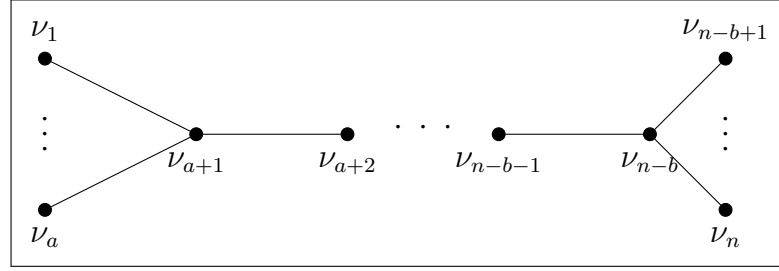


Figure 1.6: The dumbbell graph $D(n; a, b)$.

whose vertices are $\mu_0, \mu_1, \dots, \mu_{n-k-l-1}$ by connecting k pendant vertices to the vertex μ_k and l vertices to the vertex μ_l where $2 \leq \dots \leq k < l \leq \dots \leq n - k - l - 1$. As

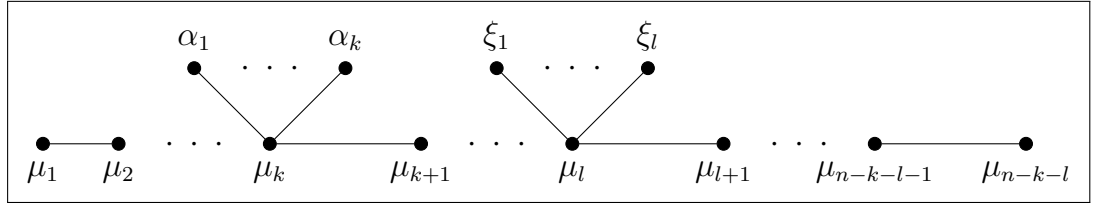


Figure 1.7: $T(n, k, l)$.

an example, $T(n, 0, 0)$ is the path graph P_n .

A *star graph* denoted by S_n is equal to $K_{1,n-1}$ (see Figure 1.8). A tree is called

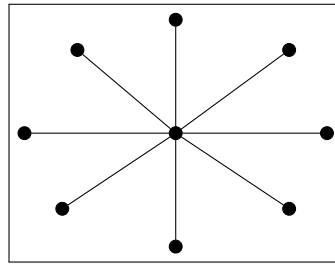


Figure 1.8: Star graph with 9 vertices.

a *starlike tree* if the tree has at most one vertex with the degree at least three. If a tree

is not a starlike tree, then it is called *non – starlike tree*. For example, a path graph P_n is a starlike tree.

The broom graph with the order n and a maximum degree k is a tree which is formed by attaching a path graph P_{n-k-1} to one of the pendant vertices of a star graph S_{k+1} (see Figure 1.9). So, a broom graph is a starlike tree. $T_{p,q}$ denotes the tree graph

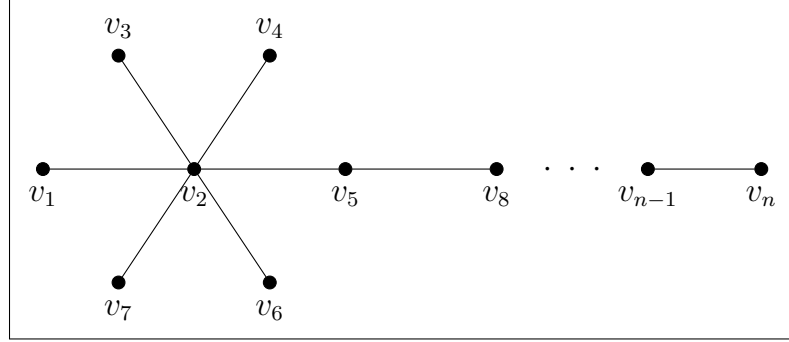


Figure 1.9: The sample of a broom graph with a maximum degree 6.

such that p pendant vertices attached to one vertex of P_2 and q pendant vertices attached to the other vertex of P_2 (see Figure 1.10), and the order of $T_{p,q}$ is $p + q + 2$. A graph

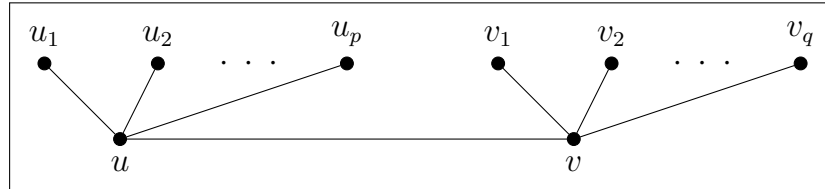


Figure 1.10: $T_{p,q}$.

G is called *unicyclic* if G has the same number of edges and vertices. Thus, unicyclic graphs include only one cycle.

The following notations will be used for unicyclic graphs. Unicyclic graphs of order a are denoted by U_a . The set of all unicyclic graphs of order a and with a cycle of length b are denoted by $U_{a,b}$. The set of all unicyclic graphs of order a with a cycle of length b and having c vertices on the cycle attached by pendant vertices are denoted by $U_{a,b,c}$, and the degree of the other vertices is 2. A connected graph is called *cactus* if any two cycles in it have at most one common vertex. $C(n, k)$ denotes the set of all cacti of order n with number of cycles k . A cactus is called a *saw graph* with order n and length l if it is obtained by replacing l cut vertices of P_{n-l} with l triangles, where

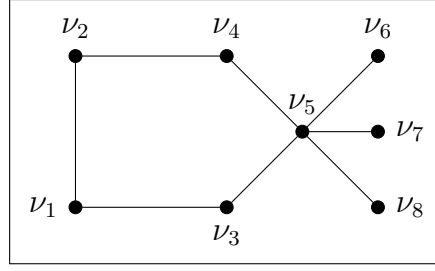


Figure 1.11: $U_{8,5,1}$.

$0 \leq l \leq \lfloor \frac{n-1}{2} \rfloor$. A saw graph is called a *proper saw graph* if its length is l and order is $2l + 1$. A vertex of degree 2 in a proper saw graph with a neighbor of degree 2 is called an *end*. Connecting an end of a proper saw graph with length a with an end of a proper saw graph with length b via a path with length c forms a saw graph, and it is denoted by $S(a, b; c)$. If a graph has p edges and q vertices where $p = q + 1$, then it

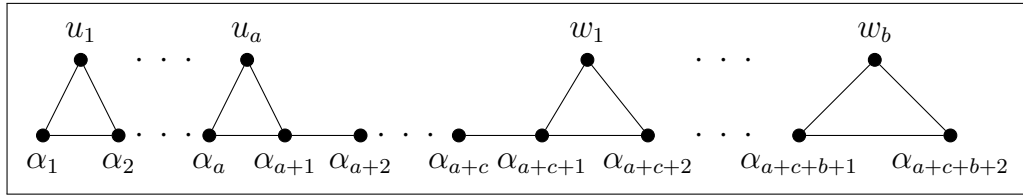


Figure 1.12: $S(a, b; c)$.

is called a bicyclic graph. B_n denotes all bicyclic graphs with n vertices. B_n^1 denotes the bicyclic graph that is obtained by adding two non-adjacent edges to the star graph S_n where the endvertices of the edges are the pendant vertices of S_n . B_n^2 denotes the bicyclic graph which is obtained by adding two adjacent edges to the star graph S_n where the endvertices of the edges are the pendant vertices of S_n (see Figures 1.13, 1.14).

The graph obtained by identifying the initial vertices and terminal vertices of three

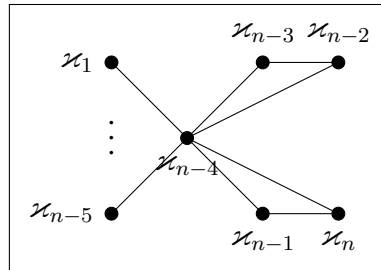


Figure 1.13: B_n^1 .

paths of lengths $p + 1$, $t + 1$, $q + 1$ whose vertices are disjoint is called a θ -graph, and it is denoted by $\theta(p; t; q)$. A θ -graph is an example of a bicyclic graph.

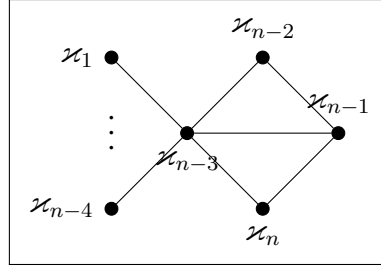


Figure 1.14: B_n^2 .

Let G and F be two graphs with vertex sets $V(G)$ and $V(F)$ and edge sets $E(G)$ and $E(F)$, respectively. If there exists a bijection $g : V(G) \rightarrow V(F)$ such that $uv \in E(G)$ if and only if $g(u)g(v) \in E(F)$ for all $u, v \in V(G)$, then G and F are called *isomorphic* and denoted by $G \cong F$. If graphs are not isomorphic, then they are called *non – isomorphic*. If an isomorphism h is defined from a graph G to itself, then it is called an *automorphism*.

Example 1.2: Let G_1 be the graph in Figure 1.15 and f be a bijection on G_1 defined in the following.

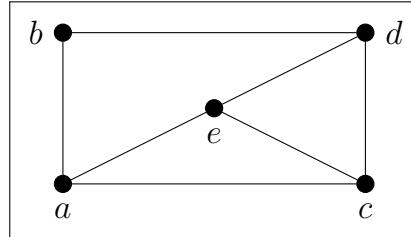


Figure 1.15: The graph G_1 in Example 1.2.

$$f : V(G_1) \rightarrow V(G_1) \quad (1.1)$$

$$a \rightarrow d \quad (1.2)$$

$$b \rightarrow b \quad (1.3)$$

$$c \rightarrow e \quad (1.4)$$

$$d \rightarrow a \quad (1.5)$$

$$e \rightarrow c \quad (1.6)$$

It can be checked

$$ab \in E(G_1) \iff db \in E(G_1), \quad (1.7)$$

$$ac \in E(G_1) \iff de \in E(G_1), \quad (1.8)$$

$$ae \in E(G_1) \iff dc \in E(G_1), \quad (1.9)$$

$$bd \in E(G_1) \iff ba \in E(G_1), \quad (1.10)$$

$$cd \in E(G_1) \iff ea \in E(G_1), \quad (1.11)$$

$$ce \in E(G_1) \iff ec \in E(G_1), \quad (1.12)$$

$$de \in E(G_1) \iff ac \in E(G_1). \quad (1.13)$$

Also, $be \notin E(G_1) \iff bc \notin E(G_1)$ and $ad \notin E(G_1) \iff da \notin E(G_1)$.

So, f is an automorphism.

If two distinct edges of a graph G have no common end vertex, then these two distinct edges are called *independent*. A *matching* of a graph G is a set of edges where each edge is pairwise independent. The maximum number of the pairwise independent edges of G is the *maximum matching* of G , and it is also called the *matching number* of G . If a vertex is in $V(M)$ then it is called *saturated* by M . A matching is a *perfect matching* if $V(M) = V(G)$.

1.3. Linear Algebra

In this chapter, some important linear algebraic structures of matrices which will be useful for this thesis are given, and some of them are explained.

The notation $M_{n \times m}$ will be used as the notation of vector spaces of all $n \times m$ matrices, and M_n as the notation of vector space of all $n \times n$ matrices.

If $A \in M_n$, then A is a *square matrix*. If $a_{i,j} = a_{j,i}$, then A is called a *symmetric matrix* where $a_{i,j}$ are the entries of A . If the entries of a matrix are all real, then the matrix is called a *real matrix*. Also, if A is a real symmetric matrix, then all of the eigenvalues of A are real. If a matrix A does not have any negative entries, then A is called a *nonnegative matrix*. If every entry a_i of A is positive, then A is called *positive matrix*, and we write $A > 0$. Roots of $\det(rI - A) = 0$ are the *eigenvalues* of A and denoted by $r(A)$.

For a square matrix A , the *spectral radius* of A is defined by

$$\rho(A) = \max\{|r| : r \in r(A)\}. \quad (1.14)$$

For a square matrix A and an eigenvalue r , if there is a vector $\vec{x} \neq \vec{0}$ that satisfies the following equation

$$A\vec{x} = r\vec{x}, \quad (1.15)$$

then the nonzero vector $\vec{x}$ is called an *eigenvector* of the matrix A corresponding r .

Let $\vec{x} = [x_1 \ x_2 \ \cdots \ x_n]$ be a vector. The *length* of $\vec{x}$ is defined by

$$\|\vec{x}\| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}. \quad (1.16)$$

Normalizing a vector means dividing a vector by its length, and the normalized vector of $\vec{x}$ is denoted by $\vec{X}$.

$$\vec{X} = \frac{[x_1 \ x_2 \ \cdots \ x_n]}{\|\vec{x}\|} \quad (1.17)$$

A normalized vector is also called a *unit vector*. The length of the unit vector is 1.

Example 1.3: Let $\vec{x} = [1 \ 2 \ 3 \ 4]$. Then, $||\vec{x}|| = \sqrt{1^2 + 2^2 + 3^2 + 4^2} = \sqrt{30}$. Normalizing $\vec{x}$, gives the following

$$\vec{X} = \frac{\vec{x}}{||\vec{x}||} = \frac{[1 \ 2 \ 3 \ 4]}{\sqrt{30}} = \left(\frac{1}{\sqrt{30}} \ \frac{2}{\sqrt{30}} \ \frac{3}{\sqrt{30}} \ \frac{4}{\sqrt{30}} \right). \quad (1.18)$$

In the previous example, it is clear to see that $||\vec{X}|| = 1$. For an eigenvalue r of any square matrix A and a normalized eigenvector $\vec{X}$ corresponding to r ,

$$r\vec{X} = A\vec{X} \quad (1.19)$$

$$\vec{X}^t r \vec{X} = \vec{X}^t A \vec{X} \quad (1.20)$$

$$r \vec{X}^t \vec{X} = \vec{X}^t A \vec{X}. \text{ Since } \vec{X}^t \vec{X} = ||\vec{X}||^2 = 1, \quad (1.21)$$

$$r = \vec{X}^t A \vec{X}. \quad (1.22)$$

Positive matrices are assumed to be the simplest and most elegant form of non-negative matrices. Oskar Perron is the one who studied positive matrices and published some fundamental discoveries in 1907. The following theorem shows some important properties of positive matrices in [1] (page 667).

Theorem 1.1: (Perron Theorem)

“ Let A be an $n \times n$ and a positive matrix. Let r be an eigenvalue of A and $\vec{x}$ be an eigenvector corresponding to r .

(i) $\rho(A)$ is an eigenvalue of A .

(ii) If $|r| = \rho(A)$, then $|\vec{x}| > 0$ and $A|\vec{x}| = \rho(A)|\vec{x}|$.

(iii) $\rho(A) > 0$.

(iv) Algebraic multiplicity of $\rho(A)$ is 1.

(v) There exists a unique positive eigenvector $\vec{x} = [x_1 \ x_2 \ \cdots \ x_n]$ where all of the components are positive and $x_1 + x_2 + \cdots + x_n = 1$ corresponding to $\rho(A)$. There are no nonnegative eigenvectors for other eigenvalues.”

Frobenius studied on this Perron's theorem, and saw the differences in terms of reducibility. Then, Frobenius related these studies to spectral properties of nonnegative and irreducible matrices. The following is Perron - Frobenius theorem which can be found in [1] (page 673).

Theorem 1.2: (Perron - Frobenius theorem)

“If A is an $n \times n$, nonnegative and irreducible matrix, then the followings are true.

(i) $\rho(A) > 0$.

(ii) Algebraic multiplicity of $\rho(A)$ is 1.

(iii) There exists a unique positive eigenvector $\vec{x} = [x_1 \ x_2 \ \cdots \ x_n]$ where all of the components are positive and $x_1 + x_2 + \cdots + x_n = 1$ corresponding to $\rho(A)$. There are no nonnegative eigenvectors for other eigenvalues.”

The following theorem is a generalized version of Perron’s theorem to nonnegative matrices which can be found in [2] (page 529).

Theorem 1.3: [2] “ If A be an $n \times n$ nonnegative matrix, then $\rho(A)$ is an eigenvalue of A and there exists a nonzero nonnegative vector $\vec{x}$ such that $A\vec{x} = \rho(A)\vec{x}$.”

Definition 1.1: [2] “ The unique normalized positive eigenvector corresponding to the spectral radius of A which is a nonnegative and irreducible $n \times n$ matrix is called the perron vector of A .” (page 526).

The following definitions are important and useful to show that for a given matrix, if the matrix is irreducible or not. The relation is explained in Theorem 1.5.

Definition 1.2: The graph G with n vertices is called a directed graph of an $n \times n$ matrix D if G is the directed graph with n vertices $\alpha_1, \alpha_2, \cdots, \alpha_n$ such that there is a directed edge in the directed graph from α_i to α_j if and only if $d_{ij} \neq 0$. The directed graph of D is denoted by $\Gamma(D)$.

Here is an example of an $n \times n$ matrix D and its directed graph $\Gamma(D)$ in the following figure.

$$D = \begin{pmatrix} 5 & 2 & 0 & 0 \\ 3 & 0 & 3 & 4 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}; \quad (1.23)$$

Definition 1.3: Let D be a square matrix with the entries d_{ij} . The indicator matrix of D is $M(D) = [\mu_{ij}]$, where $\mu_{ij} = 0$ if $d_{ij} = 0$ and $\mu_{ij} = 1$ if $d_{ij} \neq 0$.

Here is an example of an indicator matrix $M(A)$ of a given matrix A :

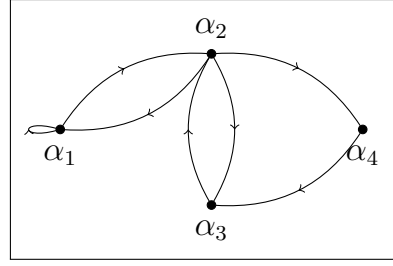


Figure 1.16: The directed graph $\Gamma(D)$ of the previous matrix D .

$$A = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 2 & 3 & 0 & 1 & 0 \\ 0 & 5 & 1 & 3 & 1 \\ 1 & 2 & 3 & 0 & 1 \\ 1 & 1 & 2 & 0 & 0 \end{pmatrix}, \quad M(A) = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 \end{pmatrix}. \quad (1.24)$$

Definition 1.4: Let D be an $n \times n$ matrix with the entries d_{ij} . If for every pair of distinct integers r, s with $1 \leq r, s \leq n$, $\exists$ a sequence of distinct integers $l_1 = r, l_2, l_3, \dots, l_m = s$ where $1 \leq m \leq n$ such that the entries $d_{l_1 l_2}, d_{l_2 l_3}, \dots, d_{l_{m-1} l_m}$ of the matrix D are nonzero, then D has a property SC.

An $n \times n$ matrix is a *permutation matrix* if only one entry of a column and a row is 1 and all of the other entries of the matrix are 0. Permutation matrices are obtained from identity matrices by permuting the rows according to the given permutation. Each permutation can be correlated with a unique permutation matrix. Therefore, there are $n!$ $n \times n$ permutation matrices. Let A be a permutation matrix, then $AA^T = I_{n \times n}$, i.e., $A^T = A^{-1}$.

Let B and A be the following matrices.

$$B = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (1.25)$$

Then,

$$ABA^t = \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix}. \quad (1.26)$$

It can be observed from above that permutation matrices permute the rows in the same way with the columns. In order to get the permutation matrices that change the

$i - th$ row with the $j - th$ row and the columns with the same way of the matrix A , the $i - th$ row of the identity matrix is changed with the $j - th$ row, and call this new matrix, obtained by changing the rows of the identity matrix, P . Now, multiply A with the matrix P by the left hand side. This will change the rows of the matrix A . Then, in order to do this for the columns, the same $i - th$ column with the $j - th$ column of the identity matrix is changed and call this new matrix, obtained by changing the columns of the identity matrix, Q . Then, multiply A with the permutation matrix Q by the right hand side. It can also be seen that $Q = P^t$. Thus, PAP^t gives the new matrix obtained from changing the $i - th$ row with the $j - th$ row and the columns in the same way of the matrix A .

Every permutation matrix can be written as multiplication of elementary matrices. For elementary matrices, $E = E^t$, but for permutation matrices $P \neq P^t$ (see Example 1.4).

Example 1.4: Let E_1, E_2 be the elementary matrices as in the following, and P be the permutation matrix such that $P = E_1E_2$.

$$E_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, E_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (1.27)$$

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, P^t = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad (1.28)$$

It can be seen from the example that $P \neq P^t$.

Let D be a matrix. If there exists a matrix D' such that $ADA^{-1} = D'$ for some permutation matrix A , then D and D' are called *similar*.

Lemma 1.4 is well-known.

Lemma 1.4: "Let D be a matrix and P be a permutation matrix. If $\vec{X}$ is an eigenvector of D , then $P\vec{X}$ is an eigenvector of D' with the same eigenvalue where $PDP^{-1} = D'$."

Proof: Let r be an eigenvalue of D and $\vec{X}$ be the corresponding eigenvector. Then, $D\vec{X} = r\vec{X}$. Now, it suffices to show that $D'P\vec{X} = rP\vec{X}$.

$D\vec{X} = r\vec{X}$. Multiply each side from the left with the permutation matrix P . Then,

$PD\vec{X} = Pr\vec{X}$. Since r is a coefficient, $Pr = rP$. So,

$PD\vec{X} = rP\vec{X}$. Since $P^{-1}P = I$, the latter becomes

$PDP^{-1}P\vec{X} = rP\vec{X}$. Since $PDP^{-1} = D'$,

$D'P\vec{X} = rP\vec{X}$.

The following definition can be found in [1].

Definition 1.5: A square matrix $A_{n \times n}$ is said to be reducible if there exists a permutation matrix H such that

$$H^T A H = \begin{pmatrix} M & N \\ 0 & Q \end{pmatrix}, \quad (1.29)$$

where M and Q are both square matrices; otherwise, A is said to be an irreducible matrix.

There is an important theorem related to irreducibility which can be found in [2] (page 403).

Theorem 1.5: [2] “Let D be an $n \times n$ matrix. Then the followings are equivalent:

- (i) D is irreducible;
- (ii) $[I + M(D)]^{n-1} > 0$;
- (iii) $\Gamma(D)$ is strongly connected;
- (iv) D has property SC.”

The following lemma is important, and it will be related with the distance matrices in the following chapters. It can be found in [3].

Lemma 1.6: [3] “Let A and B be two nonnegative, irreducible, $n \times n$ matrices and let $a_{i,j}$ and $b_{i,j}$ be the entries of the matrices A and B , respectively. If $A \geq B$, i.e., $a_{i,j} \geq b_{i,j}$ for all i, j – th entries of the matrices, then $\rho(A) \geq \rho(B)$. $\rho(A) = \rho(B)$ if and only if $A = B$ (p.38).”

2. DISTANCE MATRICES AND DISTANCE SPECTRAL RADIUS

Distance matrices of graphs have been studied extensively since the 70's because some properties of distance matrices shed light on characterizing the molecular structures (see [4] and [5]), psychology (see [6]), phylogenetics (see [7]), analysis of internet infrastructures and modelling of traffic (see [8], [9]). In the consequences of these studies and relations, researchers started to investigate the “distance spectral radius” of graphs. The studies showed that there is an important relation between “distance spectral radius” and molecules such as molecular description, inferring the extent of branching and modelling boiling points of an alkane. In this thesis, the relation between the “distance spectral radius” and others is not given, but the reader may look at the following references if interested (see [10], [11], [12], [13], [14]).

In this section, some important properties of the distance matrices will be introduced. Cayley's paper [15] is the origin of the distance matrices in 1841, but the distance matrices are begun to be studied formally during the 20 – *th* century by Young and Householder in [16] and Schoenberg in [17]. The first problem which is studied by the researchers was the realizability of the distance matrices. Hakimi and Yau were the ones who posed this problem in [18]. $D(G)$ is a *distance matrix* whose entries $d_{i,j} = d(v_i, v_j)$ where v_i, v_j are vertices of graph G . Since $d_{i,j} = d_{j,i}$, and $d_{i,j}$ is real, $D(G)$ is a real, symmetric matrix. All of the eigenvalues of a distance matrix are real since a distance matrix is a real and a symmetric matrix.

Theorem 2.1: [18] “A square, real, symmetric, nonnegative and real matrix is the distance matrix of a graph if and only if the given conditions hold.

- (i) $d_{i,j} = 0$ if $i = j$.
- (ii) $d_{i,j} \leq d_{i,k} + d_{k,j}$ where $d_{i,j}$ is the entry of the matrix.”

Graham and Pollak studied the spectral properties of distance matrices in 1971 for the first time. They determined in their first paper [19] that there is a relation between the addressing problem in data communication systems and the number of nonnegative eigenvalues of the distance matrix. In the same paper, Graham and Pollack established that the determinant of the distance matrix of a tree graph is a function of the order of

the graph only.

The set of the distinct eigenvalues of the distance matrix of a graph G with their multiplicities is called *distance spectrum* of G . Let $\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_n$ be the distinct eigenvalues of $D(G)$, and $m(\gamma_1), m(\gamma_2), \dots, m(\gamma_n)$ be their multiplicities. Then, the distance spectrum is denoted by

$$SpecG = \begin{pmatrix} \gamma_1 & \gamma_2 & \gamma_3 & \dots & \gamma_n \\ m(\gamma_1) & m(\gamma_2) & m(\gamma_3) & \dots & m(\gamma_n) \end{pmatrix}. \quad (2.1)$$

Assume γ_1 is the greatest eigenvalue. Then, it is called the “*distance spectral radius*” of G , and it is denoted by $\rho(G)$.

Distance matrices are non-negative matrices since the distance between the vertices is greater than or equal to 0.

Distance matrices have an important property which is irreducibility. It is explained below why a distance matrix is irreducible, by using the definitions in Theorem 1.5.

1. Property (ii): A distance matrix $D(G)$ is irreducible if and only if

$$[I + M(D(G))]^{n-1} > 0. \quad (2.2)$$

Let $M(D(G))$ be the indicator matrix of the distance matrix with the entries a_{ij} . $[I + M(D(G))]^{n-1} > 0$ is wanted to be shown. Then, by the definition of indicator matrices $a_{ij} = 1$ when $d_{ij} \neq 0$ and $a_{ij} = 0$ when $d_{ij} = 0$. So, the diagonal entries of $M(D(G))$ are equal to zero. Then, every entry of $[I + M(D(G))]$ is greater than zero. So, $[I + M(D(G))] > 0$. Moreover, every entry of $[I + M(D(G))]$ is 1. Hence, $[I + M(D(G))]^{n-1} > 0$.

Thus, $D(G)$ is irreducible.

Example 2.1: Let $D(G)$ be the following.

$$D(G) = \begin{pmatrix} 0 & 1 & 3 & 2 \\ 1 & 0 & 1 & 2 \\ 3 & 1 & 0 & 1 \\ 2 & 2 & 1 & 0 \end{pmatrix}. \text{ Then, } M(D(G)) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

So,

$$[I + M(D(G))] = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}. \quad (2.3)$$

$$[I + M(D(G))]^{n-1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}^{n-1} > 0. \quad (2.4)$$

2. Property (iii): Let $D(G)$ be a distance matrix and $\Gamma(D(G))$ be the directed graph of $D(G)$. Since every entry $d_{ij} \neq 0$ when $i \neq j$, there is a directed edge from a vertex v_i to another vertex v_j in the directed graph $\Gamma(D(G))$ by Definition 1.2. Then, one can find a directed path of finite length between every distinct pair of vertices. So, by the definition of being strongly connected, $\Gamma(D(G))$ is strongly connected.

Thus, $D(G)$ is irreducible.

Example 2.2: Let $D(G)$ be the distance matrix in Example 2.1. Then, the directed graph of $D(G)$ is the graph in the following figure. It can be seen in the figure that there

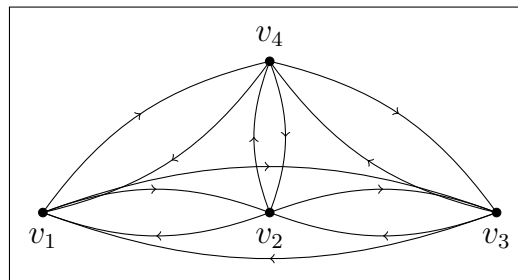


Figure 2.1: $\Gamma(D(G))$.

exists a directed path of finite length between every distinct pair of vertices.

3. Property (iv): A distance matrix has the property *SC*.

Let p and q be a pair of distinct integers with $1 \leq p, q \leq n$. So, for any sequence of distinct integers $1 \leq m \leq n$ with $k_1 = p, k_2, \dots, k_m = q$. Since all k_i 's are distinct, $k_i \neq k_j$, and so, $d_{k_i, k_j} \neq 0$. Then, $D(G)$ has the property *SC*.

Thus, $D(G)$ is irreducible.

Example 2.3: Let $D(G)$ be the distance matrix in Example 2.1. If one takes any pair of distinct integers, for example 1 and 3, then one can find a sequence $k_1 = 1, k_2 = 2$ and $k_3 = 3$ so that $d_{1,2} \neq 0, d_{1,3} \neq 0$ and $d_{2,3} \neq 0$.

Thus, $D(G)$ has the property *SC*.

Now, the following shows that a distance matrix is irreducible by using the definition of irreducibility. A distance matrix is symmetric and in this form

$$D(G) = \begin{pmatrix} A & B \\ B^t & C \end{pmatrix} \quad (2.5)$$

where A, B and C are all square matrices and only zero entries are the diagonals.

Multiplying $D(G)$ with permutation matrices, changes the rows and columns in the same way. For example, if multiplying with a permutation matrix P from the left changes the first row with the second row, then multiplying with permutation matrix P^t from the right changes the first column with the second column. So, if one changes the place of a 0 at entry a_{11} , by changing the rows, then one should put that 0 into the another diagonal entry since this operation also changes the columns. Thus, it is not possible to collect all zeros under the diagonals. Also, if the matrix is larger than 4×4 , then there are not enough 0's to get an upper triangular form. Hence, a distance matrix is irreducible.

Rayleigh quotient is stated in [1] (page 550) which is very important and useful for distance matrices and calculating the “distance spectral radius” of graphs. Rayleigh

principle is the following

$$\gamma_1 \geq \frac{\vec{x}^t D(G) \vec{x}}{\vec{x}^t \vec{x}} \geq \gamma_n \quad (2.6)$$

where $\vec{x} \neq \vec{0}$ is a vector.

Rayleigh quotient is used for distance matrices. Thus, by Rayleigh principle and Perron-Frobenius Theorem,

$$\rho(G) \geq \vec{X}^t D(G) \vec{X} \quad (2.7)$$

where $\vec{X} \in R^n$ is a normalized nonzero vector.

The previous inequality is very useful, and it is used in the following chapters to compare the “distance spectral radius” of graphs. Moreover,

$$\rho(G) = \vec{X}^t D(G) \vec{X} \quad (2.8)$$

$$= \frac{1}{2} \sum_{v_i, v_j \in V(G)} d_{ij} x_i x_j. \quad (2.9)$$

where $\vec{X} = [x_1 x_2 \cdots x_n]^t$ is the perron vector of the distance matrix $D(G)$.

Also, let G be a simple connected graph and $\vec{X} = [x_1 x_2 \cdots x_n]^t$ be the perron vector of $D(G)$, then

$$\rho(G) x_i = \sum_{v_j \in V(G)} d_{ij} x_j. \quad (2.10)$$

Now, the following is an important and a well-known lemma which will be useful for the proofs in the following chapters.

Lemma 2.2: [20] “Let v_i and v_j be twin vertices. Then, the corresponding components of the perron vector x_i and x_j are equal [Liu, 2010].”

Proof: By the perron equation,

$$\rho(G) x_i = \sum_{v_k \in V(G)} d_{ik} x_k \quad (2.11)$$

$$\rho(G)x_j = \sum_{v_k \in V(G)} d_{jk}x_k \quad (2.12)$$

$$\rho(G)x_i - \rho(G)x_j = \sum_{v_k \in V(G)} d_{ik}x_k - \sum_{v_k \in V(G)} d_{jk}x_k \quad (2.13)$$

$$\rho(G)(x_i - x_j) = \sum_{v_k \in V(G)} (d_{ik}x_k - d_{jk}x_k) \quad (2.14)$$

$$\rho(G)(x_i - x_j) = \sum_{v_k \in V(G)} x_k(d_{ik} - d_{jk}). \quad (2.15)$$

Since x_i and x_j are twin vertices, all of their neighbors are the same. So, we can say $d_{ik} = d_{jk}$. Then, $d_{ik} - d_{jk} = 0$. Thus, the latter becomes

$$\rho(G)(x_i - x_j) = \sum_{v_k \in V(G)} x_k 0 \quad (2.16)$$

$$\rho(G)(x_i - x_j) = \sum_{v_k \in V(G)} 0 \quad (2.17)$$

$$\rho(G)(x_i - x_j) = 0. \quad (2.18)$$

Since $\rho(G) > 0$, there is only one solution where $x_i - x_j = 0$. This yields that $x_i = x_j$.

The following is a result of Lemma 1.4.

Lemma 2.3: The “distance spectral radius” does not depend on the ordering.

Proof: Let B be the distance matrix of a graph H with a given ordering and λ be the “distance spectral radius” of the graph H . Now, assume that B' be the distance matrix obtained from changing the ordering of the graph H and R be the permutation matrix such that $RBR^t = B'$. It suffices to show that

$$\det(\lambda I - B') = \det(\lambda I - RBR^t). \quad (2.19)$$

$$\det(\lambda I - B') = \det(\lambda I - B')\det(R)\det(R^t) \quad (2.20)$$

$$\det(\lambda I - B') = \det(R)\det(\lambda I - B')\det(R^t) \quad (2.21)$$

$$\det(\lambda I - B') = \det(R(\lambda I - B')R^t) \quad (2.22)$$

$$\det(\lambda I - B') = \det(R\lambda I R^t - RB'R^t) \quad (2.23)$$

$$\det(\lambda I - B') = \det(\lambda R I R^t - RB'R^t) \quad (2.24)$$

$$\det(\lambda I - B') = \det(\lambda I R R^t - RB'R^t) \quad (2.25)$$

$$\det(\lambda I - B') = \det(\lambda I - RB'R^t) \quad (2.26)$$

This finishes the proof.

Permutation matrices can be used for forming the distance matrix of the graph which is reordered from another graph. The following examples will help to understand that better.

Example 2.4: Let G and G' be the following graphs with the given orderings.

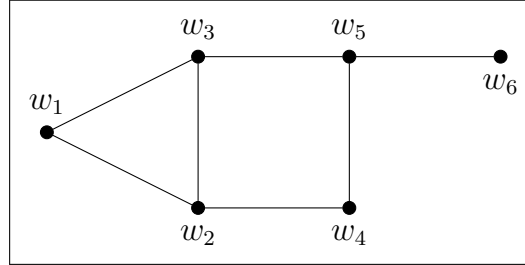


Figure 2.2: The graph G and the ordering for G : $w_1 w_2 w_3 w_4 w_5 w_6$.

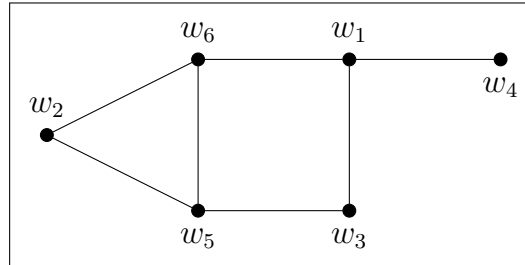


Figure 2.3: The graph G' and the ordering for G' : $w_2 w_5 w_6 w_3 w_1 w_4$.

So, the distance matrices $D(G)$ and $D(G')$ are the followings.

$$D(G) = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 & 3 \\ 1 & 0 & 1 & 1 & 2 & 3 \\ 1 & 1 & 0 & 2 & 1 & 2 \\ 2 & 1 & 2 & 0 & 1 & 2 \\ 2 & 2 & 1 & 1 & 0 & 1 \\ 3 & 3 & 2 & 2 & 1 & 0 \end{pmatrix}, D(G') = \begin{pmatrix} 0 & 2 & 1 & 1 & 2 & 1 \\ 2 & 0 & 2 & 3 & 1 & 1 \\ 1 & 2 & 0 & 2 & 1 & 2 \\ 1 & 3 & 2 & 0 & 3 & 2 \\ 2 & 1 & 1 & 3 & 0 & 1 \\ 1 & 1 & 2 & 2 & 1 & 0 \end{pmatrix} \quad (2.27)$$

Now, the proof will move on step by step.

Step 1: Change the places of w_1 and w_5 . Now, the ordering becomes $w_5 w_2 w_3 w_4 w_1 w_6$. So, the first row of $I_{6 \times 6}$ is changed with the fifth row, and this gives A_1 . The first step ends with $A_1 D(G) A_1^T$.

$$A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (2.28)$$

Step 2: Change the places of w_2 and w_5 . Now, the ordering becomes $w_2 w_5 w_3 w_4 w_1 w_6$. So, the second row of $I_{6 \times 6}$ is changed with the fifth row, and this gives A_2 . This step ends with $A_2 A_1 D(G) A_1^T A_2^T$.

$$A_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (2.29)$$

Step 3: Change the places of w_3 and w_4 . Now, the ordering becomes $w_2 w_5 w_4 w_3 w_1 w_6$. So, the third row of $I_{6 \times 6}$ is changed with the fourth row, and this gives A_3 .

This step ends with $A_3 A_2 A_1 D(G) A_1^T A_2^T A_3^T$.

$$A_3 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (2.30)$$

Step 4: Change the places of w_4 and w_6 . Now, the ordering becomes $w_2 w_5 w_6 w_3 w_1 w_4$. So, the fourth row of $I_{6 \times 6}$ is changed with the sixth row, and this gives A_4 . This step ends with $A_4 A_3 A_2 A_1 D(G) A_1^T A_2^T A_3^T A_4^T$.

$$A_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix} \quad (2.31)$$

Applying the previous steps gives that

$$A_4 A_3 A_2 A_1 D(G) A_1^T A_2^T A_3^T A_4^T = D(G'). \quad (2.32)$$

So, it is clear that $D(G)$ and $D(G')$ are similar. By Lemma 1.4, the ordering does not change the “distance spectral radius”.

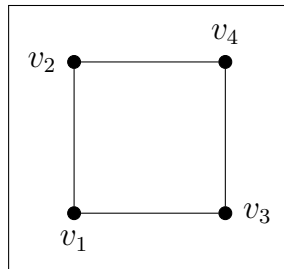


Figure 2.4: C_4 .

Example 2.5: Let C_4 be a cycle graph with the order 4 (see Figure 2.4). The distance matrix of C_4 , distance eigenvalues $(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$, and corresponding eigenvectors $\vec{X}_1, \vec{X}_2, \vec{X}_3, \vec{X}_4$ are given below.

$$D(C_4) = \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 2 & 1 \\ 1 & 2 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix} \quad (2.33)$$

$\lambda_1 = 4$ with multiplicity = 1 and $\vec{X}_1 = [1/2 \ 1/2 \ 1/2 \ 1/2]^t$.

$\lambda_2 = 0$ with multiplicity = 1 and $\vec{X}_2 = [1/2 \ -1/2 \ 1/2 \ -1/2]^t$.

$\lambda_3 = -2$ with multiplicity = 2 and $\vec{X}_3 = [1/\sqrt{2} \ 0 \ -1/\sqrt{2} \ 0]^t$ and $\vec{X}_4 = [0 \ 1/\sqrt{2} \ 0 \ -1/\sqrt{2}]^t$. Since λ_3 has multiplicity 2, $\lambda_3 = \lambda_4$ and $\vec{X}_4$ is an eigenvector of λ_3 .

From above, it can be seen that $\lambda_1 = 4$ is the “distance spectral radius”, and $\vec{X}_1 = [1/2 \ 1/2 \ 1/2 \ 1/2]^t$ is the perron vector. Entries of $\vec{X}_1$ are equal to each other i.e., $x_1 = x_2 = x_3 = x_4$. This is the only eigenvector whose all of the entries are equal to each other. There exist some automorphisms on C_4 , and the followings are some of them.

Let k be an automorphism such that $k(v_1) = v_2, k(v_2) = v_3, k(v_3) = v_4, k(v_4) = v_1$.

Let j be an automorphism such that $j(v_1) = v_3, j(v_3) = v_1, j(v_2) = v_4, j(v_4) = v_2$.

Let h be an automorphism such that $h(v_1) = v_4, h(v_4) = v_3, h(v_3) = v_2, h(v_2) = v_1$.

As it is seen above, there is a relation between automorphisms on the graph and the entries of the eigenvectors of the graph.

The following is a good example to see the relation between an automorphism on a graph and the entries of the eigenvectors of the graph.

Example 2.6: The following graph is shown in the first section as an example for

automorphism, and it is given in the following figure as a reminder. Let the ordering be $a\ b\ c\ d\ e$. Also, distance matrix $D(G_1)$, distance eigenvalues r_1, r_2, r_3, r_4, r_5 , and corresponding eigenvectors are given. The distance matrix and the eigenvectors, $\vec{X}_i = [x_a\ x_b\ x_c\ x_d\ x_e]$ where $\vec{X}_i$ denotes the eigenvector corresponding to the eigenvalue r_i , are given according to the ordering.

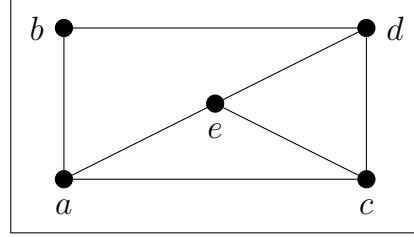


Figure 2.5: The graph G_1 in Example 2.6.

$$D(G_1) = \begin{pmatrix} 0 & 1 & 1 & 2 & 1 \\ 1 & 0 & 2 & 1 & 2 \\ 1 & 2 & 0 & 1 & 1 \\ 2 & 1 & 1 & 0 & 1 \\ 1 & 2 & 1 & 1 & 0 \end{pmatrix} \quad (2.34)$$

$r_1 \approx 5.224$ with multiplicity = 1 and $\vec{X}_1 \approx [0.43\ 0.5\ 0.44\ 0.43\ 0.44]^t$.

$r_2 \approx 0.160$ with multiplicity = 1 and $\vec{X}_2 \approx [(0.56\ -0.44\ -0.3\ 0.56\ -0.3)]^t$.

$r_3 = -1$ with multiplicity = 1 and $\vec{X}_3 = [0\ 0\ 1/\sqrt{2}\ 0\ -1/\sqrt{2}]^t$.

$r_4 = -2$ with multiplicity = 1 and $\vec{X}_4 = [1/\sqrt{2}\ 0\ 0\ -1/\sqrt{2}\ 0]^t$

$r_5 \approx -2.384$ with multiplicity = 1 and $\vec{X}_5 \approx [0.04\ 0.75\ -0.47\ 0.04\ -0.47]^t$.

Since the distance eigenvalues r_1, r_2 and r_3 are not integers, some of the components of the corresponding eigenvectors are given approximately. The main idea is to show that some of the components of the eigenvectors are equal i.e., the first components are equal to the fourth components, and the third components are equal to the fifth components. It is shown in the first chapter that there is an automorphism h for the graph G_1 where $h(a) = d, h(d) = a, h(b) = b, h(c) = e, h(e) = c$. So, for the eigenvectors $\vec{X}_1, \vec{X}_2$ and $\vec{X}_5$, it can be seen that $x_a = x_d, x_c = x_e$ and x_b equals to itself.

Lemma 2.4: [21] “ Let u and v be the vertices of a graph G . If there exists an automorphism f such that $f(u) = v$, then the corresponding components x_u and x_v of the perron vector $\vec{X}$ are equal.”

Proof: Let P be a permutation matrix with $p_{ij} = 1$ if $f(v_i) = v_j$ and $p_{ij} = 0$ otherwise where $v_i, v_j \in V(G)$. Let $\rho(G)$ be the “distance spectral radius” of G . Also, $D(G) = PD(G)P^t$ since the distance $d(i, j) = d(f(i), f(j))$, and multiplying $D(G)$ with the permutation matrices interchanges the rows and columns in the same way according to the automorphism, and this does not change $D(G)$. It is given earlier that $P^t = P^{-1}$. By the Lemma 1.4, $P\vec{X}$ is also an eigenvector of $D(G)$ for the same eigenvalue. Since $\rho(G)$ is the “distance spectral radius”, it has a unique normalized positive eigenvector.

$$\|P\vec{X}\| = (\vec{X}^t P^t P \vec{X})^{1/2} = (\vec{X}^t \vec{X})^{1/2} = \|\vec{X}\| = 1. \quad (2.35)$$

So, $P\vec{X}$ is also a normalized positive eigenvector of $\rho(G)$. Then, $P\vec{X} = \vec{X}$. The permutation matrix P interchanges the rows of $\vec{X}$. So, this proves the lemma.

Some important properties of the distance matrices are introduced. In the following chapters, some special graphs that maximizes and minimizes the “distance spectral radius” amongst some graph classes or graphs with some given properties will be introduced. Before passing to the following chapters, there is an important theorem that helps to understand the graphs that maximizes and minimizes the “distance spectral radius” better.

Theorem 2.5: “Adding an edge $e = uv$ to a graph G where $uv \notin E(G)$, decreases the distance spectral radius of the graph G . Let G' be the graph obtained by adding and edge $e = uv$ to graph G . Then, $\rho(G) > \rho(G')$.”

Proof: Adding a uv edge directly decreases the distance especially between some vertices whose shortest path between the vertices passes through the vertices u and v . This edge addition decreases some entries of the distance matrix of the graph G , but does not increase. Thus, $D(G) > D(G')$. By Lemma 1.6, $\rho(G') < \rho(G)$.

2.1. Distance Spectral Radius in Graph Classes

Extremal problems on “distance spectral radius” of graphs have been studied extensively. There are a lot of results of maximizing and minimizing the “distance spectral radius” problems on some graphs with given properties. In this section, some extremal graphs that maximizes and minimizes the “distance spectral radius” amongst trees, complements of trees, unicyclic graphs, complements of unicyclic graphs, and also, some special graphs with given properties are introduced. Moreover, every graph in this section and the sections following this section is connected since whenever the case is distance matrices, every graph has to be connected.

Let $\mathcal{F}$ be a family of graphs of order n . The following notations are given for defining the family of graphs easier.

$\max_{\text{rad}}\{\mathcal{F}\} = \max\{\rho(G) : G \in \mathcal{F}\}$ and $\max_{\text{fam}}\{\mathcal{F}\} = \{G \in \mathcal{F} : \rho(G) \geq \rho(H) \text{ for all } H \in \mathcal{F}\}$.

Also, $\min_{\text{rad}}\{\mathcal{F}\} = \min\{\rho(G) : G \in \mathcal{F}\}$ and $\min_{\text{fam}}\{\mathcal{F}\} = \{G \in \mathcal{F} : \rho(G) \leq \rho(H) \text{ for all } H \in \mathcal{F}\}$.

Ruzieh and Powers in [22] discovered the graphs in $\max_{\text{fam}}\{\mathcal{F}\}$ and $\min_{\text{fam}}\{\mathcal{F}\}$, and they are given below.

Theorem 2.6: [22] “Let $G \in \mathcal{F}$. Then, $\rho(G) \leq \rho(P_n)$.”

Theorem 2.7: [22] “Let $G \in \mathcal{F}$. Then, $\rho(G) \geq \rho(K_n)$.”

Proof: Let G be a connected graph. Adding a uv edge to the graph G where u and v are not adjacent decreases the “distance spectral radius” of G by Theorem 2.5. Applying the same procedure until there are no non-adjacent vertices, decreases the “distance spectral radius” in each step. This application ends when the graph G turns into the complete graph since all of the vertices are adjacent with each other in a complete graph. Therefore,

$$\rho(G) \geq \rho(K_n). \quad (2.36)$$

2.1.1. Trees and Complements of Trees

In this section, some extremal graphs in $\max_{\text{fam}}\{\mathcal{F}\}$ and in $\min_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees and complements of trees will be given. Also, some special graphs in $\max_{\text{fam}}\{\mathcal{F}\}$ and in $\min_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees with some properties will be shown. It is given in Theorem 2.6 that $\{P_n\} = \max_{\text{fam}}\{\mathcal{F}\}$. Since P_n is also a tree, $\{P_n\} = \max_{\text{fam}}\{\mathcal{F}\}$ if $\mathcal{F}$ consists of trees. Stevanovic and Ilic in [23] shows the graph whose “distance spectral radius” is the minimum where the graph is compared with the other graphs in the family of trees.

Theorem 2.8: [23] Let $\mathcal{F}$ consist of trees. Then,

$$\min_{\text{fam}}\{\mathcal{F}\} = \{S_n\}. \quad (2.37)$$

Stevanovic and Ilic also determined the unique tree that has the largest “distance spectral radius” among trees with a fixed maximum degree k where $3 \leq k \leq n - 2$ in [23]. For $k = 1$, there exists only one tree which is P_2 . For $k = 2$, there exists only one tree which is P_n , and for $k = n - 1$, there is only one tree which is star graph S_n .

Theorem 2.9: [23] “The broom graph (see Figure 1.9) with n vertices and a fixed maximum degree k is the unique graph that maximizes the distance spectral radius among all trees with a fixed maximum degree k where $3 \leq k \leq n - 2$.”

It is given that $\{P_n\} = \max_{\text{fam}}\{\mathcal{F}\}$. After that, it is interesting to find the unique graph that has the second largest “distance spectral radius” amongst trees, and this problem is solved by Lin and Zhang in [24].

Theorem 2.10: [24] “The graph G where 2 pendant vertices attached to one end of a path P_{n-2} has the second maximum distance spectral radius among all trees.” (See Figure 2.6).

The graph in $\max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees which are non-starlike and the graph in $\max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees which are non-caterpillar are determined by Zhou et al. in [25]. They posed a conjecture about finding the graph in $\max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees which are non-caterpillar non-starlike. This conjecture was proved later by Wang et al in [26].

Theorem 2.11: [26] “If $\mathcal{F}$ consists of non-caterpillar non-starlike trees of order $n \geq 8$, then $\max_{\text{fam}}\{\mathcal{F}\} = \{P(n; 2, n - 5)\}$ (see Figure 2.7).”

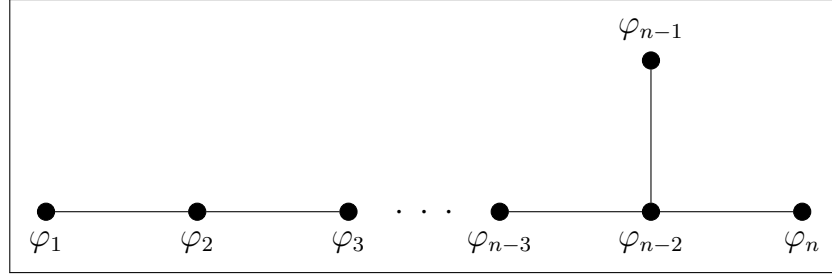


Figure 2.6: The graph G in Theorem 2.10.

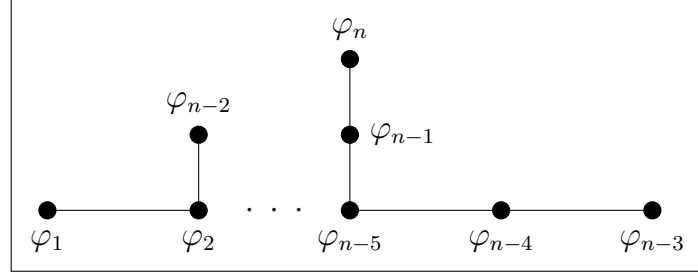


Figure 2.7: $P(n; 2, n - 5)$.

Ilic [27] conjectured that the dumbbell graph $\{D(n, \lceil \frac{n+1}{2} \rceil - l, \lfloor \frac{n+1}{2} \rfloor - l)\} = \max_{\text{fam}}\{\mathcal{F}\}$ if the graphs in $\mathcal{F}$ are trees and their matching number is l (see Figure 1.6 for $D(n; a, b)$). This conjecture is proved later by Nath and Paul [28] in 2013.

Yu et al. in [29] posed the following conjecture for finding the graph in $\max_{\text{fam}}\{\mathcal{F}\}$ where the graphs in $\mathcal{F}$ have m pendant vertices.

Conjecture 2.12: [29] $\{D(n, \lceil \frac{m}{2} \rceil, \lfloor \frac{m}{2} \rfloor)\} = \max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ has m pendant vertices.

Nath and Paul found the unique graph in $\max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees with m pendant vertices in [28].

Theorem 2.13: [28] The dumbbell graph $\{D(n, \lceil \frac{m}{2} \rceil, \lfloor \frac{m}{2} \rfloor)\} = \max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees with m pendant vertices.

It is known that the “distance spectral radius” of graphs attains its maximum if the graph is a tree.

Lin and Zhou in [30] posed the following theorem which shows the graph in $\max_{\text{fam}}\{\mathcal{F}\}$ if the graphs in $\mathcal{F}$ has the fixed number of vertices with maximum degree 3.

Theorem 2.14: [30] “ $T(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)$ is the unique graph that maximizes the distance spectral radius among trees with the order n and with k vertices of maximum degree 3, where $1 \leq k \leq \lfloor \frac{n-2}{2} \rfloor$.” (see Figure 1.7 for $T(n, i, j)$).

Lin and Zhou also determined in [31] that the graph in $\max_{\text{fam}}\{\mathcal{F}\}$ if $\mathcal{F}$ consists of trees, and the vertices with degree 2 of the graphs in $\mathcal{F}$ are given.

Theorem 2.15: [31] “If $n - m$ is even, then $\{T(n, \lfloor \frac{n-2-m}{4} \rfloor, \lceil \frac{n-2-m}{4} \rceil)\} = \max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of trees with m vertices of degree 2 where $0 \leq m \leq n - 4$.”

Lin et al. in [32] showed the graphs with the maximum and the minimum “distance spectral radius” in a graph family of connected complements of trees. Theorems 2.16 and 2.17 show these graphs.

Theorem 2.16: [32] If $\mathcal{F}$ consists of connected complements of trees, then $\overline{T_{1,n-3}} = \max_{\text{fam}}\{\mathcal{F}\}$ (see Figure 1.10 for $T_{p,q}$). In other words,

$$\rho(\overline{T_{1,n-3}}) \geq \rho(\overline{T}) \quad (2.38)$$

where $T \in \mathcal{F}$ $T \not\cong K_{1,n-1}$.

Theorem 2.17: [32] If $\mathcal{F}$ consists of connected complements of trees, then $\overline{P_n} = \min_{\text{fam}}\{\mathcal{F}\}$.

For trees with $n = 4$, there are 2 non-isomorphic graphs which are P_4 and S_4 with the distance spectral radii $\rho(P_4) \approx 5.1623$ and $\rho(S_4) \approx 4.6457$. The complement of P_4 , $\overline{P_4}$, is again a P_4 i.e., $\overline{P_4} \cong P_4$. The complement of a star graph is not connected since there is a vertex $v \in S_n$ which is attached to every other vertices in S_n . So, v is not adjacent to any other vertices in $\overline{S_n}$. Thus, v becomes isolated, and this yields that $\overline{S_n}$ is disconnected. Thus, S_n will not be compared.

For trees with $n = 5$, there are 3 non-isomorphic graphs which are S_5 , P_5 and T in Figure 2.8. Since the complement of S_5 is not connected, $\overline{S_5}$ is not compared. Thus, comparing the complements of P_5 and T , $\rho(\overline{T}) > \rho(\overline{P_5})$.

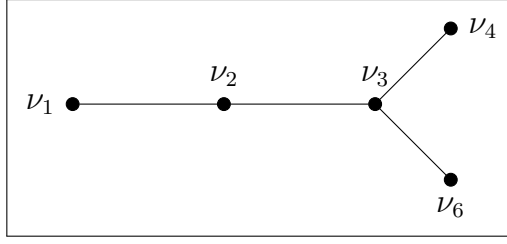


Figure 2.8: The graph T in Theorem 2.17.

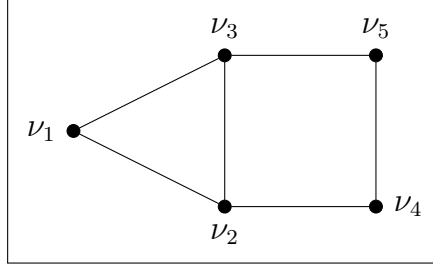


Figure 2.9: The complement $\overline{T}$ of the graph in Figure 2.8.

2.1.2. Unicyclic Graphs

In this section, some extremal graphs that maximize and minimize the “distance spectral radius” among unicyclic graphs and their complements will be given.

Theorem 2.18: [33] “Let $G \in C(n, l)$ be a graph. G has the maximum distance spectral radius if $G \cong S(a, b; c)$, where $a + b = l$ and $c = n - 2l - 1$.”

$C(n, 1) \in U_n$. Thus, according to Theorem 2.18, putting $l = 1$ gives that either $a = 1$ and $b = 0$ or $a = 0$ and $b = 1$. This yields that $\{S(1, 0; n - 3)\} = \max_{\text{fam}}\{C(n, 1)\}$. Thus, $\{S(1, 0; n - 3)\} = \max_{\text{fam}}\{\mathcal{F}\}$ if the graphs in $\mathcal{F}$ are unicyclic graphs.

Qin et al. in [34] studied the “distance spectral radius” of complements of unicyclic graphs, and posed the following.

Theorem 2.19: [34] “Let $G \in U_n$ where $n \geq 5$. If $\overline{G}$ is connected, then $\rho(\overline{G}) \leq \rho(\overline{U_{n,4,1}})$.

$\rho(\overline{G}) = \rho(\overline{U_{n,4,1}})$ if and only if $\overline{G} \cong \overline{U_{n,4,1}}$ (see Figure 2.10).”

Yu et al. in [35] showed the graphs in $\min_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of U_n .

Theorem 2.20: [35] Let $G \in U_n$ where $4 \leq n$.

(i) For $n = 4, 5$, $C_n = \min_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of U_n .

(ii) For $n \geq 6$, $G = \min_{\text{fam}} \{\mathcal{F}\}$ where G is the graph that an edge e attached to any two leaves of the star graph S_n if $\mathcal{F}$ consists of unicyclic graphs.

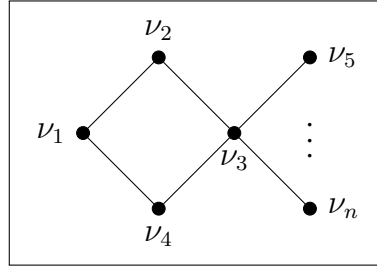


Figure 2.10: $U_{n,4,1}$.

3. BICYCLIC GRAPHS

In this chapter, the unique graph in $\max_{\text{fam}} \{B_n\}$ is investigated. Also, the unique graphs with minimum and second minimum “distance spectral radius” are given. Firstly, to understand the class of bicyclic graphs, it is necessary to identify the bicyclic graphs. The following lemma shows that bicyclic graphs can be divided into two subclasses.

Lemma 3.1: If a graph is bicyclic, then it is either a cactus graph with two cycles or it contains a theta graph.

Proof: Let G be a bicyclic graph. Every bicyclic graph is obtained from a unicyclic graph by adding a new edge. Let G be obtained from a unicyclic graph H by adding a new edge $e \notin E(H)$ with endvertices u and v . Let C be the unique cycle in H . Now, the proof continues with several cases.

Case 1 : $u, v \in V(C)$. Let P^1 and P^2 be two shortest u, v paths in H . Now, the paths P^1 , P^2 and the edge e form a theta graph $\theta(1; |E(P^1)|; |E(P^2)|)$ (see Figure 3.1). Case 2 : $u \in V(C)$ and $v \notin V(C)$.

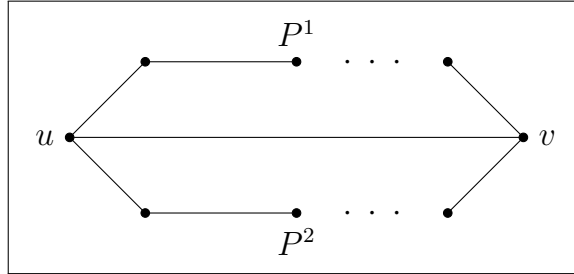


Figure 3.1: Theta Graph for Case 1.

Let v' be a vertex of C which is closest to the vertex $v \in H$. Now, this case is considered in two subcases. The first is when $v' = u$, and the second is when $v' \neq u$.

Subcase 2.1 : $v' = u$. Let P^1 be the unique path between vertex u and vertex v . Adding a new edge $e \notin E(H)$ with endvertices u and v forms a cycle C' including P^1 . So, this gives that two cycles C and C' . Since $u \in C$ and $u \in C'$, then $C \cap C' = u$. Thus, G is a cactus (see Figure 3.2). Subcase 2.2 : $v' \neq u$. There exist two paths in C from vertex u to v' which are $P^1 = up_1p_2v'$ and $P^2 = uq_1q_2v'$.

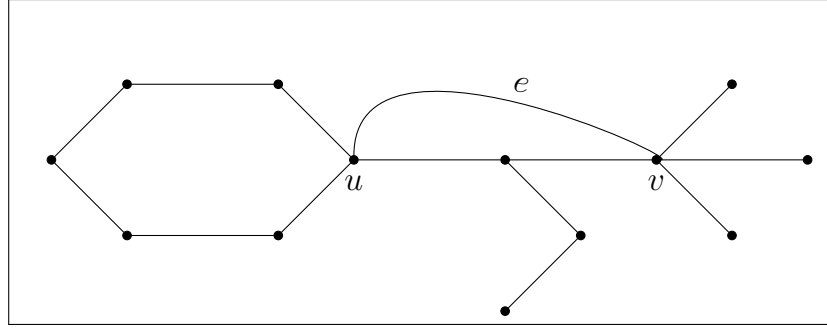


Figure 3.2: Cactus Graph for Case 2.1.

Since there exists a path between vertices v and v' , adding a new edge $e \notin E(H)$ with the endvertices u and v forms another path, P^3 , from vertex u to vertex v' . Now, the paths P^1 , P^2 and P^3 form a theta graph $\theta(|E(P^1)|; |E(P^2)|; |E(P^3)|)$ (see Figure 3.3). Case 3 : $u \notin V(C)$, $v \notin V(C)$. Let P be a shortest $u - v$ path in H . This case

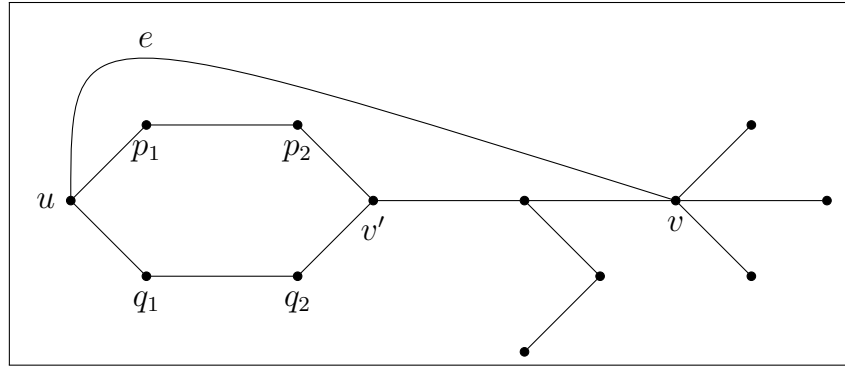


Figure 3.3: Graph in Subcase 2.2.

is considered in three subcases. The first is when P contains only one vertex of C , the second is when P contains more than one vertex of C , and the third is when P does not contain any vertices of C .

Subcase 3.1 : Let P contain only one vertex of C , and call it v' . Adding a new edge $e \notin E(H)$ with the endvertices u and v forms a new cycle C' which includes v' . Then, since $C \cap C' = v'$, it can be said that G includes two cycles with one common vertex. Thus, G is a cactus.

Subcase 3.2 : If P contains more than one vertex of C , then P is passing through some part of cycle C . Let u' and v' be the vertices contained in C , and let P pass through these vertices. Also, let u' be the closest to the vertex u and v' be the closest vertex to the vertex v . Since $u', v' \in V(C)$, there exist two paths P^1 and P^2

connecting u' and v' . Also, since $u, u', v, v' \in V(P)$, there exist $u - u'$ and $v - v'$ paths. Adding a new edge $e \notin E(H)$ with the endvertices u and v forms another path P^3 between the vertices u' and v' . Thus, the paths P^1 , P^2 and P^3 form a theta graph $\theta(|E(P^1)|; |E(P^2)|; |E(P^3)|)$.

Subcase 3.3 : If P does not contain any vertices of C , then it is clear that adding a new edge $e \notin E(H)$ with the endvertices u and v forms another cycle C' which has no common vertex with the cycle C . Thus, G is a cactus.

3.1. Maximal Distance Spectral Radius

In this section, the unique graph that maximizes the “distance spectral radius” is given. It is given earlier that if a graph is a bicyclic graph, then it is either a cactus with two cycles or a graph which includes a theta graph in Lemma 3.1. If the graph is a cactus with two cycles, then either $\{S(1, 1; n - 5)\} = \max_{\text{fam}}\{\mathcal{F}\}$ or $\{S(2, 0; n - 5)\} = \max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of cactus graphs with two cycles by Theorem 2.18. Paul in [36] determined the bicyclic graph that maximizes the “distance spectral radius” amongst B_n which includes a θ -graph as an induced subgraph.

Theorem 3.2: [36] “The graph which contains a $\theta(2; 1; 2)$ graph as an induced subgraph and a path graph P_{n-4} attached one of the vertices of $\theta(2; 1; 2)$ with degree 2 is the graph that maximizes the distance spectral radius among all bicyclic graphs with n vertices which contain a θ -graph as an induced subgraph.”

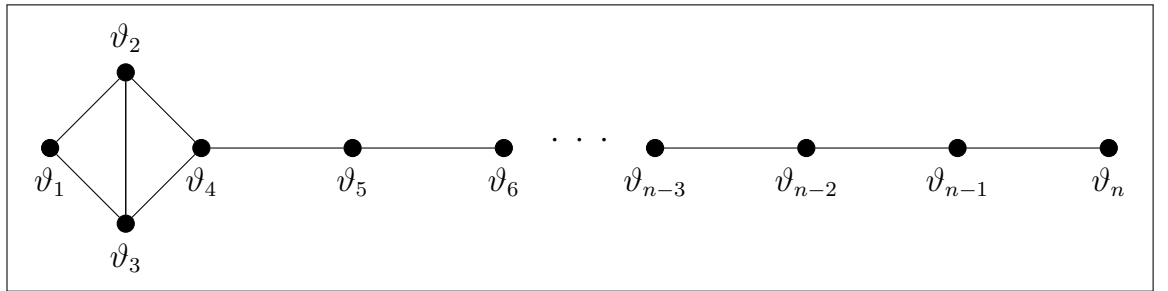


Figure 3.4: G_1 .

Since comparing the “distance spectral radii” of the graphs $S(1, 1; n - 5)$ and $S(2, 0; n - 5)$ is difficult, the “distance spectral radius” of the graph in Theorem 3.2 is compared with the “distance spectral radii” of the saw graphs $S(1, 1; n - 5)$ and $S(2, 0; n - 5)$ separately.

Lemma 3.3: Let G_1 be the graph in Figure 3.4, and G_2 be the saw graph $S(1, 1; n - 5)$ (see Figure 3.5). Then $\rho(G_1) > \rho(G_2)$.

Proof: Let $\vec{X}^t = [x_1 \ x_2 \ x_3 \ \dots \ x_n]$ be the perron vector of the graph G_2 . So,

$$\rho(G_1) - \rho(G_2) \geq \vec{X}^t (D(G_1) - D(G_2)) \vec{X} \quad (3.1)$$

$$= \vec{X}^t \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & \cdots & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & -1 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & \cdots & 1 & 0 & 0 \end{pmatrix} \vec{X} \quad (3.2)$$

$$= 2[x_n(x_1 + x_3 + \dots + x_{n-2}) - x_2(x_4 + x_5 + \dots + x_{n-1})]. \quad (3.3)$$

v_1 and v_2 in G_2 are twin vertices since all of their neighbors are the same. So, the corresponding components of perron vector x_1 and x_2 are the same by Lemma 2.2 i.e., $x_1 = x_2$. Also, v_{n-1} and v_n are twin vertices, so $x_{n-1} = x_n$. In G_2 , there exists an automorphism f such that $f(v_1) = v_n$, $f(v_2) = v_{n-1}$, $f(v_3) = v_{n-2}$, $f(v_4) = v_{n-3}$, $\dots$, $f(v_{\lfloor n/2 \rfloor}) = v_{\lceil n/2 \rceil}$, $\dots$, $f(v_n) = v_1$. By Lemma 2.4, $x_1 = x_n$. Thus, x_1, x_2, x_{n-1}, x_n are all equal.

Since x_1, x_2, x_{n-1}, x_n are equal,

$$\vec{X}^t (D(G_1) - D(G_2)) \vec{X} = 2[x_2(x_1 + x_3 - x_{n-1})] \quad (3.4)$$

$$= 2x_2x_3 > 0. \quad (3.5)$$

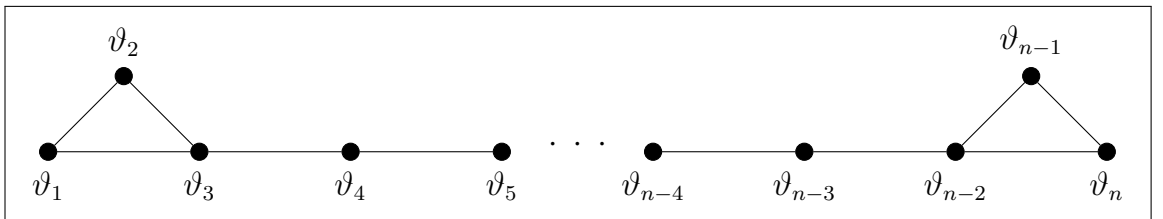


Figure 3.5: $G_2 = S(1, 1, n - 5)$.

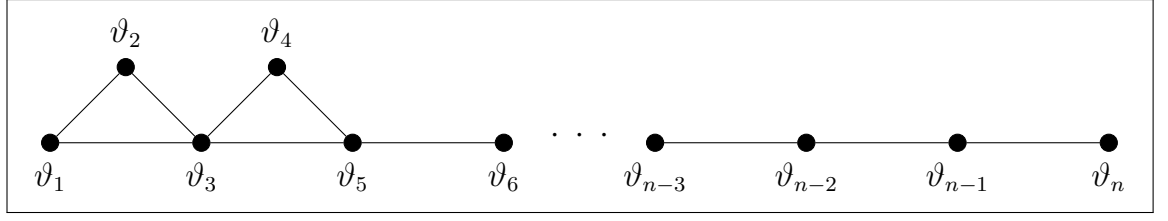


Figure 3.6: $G_3 = S(2, 0; n - 5)$.

Lemma 3.4: Let G_1 be the graph (see Figure 3.4), and G_3 be the saw graph $S(2, 0; n-5)$ (see Figure 3.6). Then $\rho(G_1) > \rho(G_3)$.

Proof: This lemma is investigated in 3 cases. It is better to start with when $n = 5$ since $|G_3| \geq 5$. In this case, $G_3 = S(2, 0; 0)$ (see Figure 3.7). Then, the proof continues with cases for $n = 6$, and for $n \geq 7$. The distance spectral radii of the graphs for $n = 5$ and $n = 6$ are easy to find by using a computer.

Case 1 : For $n = 5$,

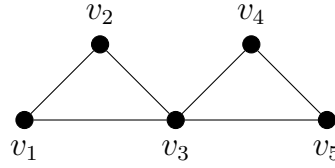


Figure 3.7: $G_3 = S(2, 0; 0)$.

$$D(S(2, 0; 0)) = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 \\ 1 & 0 & 1 & 2 & 2 \\ 1 & 1 & 0 & 1 & 1 \\ 2 & 2 & 1 & 0 & 1 \\ 2 & 2 & 1 & 1 & 0 \end{pmatrix} \quad (3.6)$$

Based on computer results,

$\rho(S(2, 0; 0)) \approx 5,7016$, and $\rho(G_1) \approx 6,2161$ when $|G_1| = 5$.

So, $\rho(G_1) > \rho(S(2, 0; 0))$.

Case 2 : For $n = 6$, $G_3 = S(2, 0; 1)$.

$$D(S(2, 0; 1)) = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 & 3 \\ 1 & 0 & 1 & 2 & 2 & 3 \\ 1 & 1 & 0 & 1 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 & 2 \\ 2 & 2 & 1 & 1 & 0 & 1 \\ 3 & 3 & 2 & 2 & 1 & 0 \end{pmatrix} \quad (3.7)$$

By using a computer, calculating the eigenvalues of the distance matrix $D(S(2, 0; 1))$ gives that $\rho(S(2, 0; 1)) \approx 8, 5936$. When $|G_1| = 6$, $\rho(G_1) \approx 9, 6964$. It is clear that $\rho(G_1) > \rho(S(2, 0; 1))$.

Case 3 : For $n \geq 7$,

Let $\vec{X}^t = [x_1 \ x_2 \ x_3 \ \dots \ x_n]$ be the perren vector of the graph G_3 . So,

$$\rho(G_1) - \rho(G_3) \geq \vec{X}^t (D(G_1) - D(G_3)) \vec{X} \quad (3.8)$$

$$= \vec{X}^t \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & \dots & 1 & 1 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & \dots & 1 & 1 & 1 \\ 0 & -1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} \vec{X} \quad (3.9)$$

$$= 2[(x_1 + x_3)(x_5 + \dots + x_n) - x_2 x_4]. \quad (3.10)$$

Since $\vartheta_1 = \vartheta_2$ are twin vertices, $x_1 = x_2$ by Lemma 2.2. Thus, the latter becomes

$$2[(x_1 + x_3)(-x_4 + x_5 + x_6 + \dots + x_n) + x_3 x_4]. \quad (3.11)$$

It suffices to show that $-x_4 + x_5 + x_6 + x_7 > 0$ because x_i 's are all positive.

Using the eigenequation $\rho(G_3)x_i = \sum_{\vartheta_j \in V(G_3)} d_{(i,j)}x_j$, the proof is formed as follows

$$\rho(G_3)x_4 = 2x_1 + 2x_2 + x_3 + x_5 + 2x_6 + \cdots + (n-4)x_n \quad (3.12)$$

$$\rho(G_3)x_5 = 2x_1 + 2x_2 + x_3 + x_4 + x_6 + \cdots + (n-5)x_n \quad (3.13)$$

$$\rho(G_3)x_6 = 3x_1 + 3x_2 + 2x_3 + 2x_4 + x_5 + x_7 + \cdots + (n-6)x_n \quad (3.14)$$

$$\rho(G_3)x_7 = 4x_1 + 4x_2 + 3x_3 + 3x_4 + 2x_5 + x_6 + \cdots + (n-7)x_n. \quad (3.15)$$

Adding the latter equations side by side gives the following

(i) If $n = 7$, then

$$\rho(G_3)(-x_4 + x_5 + x_6 + x_7) = 7x_1 + 7x_2 + 5x_3 + 6x_4 + 2x_5. \quad (3.16)$$

(ii) If $n \geq 7$,

$$\begin{aligned} \rho(G_3)(-x_4 + x_5 + x_6 + x_7) &= 7x_1 + 7x_2 + 5x_3 + 6x_4 + 2x_5 \\ &\quad + 3x_8 + \cdots + (2n-14)x_n > 0. \end{aligned} \quad (3.17)$$

This yields that

$$\rho(G_3)(-x_4 + x_5 + x_6 + \dots + x_n) > 0. \quad (3.18)$$

Hence, in each case, it is proven that $\rho(G_1) > \rho(G_3)$.

Theorem 3.5: $\{G_1\} = \max_{\text{fam}}\{B_n\}$.

Proof: Let $G \in B_n$. Then, G is either cactus with two cycles i.e., $G \in C(n, 2)$ or G contains a theta graph by Lemma 3.1. So, $\{S(1, 1; n-5)\} = \max_{\text{fam}}\{C(n, 2)\}$ or $\{S(2, 0; n-5)\} = \max_{\text{fam}}\{C(n, 2)\}$ by Theorem 2.18. Let $G_2 = S(1, 1; n-5)$ (see Figure 3.5) and $G_3 = S(2, 0; n-5)$ (see Figure 3.6). Comparing these two graphs G_2 and G_3 with G_1 (see Figure 3.4) will give a result since it is known that $\{G_1\} = \max_{\text{fam}}\{\mathcal{F}\}$ where $\mathcal{F}$ consists of B_n containing a θ -graph as an induced subgraph by Theorem 3.2. In Lemmas 3.3 and 3.4, the graph G_1 is compared with the graphs G_2 and G_3 . By the results of these lemmas, it is shown that $\{G_1\} = \max_{\text{fam}}\{B_n\}$.

3.2. Minimal Distance Spectral Radius

In this part, an interesting result that is done by Xing and Zhou in [21] is introduced. Their result gives the graph in $\min_{\text{fam}}\{B_n\}$ and the graph that has the second smallest “distance spectral radius” in B_n .

Theorem 3.6: [21] Let $G \in B_n$ where $5 \leq n$.

(i) *For $n = 5$, $\theta(1; 2; 3) < \rho(B_5^1) < \rho(B_5^2) < \rho(G)$ where $G \not\cong (B_5^1) \not\cong (B_5^2) \not\cong \theta(1; 2; 3)$.*

(ii) *For $n = 6$, $\theta(2; 2; 3) < \rho(B_6^1) < \rho(B_6^2) < \rho(G)$ where $G \not\cong (B_6^1) \not\cong (B_6^2) \not\cong \theta(2; 2; 3)$.*

(iii) *For $n \geq 7$, $\rho(B_n^1) < \rho(B_n^2) < \rho(G)$ where $G \not\cong (B_n^1) \not\cong (B_n^2)$.*

4. CONCLUSION

In the section of bicyclic graphs, the graph in $\max_{\text{fam}}\{B_n\}$ is determined. Also, the graph in $\min_{\text{fam}}\{B_n\}$ and the graph that has the second smallest “distance spectral radius” among bicyclic graphs are given. In this section, the graph in $\max_{\text{fam}}\{\overline{B}_n\}$ is investigated. Since graphs in B_n have $n + 1$ edges, their complements have $\binom{n}{2} - n - 1$ edges. Some results for complements of bicyclic graphs with 6, 7 and 8 vertices are found based on computer calculations. There are 22 non-isomorphic graphs for 6 vertices and 8 edges, and 95 non-isomorphic graphs with 7 vertices and 13 edges. There are 234 non-isomorphic graphs for 8 vertices. For the graphs $\{\overline{G}_1\} = \max_{\text{fam}}\{\overline{B}_6\}$, $\{\overline{G}_2\} = \max_{\text{fam}}\{\overline{B}_7\}$, $\{\overline{G}_3\} = \max_{\text{fam}}\{\overline{B}_8\}$, see Figures 4.1, 4.3, 4.5, respectively.

Taking the complements of $\overline{G}_1$, $\overline{G}_2$ and $\overline{G}_3$, gives G_1 , G_2 and G_3 , respectively.

For $n = 6$ and $m = 8$: It is found that $\overline{G}_1$ which has 8 edges, and $\{\overline{G}_1\} = \max_{\text{fam}}\{\overline{B}_6\}$ (see Figures 4.1, 4.2).

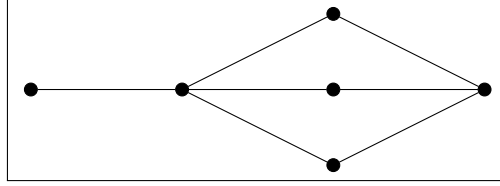


Figure 4.1: G_1 .

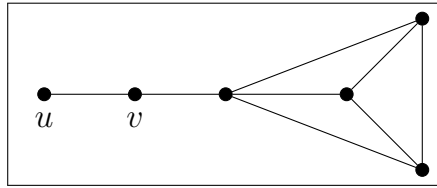


Figure 4.2: The graph $\overline{G}_1$ and $\rho(\overline{G}_1) = 8.6279$.

For $n = 7$ and $m = 13$ edges: It is found that $\{\overline{G}_2\} = \max_{\text{fam}}\{\overline{B}_7\}$ (see Figures 4.3, 4.4).

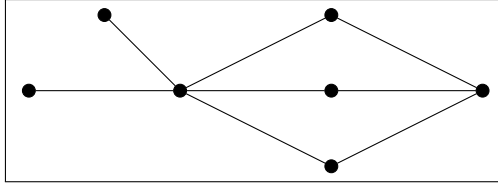


Figure 4.3: G_2 .

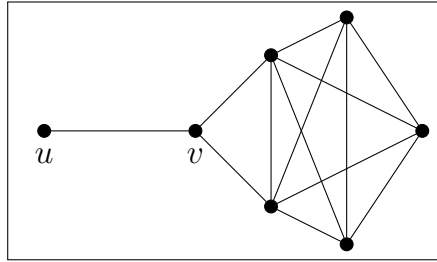


Figure 4.4: The graph $\overline{G_2}$ and $\rho(\overline{G_2}) = 9.5415$.

For $n = 8$ and $m = 19$: Comparing the complements of bicyclic graphs with the order 8, $\{\overline{G_3}\} = \max_{\text{fam}}\{\overline{B_8}\}$ (see Figures 4.5, 4.6). Now, see the graphs G_1 ,

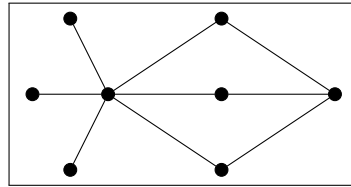


Figure 4.5: The graph G_3 .

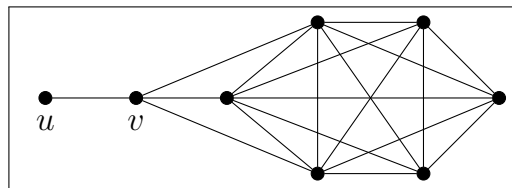


Figure 4.6: The graph $\overline{G_3}$ and $\rho(\overline{G_3}) = 10.4726$.

G_2 and G_3 in Figures 4.2, 4.4, 4.6 respectively. It can be seen that for $n = 6, 7, 8$, the complements of connected bicyclic graphs which include a $\theta(2; 2; 2)$ as an induced subgraph and $n - 5$ pendant vertices attached to one of the vertices with degree 3 of $\theta(2; 2; 2)$ maximize the “distance spectral radius” in $\overline{B_6}, \overline{B_7}, \overline{B_8}$, respectively.

Conjecture 4.1: $\{G_0\} = \max_{\text{fam}}\{\overline{B_n}\}$ where G_0 has a K_{n-2} and a vertex v which is attached to $n - 5$ vertices of the K_{n-2} and a pendant vertex u attached to v .

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BIOGRAPHY

Ahmet Tugay KUZU was born on 24th of November 1993 in Istanbul, TURKEY. He received his bachelor of science degree in mathematics at Middle East Technical University in 2018. Then, he started his master's education in mathematics at the Graduate School of Natural and Applied Sciences in Gebze Technical University in 2018. He has been working as a part-time mathematics teacher in different private schools.