

Spectral radii of matrices associated with graphs

by

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Abstract

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The spectral radius of a graph is defined as the largest absolute value of the eigenvalues of a matrix associated with the graph. In this thesis, we study the spectral radii of the adjacency matrix, the distance matrix and a matrix related to the distance matrix associated to simple graphs.

For the adjacency matrix, we determine the spectral radii of some classes of graphs. We prove that the spectral radius can be used to estimate the number of walks and closed walks in the graph. Furthermore, we present bounds on the spectral radius in terms of some graph parameters. We then proceed to show that the greedy tree, the Volkmann tree and the extended star graph maximise the spectral radius among all trees with prescribed degree sequence, maximum degree and number of leaves respectively.

We also collect results on the spectral radii of the distance matrices of some classes of graphs. We investigate a matrix that is related to the distance matrix where we proved that the greedy tree, the Volkmann tree and the extended star graph maximise its spectral radius among all trees with prescribed degree sequence, maximum degree and number of leaves respectively.

Uittreksel

Spektraalradiusse van matrikse wat met grafieke geassosieer word

(“Spectral radii of matrices associated with graphs”)

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Die spektraalradius van 'n grafiek word gedefinieer as die grootste absolute waarde van die eiewaardes van 'n matriks wat met die grafiek geassosieer word. In hierdie tesis bestudeer ons die spektraalradiusse van die nodusmatriks, die afstandsmatriks en 'n matriks wat aan die afstandsmatrix verwant is, vir eenvoudige grafieke.

Vir die nodusmatriks bepaal ons die spektraalradiusse van sommige klasse van grafieke. Ons bewys dat die spektraalradius gebruik kan word om die aantal wandelings of geslote wandelings in 'n grafiek af te skat. Verder gee ons grense vir die spektraalradius in terme van sekere grafiekparameters. Ons wys ook dat die gulsige boom, die Volkmann-boom en die uitgebreide stergrafiek die spektraalradius maksimeer onderskeidelik in die versameling van bome met voorgeskrewe graadry, maksimaalgraad en aantal blare. Ons versamel ook verskillende resultate oor die spektraalradiusse van die afstandsmatrikse van sommige klasse van grafieke. Ons ondersoek 'n matriks wat verwant is aan die afstandsmatriks en ons bewys dat die gulsige boom, die Volkmann-boom en die uitgebreide stergrafiek sy spektraalradius

maksimeer, ook onderskeidelik in die versameling van bome met voorgeskrewe graadry, maksimaalgraad en aantal blare.

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Dedications

To my dearest mother, Florence Dumoga Collymore

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Nomenclature

Linear Algebra

- $\mathbb{R}^{n \times n}$ The set of all $n \times n$ matrices with real entries.
- \mathbb{R}^n The set of all vectors of size n with real entries.
- J A square matrix with all entries equal to one.
- O A square matrix with all entries equal to zero.
- $\mathbf{1}$ A vector with all entries equal to one.
- $\mathbf{0}$ A vector with all entries equal to zero.
- I An identity matrix.
- $\Phi_A(\lambda)$ The characteristic polynomial of the matrix A .
- $\det(A)$ The determinant of the matrix A .

Graph Theory

- $V(G)$ The set of vertices of a graph G .
- $E(G)$ The set of edges of a graph G .
- $|V(G)|$ The order, the number of vertices, of the graph G .
- $|E(G)|$ The size, the number of edges, of the graph G .

Chapter 1

Introduction

Spectral graph theory is concerned with the relationship between graph properties and the spectrum of matrices associated with graphs. These include the adjacency matrix, the distance matrix, the signed and unsigned Laplacian.

Our research is mainly focussed on the spectral radius, which is the largest of the absolute values of the eigenvalues of a given matrix associated with a graph. The matrices we shall be discussing include the adjacency matrix, the distance matrix and a matrix related to the distance matrix. All these matrices are real and symmetric so have real eigenvalues. We will see that the spectral radius is actually the largest eigenvalue.

The aim of this thesis is to come up with explicit formulas to easily compute the spectral radii of these matrices associated to some classes of simple graphs. Our next goal is to investigate the relationship between some graph parameters and the spectral radius. Thirdly, we shall determine upper and lower bounds for the spectral radii of different matrices and also determine the extremal graphs, i.e., graphs that minimise or maximise the spectral radius in a given class of graphs.

In Chapter 2, we review some facts and concepts about symmetric matrices and simple graphs that will aid us in achieving our goal. In Chapter 3, we determine the spectral radii of the adjacency matrices associated to some classes of simple graphs, namely the complete graphs, paths, cycles, regular graphs, semi-regular graphs and the extended star graphs. We show that the spectral radius provides information on the growth of the number of walks and closed walks in a graph and can also be used as an upper bound for the chromatic number of a graph. We also provide upper and lower

bounds on the spectral radius in terms of the order, size, number of walks and the number of pendant vertices in the graph. On the problem of determining extremal graphs, we prove that the greedy tree, the Volkmann tree and the extended star graph maximise the spectral radius among all trees with prescribed degree sequence, maximum degree and number of leaves respectively. Motivated by this results, we study the extended star graph and obtain an upper bound on the spectral radius of trees in terms of the number of leaves. Finally, in Chapter 4, we also determine the spectral radii of the distance matrices of vertex-transitive graphs and complete bipartite graphs. In addition, we provide lower bounds on the distance spectral radius of a graph in terms of the Wiener index and the order. We proceed to show that a caterpillar maximises the distance spectral radius among all trees a given degree sequence. We study a matrix related to the distance matrix and prove that the greedy tree, the Volkmann tree and the extended star graph maximise its spectral radius among all trees with prescribed degree sequence, maximum degree and number of leaves respectively.

Chapter 2

Basic notions

This chapter presents some basic definitions and theorems on graphs and matrices. Specifically, simple undirected graphs (no loops or multiple edges) and symmetric matrices with real entries. It is important to note that some of these results also hold for graphs and matrices in general. Throughout this work we will let $\mathbb{R}^{n \times n}$ denote the set of all $n \times n$ matrices with real entries, and \mathbb{R}^n represents the set of all vectors of size n with real entries.

2.1 Some definitions and results in Linear Algebra

Definition 2.1.1. Let $A \in \mathbb{R}^{n \times n}$, I be the n -dimensional identity matrix, λ a scalar and \mathbf{x} an $n \times 1$ non-zero vector. We call λ an eigenvalue of A and \mathbf{x} its corresponding eigenvector if it satisfies the equation

$$A\mathbf{x} = \lambda\mathbf{x}, \quad (2.1)$$

which is equivalent to

$$(A - \lambda I)\mathbf{x} = \mathbf{0} \quad \text{or} \quad (\lambda I - A)\mathbf{x} = \mathbf{0}. \quad (2.2)$$

The set of all the eigenvalues of the matrix A is referred to as the spectrum of A . Also, the set of all eigenvectors of A corresponding to an eigenvalue λ is called the eigenspace of λ . The dimension of the eigenspace of λ is referred to as the geometric multiplicity of λ .

We define the null space of A as the set $\{\mathbf{x} : A\mathbf{x} = \mathbf{0}\}$. Its dimension is referred to as the nullity of A . Therefore, we can deduce from equation

(2.2) that the geometric multiplicity of λ is equal to the nullity of $A - \lambda I$ or $\lambda I - A$. In particular, if zero is an eigenvalue of A then its geometric multiplicity is exactly the nullity of A .

The dimension of the column or row space of A is called the rank of A . It is well known that the nullity of A plus its rank equals n (the size of A).

Proposition 2.1.2 ([20], p. 14). *For any matrix $A \in \mathbb{R}^{n \times n}$, the following statements are equivalent:*

1. A is singular;
2. The determinant of A is zero;
3. A is not invertible;
4. The rank of A is less than n ;
5. Zero is an eigenvalue of A .

Note that if A is non-singular then its rank is equal to n , and hence it does not have zero as an eigenvalue (thus the nullity of A is zero).

Now considering equation (2.2), if we multiply both sides by the inverse of the matrix $\lambda I - A$ (if it exists) then we get $\mathbf{x} = \mathbf{0}$ which contradicts the definition of eigenvectors. Hence the matrix $\lambda I - A$ is not invertible. It then follows that all possible values of λ such that $\det(\lambda I - A) = 0$ form the spectrum of A . The equation

$$\det(\lambda I - A) = 0 \tag{2.3}$$

is called the characteristic equation of A . The left hand side of equation (2.3) is a polynomial of degree n and it is called the characteristic polynomial of A . We will denote it by $\Phi_A(\lambda)$.

The roots of $\Phi_A(\lambda)$ are the eigenvalues of A and they are all not necessarily distinct. So if we let $\lambda_1, \lambda_2, \dots, \lambda_k$ be the distinct eigenvalues of A , then we can write its characteristic polynomial as

$$\begin{aligned} \Phi_A(\lambda) &= \det(\lambda I - A) \\ &= (\lambda - \lambda_1)^{m_1} (\lambda - \lambda_2)^{m_2} \cdots (\lambda - \lambda_k)^{m_k}, \end{aligned} \tag{2.4}$$

where $m_i, 1 \leq i \leq k$, is the number of times the eigenvalue λ_i appears as root of $\Phi_A(\lambda)$. The exponent m_i is called the algebraic multiplicity of λ_i . Note that

$$\sum_{i=1}^k m_i = n,$$

and also that the eigenvalues might be complex. Furthermore, the geometric multiplicity of an eigenvalue λ_i is always less than or equal to its algebraic multiplicity [32, p. 295]. Since there are n roots of $\Phi_A(\lambda)$, it is obvious that the number of non-zero eigenvalues of A is equal to its rank.

If we set $\lambda = 0$ in equation (2.4), then we get

$$\det(A) = (\lambda_1)^{m_1} (\lambda_2)^{m_2} \cdots (\lambda_k)^{m_k}.$$

Thus, the product of the eigenvalues (with algebraic multiplicities) is equal to the determinant of the matrix. This also justifies the fact that zero is an eigenvalue of a singular matrix.

Now that the notions of eigenvalues and eigenvectors have been introduced, we can now talk about the spectral radius of a given matrix.

Definition 2.1.3. Let $A \in \mathbb{R}^{n \times n}$ and $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A . We define the spectral radius of A , which we shall denote by $\rho(A)$, as

$$\rho(A) = \max\{|\lambda_i| : 1 \leq i \leq n\}.$$

By definition, the spectral radius of a matrix is not necessarily its largest positive eigenvalue (even if positive eigenvalues exist). However, it is clear that if all its eigenvalues are non-negative or positive reals then the largest eigenvalue is the spectral radius.

Example 2.1.4. Consider the matrix $A \in \mathbb{R}^{4 \times 4}$ given by

$$A = \begin{pmatrix} 0 & 2 & 1 & 1 \\ 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 \\ 1 & 1 & 2 & 0 \end{pmatrix}.$$

Then, its characteristic polynomial is given by

$$\begin{aligned}\Phi_A(\lambda) &= \begin{vmatrix} \lambda & -2 & -1 & -1 \\ -2 & \lambda & -1 & -1 \\ -1 & -1 & \lambda & -2 \\ -1 & -1 & -2 & \lambda \end{vmatrix} \\ &= \lambda^4 - 12\lambda^2 - 16\lambda \\ &= \lambda(\lambda - 4)(\lambda + 2)^2.\end{aligned}$$

Therefore, the eigenvalues of A are $-2, 0, 4$ and clearly its spectral radius $\rho(A)$ is equal to 4.

Now, we state and prove some well known results about the spectrum of some matrices which are relevant to our work.

Theorem 2.1.5. *Suppose the eigenvalues of $A \in \mathbb{R}^{n \times n}$ are λ_i ($i = 1, \dots, n$), then for a scalar α , the eigenvalues of the matrix $A \pm \alpha I$ are $\lambda_i \pm \alpha$ ($i = 1, \dots, n$).*

Proof. Let the eigenvalues of the matrix A be λ_i ($i = 1, \dots, n$), and their corresponding eigenvectors be \mathbf{x}_i ($i = 1, \dots, n$). Then by definition we know that $A\mathbf{x}_i = \lambda_i\mathbf{x}_i$. Now, for a scalar α and the identity matrix I we have that

$$\begin{aligned}(A \pm \alpha I)\mathbf{x}_i &= A\mathbf{x}_i \pm \alpha I\mathbf{x}_i \\ &= \lambda_i\mathbf{x}_i \pm \alpha\mathbf{x}_i \\ &= (\lambda_i \pm \alpha)\mathbf{x}_i.\end{aligned}$$

This shows that $\lambda_i \pm \alpha$ are eigenvalues of $A \pm \alpha I$. Note that every non-zero vector is an eigenvector of the identity matrix I . \square

A set of vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$ is said to be linearly dependent if there exist some scalars c_1, c_2, \dots, c_k , not all equal to zero, such that

$$c_1\mathbf{x}_1 + c_2\mathbf{x}_2 + \dots + c_k\mathbf{x}_k = \mathbf{0}. \quad (2.5)$$

Linearly dependent vectors have the property that at least one of them can be expressed as a linear combination of the others since not all of the scalars are equal to zero. However, if the only way for equation (2.5) to be satisfied is when all the scalars are equal to zero then the vectors are said to be linearly independent.

Two vectors \mathbf{x} and \mathbf{y} are said to be orthogonal if $\mathbf{x}^T \mathbf{y} = \mathbf{y}^T \mathbf{x} = 0$. We therefore refer to a set of vectors as an orthogonal set if any pair of its vectors is orthogonal. Moreover, if a set of vectors S is orthogonal and each vector in S has unit length, thus $\mathbf{x}^T \mathbf{x} = 1$ for $\mathbf{x} \in S$, then S is called orthonormal. Furthermore, if we let $\mathbf{x}_1, \dots, \mathbf{x}_n$ be linearly independent vectors then by the Gram-Schmidt orthogonalization method we can obtain orthonormal vectors $\mathbf{q}_1, \dots, \mathbf{q}_n$, [32, p. 223-224]. Thus, for $i, j \in \{1, \dots, n\}$,

$$\mathbf{q}_i^T \mathbf{q}_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

In the context of matrices, we say a matrix is orthogonal if its column or row vectors form an orthonormal set. By definition, it is clear that if Q is an orthogonal matrix then $Q^T Q = Q Q^T = I$. So $Q^T = Q^{-1}$.

Theorem 2.1.6 ([32], p. 290). *If the eigenvalues of a matrix are all distinct then their corresponding eigenvectors are linearly independent.*

Proof. Let the distinct eigenvalues of a matrix A be $\lambda_1, \lambda_2, \dots, \lambda_n$ and their corresponding eigenvectors be $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$. We assume that the eigenvectors are linearly dependent. Then by definition of linear independent vectors we have that

$$c_1 \mathbf{x}_1 + c_2 \mathbf{x}_2 + \dots + c_n \mathbf{x}_n = \mathbf{0}, \quad (2.6)$$

where c_1, c_2, \dots, c_n , are scalars and not all them are zero. Multiplying both sides of equation (2.6) by $\prod_{i=2}^n (I\lambda_i - A)$ and applying the definition of eigenvalues, i.e., $A\mathbf{x}_i = \lambda_i \mathbf{x}_i$, we get

$$\begin{aligned} c_1 \prod_{i=2}^n (I\lambda_i - A) \mathbf{x}_1 &= \mathbf{0} \\ c_1 \prod_{i=2}^n (\lambda_i - \lambda_1) \mathbf{x}_1 &= \mathbf{0} \end{aligned} \quad (2.7)$$

Equation (2.7) implies that $c_1 = 0$. Following a similar approach, we can show that the scalars $c_k, k = 2, \dots, n$, are also zero, by multiplying both sides of equation (2.6) by

$$\prod_{\substack{i=1 \\ i \neq k}}^n (I\lambda_i - A).$$

Since all the scalars are zero, this contradicts our assumption. So the eigenvectors are linearly independent. \square

Definition 2.1.7. An $n \times n$ matrix A is symmetric if $A = A^T$, where A^T is the transpose of A . This implies that its ij -th entry a_{ij} is equal to its ji -th entry a_{ji} , for $1 \leq i \leq n$ and $1 \leq j \leq n$.

Theorem 2.1.8 ([32], p. 320). The eigenvalues of a real symmetric matrix are real.

Proof. Consider $A \in \mathbb{R}^{n \times n}$ and assume that λ is a complex eigenvalue of A with eigenvector \mathbf{x} . Note that components of \mathbf{x} can be complex. By definition, we know that

$$A\mathbf{x} = \lambda\mathbf{x}. \quad (2.8)$$

Taking the conjugate transpose of both side yields

$$\overline{\mathbf{x}}^T A^T = \overline{\lambda} \overline{\mathbf{x}}^T. \quad (2.9)$$

Left multiplying both sides of equation (2.8) by $\overline{\mathbf{x}}^T$ and right multiplying both sides of equation (2.9) by \mathbf{x} yields

$$\overline{\mathbf{x}}^T A\mathbf{x} = \lambda \overline{\mathbf{x}}^T \mathbf{x} \quad (2.10)$$

$$\overline{\mathbf{x}}^T A^T \mathbf{x} = \overline{\lambda} \overline{\mathbf{x}}^T \mathbf{x} \quad (2.11)$$

Since A is symmetric, we can deduce from equations (2.10) and (2.11) that $\lambda \overline{\mathbf{x}}^T \mathbf{x} = \overline{\lambda} \overline{\mathbf{x}}^T \mathbf{x}$ implying that $\lambda = \overline{\lambda}$. This proves that λ must be a real number.

□

Theorem 2.1.9 ([32], p. 321). The eigenvectors corresponding to the eigenvalues of a real symmetric matrix are orthogonal and hence can be made orthonormal.

Proof. Let λ_1 and λ_2 be two distinct eigenvalues of a real symmetric matrix A , and let their corresponding eigenvectors be \mathbf{x} and \mathbf{y} respectively. We know that

$$\begin{aligned} A\mathbf{x} &= \lambda_1\mathbf{x} \\ \mathbf{y}^T A\mathbf{x} &= \lambda_1\mathbf{y}^T \mathbf{x} \\ (A^T \mathbf{y})^T \mathbf{x} &= \lambda_1\mathbf{y}^T \mathbf{x}. \end{aligned}$$

Since A is symmetric, we get

$$\begin{aligned} (A\mathbf{y})^T \mathbf{x} &= \lambda_1 \mathbf{y}^T \mathbf{x} \\ (\lambda_2 \mathbf{y})^T \mathbf{x} &= \lambda_1 \mathbf{y}^T \mathbf{x} \\ (\lambda_2 - \lambda_1) \mathbf{y}^T \mathbf{x} &= 0, \\ \Rightarrow \mathbf{y}^T \mathbf{x} &= 0 \end{aligned}$$

since λ_1 and λ_2 are distinct. Therefore, \mathbf{x} and \mathbf{y} are orthogonal. So, if all the eigenvalues of A are distinct then we know that their corresponding eigenvectors are mutually orthogonal. Now, we shall consider eigenvalues with algebraic multiplicity of more than one.

Suppose we let λ_1 be an eigenvalue of a symmetric matrix $A \in \mathbb{R}^{n \times n}$ with algebraic multiplicity $m_1 \geq 2$. We want to show that its eigenspace contains m_1 orthonormal eigenvectors. Let $U \in \mathbb{R}^{n \times n}$ be an orthogonal matrix whose columns are the vectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, where \mathbf{x}_1 is an eigenvector corresponding to λ_1 . For simplicity, we let X be a submatrix obtained from U by deleting the eigenvector \mathbf{x}_1 . So, if we let $C = U^T A U$ we get

$$C = \begin{pmatrix} \lambda_1 \mathbf{x}_1^T \mathbf{x} & \mathbf{x}_1^T A X \\ \lambda_1 X^T \mathbf{x}_1 & X^T A X \end{pmatrix}.$$

Since U is orthogonal and A is symmetric we have $\lambda_1 \mathbf{x}_1^T \mathbf{x} = \lambda_1$, $\lambda_1 X^T \mathbf{x}_1 = \mathbf{0}$ and $\mathbf{x}_1^T A X = (A^T \mathbf{x}_1)^T X = (A \mathbf{x}_1)^T X = \lambda_1 \mathbf{x}_1^T X = \mathbf{0}$. Also, $U^T = U^{-1}$. So we can say that A and C are similar and hence have the same characteristic polynomial and eigenvalues. Therefore,

$$\begin{aligned} C &= \begin{pmatrix} \lambda_1 & 0 \\ 0 & X^T A X \end{pmatrix}, \\ \Phi_C(\lambda) &= \det(\lambda I - C) \\ &= (\lambda - \lambda_1) \det(\lambda I - X^T A X). \end{aligned}$$

Now, if $m_1 \geq 2$, then we can still obtain the factor $(\lambda - \lambda_1)$ from the polynomial $\det(\lambda I - X^T A X)$, hence $\det(\lambda_1 I - X^T A X) = 0$. This implies that the rank of the matrix $\lambda_1 I - C$ is at most $n - 2$ so its nullity is at least 2. Precisely, if $m_1 = 2$ then the nullity of $\lambda_1 I - C$ is 2 and hence there exist two linearly independent eigenvectors in the eigenspace of λ_1 . However, if $m_1 = 3$ then we know that there are at least two linearly independent

eigenvectors, namely $x_1 = y_1, y_2$ in the eigenspace of λ_1 . So if we let our orthogonal matrix U be defined by $U = (y_1 y_2 Y)$, where $Y = (y_3 \cdots y_n)$, and repeat the same idea then we can show that the eigenspace of λ_1 contains 3 orthonormal eigenvectors. The process continues similarly for all $m_1 \geq 2$. We have shown that if an eigenvalue λ of A has algebraic multiplicity of $m_1 \geq 2$ then there exist m_1 linearly independent eigenvectors in its eigenspace, which by Gram-Schmidt orthogonalization method can be made orthogonal. Note that it is not possible to get more than m_1 orthonormal eigenvectors corresponding to λ since there are only n orthonormal eigenvectors for $A \in \mathbb{R}^{n \times n}$. \square

It then follows that each eigenvalue of a symmetric matrix has its algebraic multiplicity equal to its geometric multiplicity. So if λ is an eigenvalue of a symmetric matrix then we shall refer to its algebraic multiplicity or geometric multiplicity as the multiplicity of λ , for the sake of simplicity.

A diagonal matrix is a matrix with all non-diagonal entries equal to zero. We will let $\text{diag}(d_1, d_2, \dots, d_n)$ denote an $n \times n$ diagonal matrix with diagonal entries d_1, d_2, \dots, d_n . The diagonal entries are all not necessarily non-zero. It is an important fact that the eigenvalues of a diagonal matrix are exactly its diagonal entries. Therefore, if one can decompose or reduce a given square matrix to a diagonal matrix, then the spectrum of the matrix can easily be obtained.

Definition 2.1.10. *Two matrices A, B are said to be similar if there exists an invertible matrix Q such that $A = Q^{-1}BQ$.*

Similar matrices have the same characteristic polynomials and hence the same set of eigenvalues [32, p. 343-345].

Definition 2.1.11. *A matrix M is diagonalisable if it is similar to a diagonal matrix D .*

The procedure described in the proof of Theorem 2.1.9 shows that every symmetric matrix can be diagonalised. In particular, if we let the n orthonormal eigenvectors of an $n \times n$ symmetric matrix A be x_1, x_2, \dots, x_n and their respective eigenvalues be $\lambda_1, \lambda_2, \dots, \lambda_n$, then we can form an orthogonal matrix $M = (x_1 x_2 \cdots x_n)$ such that

$$D = M^T A M,$$

where $D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$.

Definition 2.1.12. A Jordan block $J_{\lambda, m}$ is a $m \times m$ matrix whose diagonal entries are equal to λ , superdiagonal entries are equal to 1 and all other entries are 0, i.e.,

$$J_{\lambda, m} = \begin{pmatrix} \lambda & 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & \ddots & \ddots & 1 \\ 0 & \cdots & \cdots & 0 & \lambda \end{pmatrix}.$$

A Jordan normal form J is a block matrix whose block diagonal consists of Jordan blocks and all other entries are 0. It is nearly a diagonal matrix.

There is a generalisation of diagonalisability which states that every square matrix is similar to a matrix in a Jordan normal form J . In particular, if an $n \times n$ matrix A has k linearly independent eigenvectors, then it is similar to a matrix in a Jordan normal form J with k Jordan blocks, i.e.,

$$J = \begin{pmatrix} J_{\lambda, m_1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & J_{\lambda, m_k} \end{pmatrix},$$

such that $\sum_{i=1}^k m_i = n$ and the λ 's form the set of eigenvalues of A [32, p. 346-347].

Let us denote the trace of a matrix A by $\text{tr}(A)$. Now, suppose that P is an $n \times m$ matrix and Q an $m \times n$ matrix. Then

$$\begin{aligned} \text{tr}(PQ) &= \sum_{i=1}^n \sum_{j=1}^m p_{ij} q_{ji} \\ &= \sum_{j=1}^m \sum_{i=1}^n q_{ji} p_{ij} \\ &= \text{tr}(QP). \end{aligned}$$

Therefore, considering an $n \times n$ matrix A and an invertible matrix M such

that $A = MJM^{-1}$, we have that

$$\begin{aligned}\operatorname{tr}(A) &= \operatorname{tr}(MJM^{-1}) \\ &= \operatorname{tr}(M^{-1}MJ) \\ &= \operatorname{tr}(J) \\ &= \sum_{i=1}^n \lambda_i,\end{aligned}$$

where $\lambda_i, i = 1, \dots, n$, form the set of eigenvalues of A . We then obtain the fact that the sum of the eigenvalues of a matrix is equal to its trace.

Theorem 2.1.13 ([32], p. 296). *Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of a matrix A . Then for $k \geq 2$, the eigenvalues of A^k are $\lambda_1^k, \lambda_2^k, \dots, \lambda_n^k$.*

Proof. From the generalisation of diagonalisability, we know that for an $n \times n$ matrix A , there exist an invertible matrix such that $J = M^{-1}AM$, where J is a matrix in a Jordan normal form. Therefore

$$\begin{aligned}A^k &= AA \cdots A \\ &= MJM^{-1}MJM^{-1} \cdots MJM^{-1} \\ &= MJ^kM^{-1} \\ &= M \begin{pmatrix} \lambda_1^k & * & \cdots & * \\ 0 & \lambda_2^k & \cdots & * \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^k \end{pmatrix} M^{-1}.\end{aligned}$$

J^k as shown above is an upper triangular matrix with $*$ denoting real values. We therefore obtain the eigenvalues of A^k to be $\lambda_1^k, \lambda_2^k, \dots, \lambda_n^k$. \square

Now, we introduce a representation for the largest and smallest eigenvalues of a symmetric matrix and also some bounds on its spectral radius.

Definition 2.1.14. *The Rayleigh quotient of an $n \times n$ matrix A on a nonzero vector \mathbf{x} , denoted by $R_A(\mathbf{x})$, is given by*

$$R_A(\mathbf{x}) = \frac{\langle A\mathbf{x}, \mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle} = \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}},$$

where $\langle \cdot, \cdot \rangle$ is the scalar product. Let a_{ij} denote the ij -th entry of A and x_i denote the i -th entry of the vector \mathbf{x} . Then

$$\mathbf{x}^T A \mathbf{x} = \sum_{i,j=1,\dots,n} a_{ij} x_i x_j.$$

Theorem 2.1.15 ([3], p. 37). *Suppose A is an $n \times n$ symmetric matrix whose eigenvalues are given as $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ and \mathbf{x} denotes a non-zero vector. Then we have*

$$\lambda_n \leq \min_{\mathbf{x} \neq 0} R_A(\mathbf{x}) \leq \max_{\mathbf{x} \neq 0} R_A(\mathbf{x}) \leq \lambda_1.$$

It is important to note that the maximum or minimum value is attained when the vector \mathbf{x} is the respective eigenvector.

Proof. We let Q be an orthogonal matrix that diagonalises A . That is $A = Q^T D Q$, where $D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. Note that since Q is an orthogonal matrix $Q^T = Q^{-1}$, so $Q^T Q = Q Q^T = I$.

Now, for a vector $\mathbf{x} \neq 0$, and its entries given by x_1, x_2, \dots, x_n , we have

$$\begin{aligned} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} &= \frac{\mathbf{x}^T Q^T D Q \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \\ &= \frac{(Q \mathbf{x})^T D (Q \mathbf{x})}{\mathbf{x}^T \mathbf{x}}. \end{aligned}$$

If we let $Q \mathbf{x} = (y_1, y_2, \dots, y_n)^T$ then we get

$$\begin{aligned} (Q \mathbf{x})^T D (Q \mathbf{x}) &= (y_1 \ y_2 \ \dots \ y_n) \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \lambda_n \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \\ &= \lambda_1 y_1^2 + \lambda_2 y_2^2 + \dots + \lambda_n y_n^2. \end{aligned}$$

Also,

$$\begin{aligned} \mathbf{x}^T \mathbf{x} &= \mathbf{x}^T Q^T Q \mathbf{x} \\ &= (Q \mathbf{x})^T (Q \mathbf{x}) \\ &= y_1^2 + y_2^2 + \dots + y_n^2. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} &= \frac{\lambda_1 y_1^2 + \lambda_2 y_2^2 + \dots + \lambda_n y_n^2}{y_1^2 + y_2^2 + \dots + y_n^2} \\ &\leq \frac{\lambda_1 (y_1^2 + y_2^2 + \dots + y_n^2)}{y_1^2 + y_2^2 + \dots + y_n^2} \\ &= \lambda_1. \end{aligned}$$

But if \mathbf{x} is an eigenvector corresponding to λ_1 then we have

$$\frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \frac{\mathbf{x}^T (\lambda_1 \mathbf{x})}{\mathbf{x}^T \mathbf{x}} = \lambda_1.$$

Also,

$$\begin{aligned} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} &\geq \frac{\lambda_n (y_1^2 + y_2^2 + \cdots + y_n^2)}{y_1^2 + y_2^2 + \cdots + y_n^2} \\ &= \lambda_n \end{aligned}$$

for every vector $\mathbf{x} \neq 0$, and if \mathbf{x} is an eigenvector corresponding to λ_n then we have

$$\frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \frac{\mathbf{x}^T (\lambda_n \mathbf{x})}{\mathbf{x}^T \mathbf{x}} = \lambda_n.$$

□

Theorem 2.1.16 (Cauchy-Schwarz inequality,[20], p. 15). *For all vectors \mathbf{x} and \mathbf{y} of an inner product space, the following inequality holds:*

$$|\langle \mathbf{x}, \mathbf{y} \rangle|^2 \leq \langle \mathbf{x}, \mathbf{x} \rangle \cdot \langle \mathbf{y}, \mathbf{y} \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product (scalar product) and $|\langle \cdot, \cdot \rangle|$ is the absolute value of the inner product.

Theorem 2.1.17. *Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix; then its spectral radius satisfies*

$$\rho(A) \leq \sqrt{n \cdot \text{tr}(A^2)}.$$

Proof. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A . So by the Cauchy-Schwarz inequality, if we consider the vectors $\mathbf{x} = (\lambda_1, \dots, \lambda_n)$ and $\mathbf{y} = \mathbf{1}$, then we get

$$\left[\sum_{i=1}^n |\lambda_i| \right]^2 \leq n \sum_{i=1}^n \lambda_i^2.$$

But we know from Theorem 2.1.13 that the eigenvalues of A^2 are $\lambda_i^2, 1 \leq i \leq n$ and hence the sum gives its trace. Therefore

$$\rho(A) \leq \sum_{i=1}^n |\lambda_i| \leq \sqrt{n \cdot \text{tr}(A^2)}.$$

This completes the proof. □

Definition 2.1.18. An $n \times n$ matrix A is reducible if and only if it contains a zero submatrix whose row indices i_1, i_2, \dots, i_s , and respectively column indices j_1, j_2, \dots, j_t are such that

$$\{i_1, i_2, \dots, i_s\} \cap \{j_1, j_2, \dots, j_t\} = \{\}$$

and

$$\{i_1, i_2, \dots, i_s\} \cup \{j_1, j_2, \dots, j_t\} = \{1, 2, \dots, n\}.$$

A matrix that is not reducible is called irreducible.

Theorem 2.1.19 (Perron-Frobenius Theorem, [25], p. 673). *If a matrix M is irreducible and has non-negative entries, then its spectral radius $\rho(M)$ is an eigenvalue of multiplicity one. It corresponds to a unique positive unit eigenvector \mathbf{x} that we call the Perron vector of M .*

In this work, we shall use the Perron-Frobenius Theorem as a tool in computing the spectral radii of some of the matrices associated to graphs. In particular, if a positive vector is an eigenvector then its corresponding positive eigenvalue is the spectral radius.

Theorem 2.1.20. *Suppose A and B are two irreducible matrices with non-negative entries. Let a_{ij} and b_{ij} denote the ij -th entry of A and B respectively. If $a_{ij} \geq b_{ij}$ for all $i, j = 1, \dots, n$, then*

$$\rho(A) > \rho(B),$$

where $\rho(A)$ and $\rho(B)$ are the respective spectral radii of A and B .

Proof. Assume that $a_{ij} \geq b_{ij}$ for all $i, j = 1, \dots, n$. Let \mathbf{f} be a unit Perron vector of B . So

$$R_A(\mathbf{f}) - R_B(\mathbf{f}) = \sum_{i,j=1,\dots,n} (a_{ij} - b_{ij})f(i)f(j).$$

By our assumption and the fact that \mathbf{f} is positive from the Perron-Frobenius Theorem, we have

$$R_A(\mathbf{f}) - R_B(\mathbf{f}) \geq 0.$$

Note that $R_A(\mathbf{f}) - R_B(\mathbf{f}) = 0$ if $a_{ij} = b_{ij}$ for all $i, j = 1, \dots, n$, which would imply that $A = B$. Therefore, by Theorem 2.1.15 and the Perron-Frobenius

Theorem we have

$$\begin{aligned} R_A(\mathbf{f}) - R_B(\mathbf{f}) &> 0, \\ \rho(A) &\geq R_A(\mathbf{f}) > R_B(\mathbf{f}) = \rho(B), \\ &\Rightarrow \rho(A) > \rho(B). \end{aligned}$$

□

2.2 Some definitions and results in Graph Theory

A graph is an ordered pair $G = (V(G), E(G))$, where $V(G)$ is a finite set of vertices of G and $E(G)$ is a set of 2-element subsets of $V(G)$ called edges of G . The order and size of G are $|V(G)|$ and $|E(G)|$ respectively. For the sake of simplicity, an edge (u, v) will be denoted by uv . Suppose $u, v \in V(G)$ and $uv \in E(G)$. Then we say u and v are adjacent.

Graphs as defined above are also called simple graphs: they do not have loops or multiple edges, see Figure 2.1. In this thesis, we will only be discussing simple graphs.

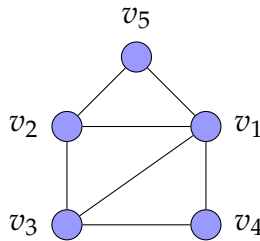


Figure 2.1: A simple graph G .

Let G be a simple graph of order n and size m . The total number of possible edges in G is equal to the number of ways of choosing a subset of 2 elements from the vertex set $V(G)$ which is given by $\binom{n}{2} = \frac{n(n-1)}{2}$. Therefore, we have

$$m \leq \frac{n(n-1)}{2}.$$

Equality holds when each vertex is adjacent to all the other vertices. Such graphs are called complete graphs K_n .

The neighbourhood of a vertex u in G , denoted by $N(u)$, is the set of all vertices in G that are adjacent to u . The cardinality of $N(u)$ is called the degree of u , which we shall denote by $d(u)$. A vertex with degree 1 is called a pendant vertex. Among all the degrees of the vertices in a graph G , we shall let δ_G and Δ_G represent the minimum and maximum degree in G respectively. Suppose G is a simple graph of order n with $V(G) = \{v_1, \dots, v_n\}$ and $d(v_i)$ denotes the degree of vertex v_i , $1 \leq i \leq n$. Then we call $(d(v_1), \dots, d(v_n))$ the degree sequence of G . We can assume that $d(v_1) \geq d(v_2) \geq \dots \geq d(v_n)$.

Theorem 2.2.1. *In a graph, the sum of all the degrees of its vertices is equal to twice the cardinality of its edge set.*

Proof. In a graph G , let $e \in E(G)$ such that $e = uv$, where $u, v \in V(G)$. When we sum the degrees of the vertices, the edge e is counted twice. Once in the degree of u and once in the degree of v . This holds for all the edges in G . Hence the result follows. \square

Example 2.2.2. *Considering the graph G in Figure 2.1, $|E(G)| = 7$ and the degree sequence of G is given by $(4, 3, 3, 2, 2)$, which sums up to 14. Also, $\delta_G = 2$ and $\Delta_G = 4$.*

Definition 2.2.3. *Suppose G is a simple graph of order n with degree sequence $(d(v_1), \dots, d(v_n))$. Then the average degree, denoted by \mathcal{D} , is given by*

$$\mathcal{D} = \frac{1}{n} \sum_{i=1}^n d(v_i).$$

By Theorem 2.2.1 we can redefine the average degree of a graph G of order n and size m as

$$\mathcal{D} = \frac{2m}{n}.$$

Definition 2.2.4. *A graph H is a subgraph of a graph G , written as $H \subseteq G$, if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.*

Definition 2.2.5. *A path P_n is a simple graph of order n with vertex set $V(P_n) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(P_n) = \{v_i v_{i+1} : i = 1, 2, \dots, n-1\}$.*

Definition 2.2.6. *An n -cycle C_n is a simple graph of order n with vertex set $V(C_n) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(C_n) = \{v_i v_{i+1} : i = 1, 2, \dots, n-1\} \cup \{v_1 v_n\}$. Each vertex has degree 2.*

Cycles contain two distinct paths between any pair of its vertices. The length of a path (or cycle) is the number of edges in the path (or cycle). We let $P(u, v)$ denote a path from a vertex u to a vertex v in a graph G .

Definition 2.2.7. *The distance $d_G(u, v)$ between two vertices u and v is the length of the shortest path $P(u, v)$ in a graph G .*

Definition 2.2.8. *A graph G is connected if there exists a path between any pair of its vertices. Otherwise, G is disconnected.*

Figure 2.1 is an example of a connected graph. A graph with no cycle is called an acyclic graph. A connected acyclic graph is called a tree. A forest is a simple graph whose connected components are trees. In particular, if a forest has only one connected component then it is called a tree. We call a pendent vertex in a tree or a forest a leaf. A rooted tree is a tree in which one of its vertices is marked and referred to as the root r of the tree. In a rooted tree T , we call the distance from a vertex u to its root r the height of the vertex, denoted by $h_T(u)$.

In a tree, any two vertices are connected by only one path since there are no cycles. Later in this thesis, we shall talk about the spectral radius of trees. Meanwhile, we introduce the following well known results about trees which we will use later in this thesis.

Proposition 2.2.9. *Let T be a tree of order n and size m . Then we have $m = n - 1$.*

Proof. We prove this Proposition by induction on the order n of T . For our base case, we let $n = 1$ and it is clear that T has size $m = 0$. Now, we assume it holds for all trees of order $k < n$. Let the order of T be n . Let $uv \in E(T)$. We remove the edge uv from T to obtain two connected components T_1 and T_2 , which are also trees. So by our hypothesis, we have $|E(T_1)| = |V(T_1)| - 1$ and $|E(T_2)| = |V(T_2)| - 1$. Therefore,

$$\begin{aligned} |E(T)| &= |E(T_1)| + |E(T_2)| + 1 \\ &= |V(T_1)| - 1 + |V(T_2)| - 1 + 1 \\ &= |V(T)| - 1. \end{aligned}$$

□

The following proposition talks about the degree sequence of trees.

Proposition 2.2.10. *A sequence (d_1, d_2, \dots, d_n) of positive integers is a degree sequence of a tree of order n if and only if*

$$\sum_{i=1}^n d_i = 2(n-1). \quad (2.12)$$

Proof. Let (d_1, d_2, \dots, d_n) be a degree sequence of a tree of order n . From Proposition 2.2.9 and Theorem 2.2.1, we have

$$\sum_{i=1}^n d_i = 2(n-1).$$

This proves the first part of Proposition 2.2.10.

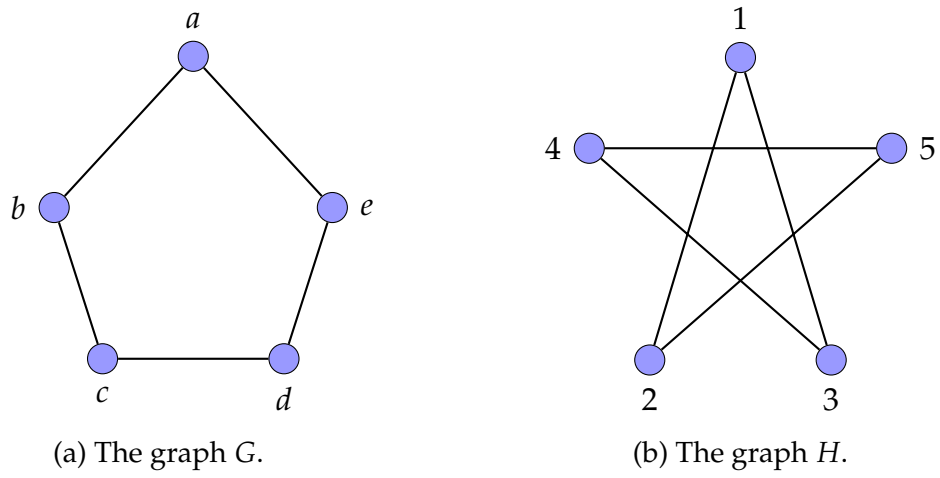
Now, we need to show that if (d_1, d_2, \dots, d_n) satisfies equation (2.12), then it is a degree sequence of a tree of order n . We prove this by induction on n . For $n = 2$, we have $(1, 1)$ to be the only positive sequence satisfying equation (2.12). This sequence is the degree sequence of a tree of order 2. Now, we assume our assertion holds for $k \leq n$ and prove that it also holds for $n + 1$. If we let $(d_1, d_2, \dots, d_{n+1})$ be a sequence satisfying equation (2.12), then there exist i, j such that $d_i > 1$ and $d_j = 1$. Otherwise, the sum $d_1 + \dots + d_{n+1}$ would be at least $2(n+1) > 2n$ or equal to $n+1 < 2n$. By deleting d_j and subtracting 1 from d_i , we obtain a sequence of n positive integers satisfying equation (2.12). Then by our hypothesis, we have a degree sequence for a tree T of order n . By attaching a pendant vertex to the vertex u in T with degree $d_i - 1$, we obtain another tree of order $n + 1$ with degree sequence $(d_1, d_2, \dots, d_{n+1})$. This completes the proof. \square

Definition 2.2.11. *Two graphs G and H are said to be isomorphic, written as $G \cong H$, if there is a bijection $f : V(G) \rightarrow V(H)$ which preserves adjacency and non-adjacency. Thus, $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$.*

Example 2.2.12. *In Figure 2.2, we define f by $f(a) = 1, f(b) = 2, f(c) = 5, f(d) = 4$ and $f(e) = 3$. It is easy to check that $ab \mapsto 12, bc \mapsto 25, cd \mapsto 54, de \mapsto 43, ea \mapsto 31$, where*

$$E(G) = \{ab, bc, cd, de, ea\} \quad \text{and} \quad E(H) = \{12, 25, 54, 43, 31\}.$$

The main theme of this thesis is to represent the properties of a given simple undirected graph G by a matrix M and investigate the spectral radius of M . Two graph properties, namely adjacency and distances among the vertices of a graph, will play an important role.

Figure 2.2: Isomorphic graphs G and H .

Chapter 3

The Adjacency Matrix

3.1 Introduction

Let G be a simple graph of order n with vertex set $V(G) = \{v_1, \dots, v_n\}$. The adjacency matrix of G denoted by A_G is a symmetric matrix whose entries are

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The rows and columns of A_G are associated with the vertices of the graph G . A_G is symmetric hence its eigenvalues are real. These eigenvalues sum up to zero (since the trace is equal to zero). Throughout this section, we shall denote the spectral radius of the adjacency matrix of a graph G by $\rho(G)$. For the sake of simplicity, we will call $\rho(G)$ the spectral radius of G .

It is important to note that relabelling the vertices of G do not affect its spectral radius. In particular, if we let G_1 be the resulting graph after relabelling the vertices of the graph G , then there exists a permutation matrix P such that $A_{G_1} = P^T A_G P$, implying that A_{G_1} is similar to A_G . Therefore, A_G and A_{G_1} have the same spectrum and hence same spectral radius. An example of the adjacency matrix A_G of a graph G is shown in Figure 3.1.

By the definition of an adjacency matrix, we have that the sum of the entries of a row or a column associated with a vertex gives us the degree of the vertex. Suppose A_G is the adjacency matrix of a graph G of order n and size m . Then by Theorem 2.2.1, we have

$$\mathbf{1}^T A_G \mathbf{1} = \sum_{i=1}^n d(v_i) = 2m,$$

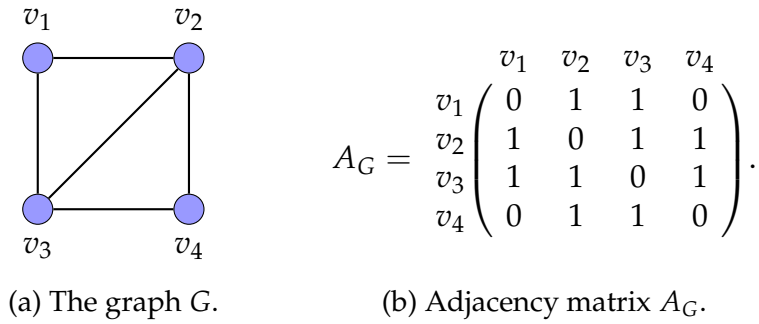


Figure 3.1: A graph and its adjacency matrix.

where $d(v_i)$ is the degree of the vertex v_i .

Proposition 3.1.1 ([12], p.15). *The adjacency matrix A_G of a graph G is irreducible if G is connected.*

Proof. Let G be a connected graph of order n with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and whose adjacency matrix A_G is reducible. Recall that the rows and columns of A_G are associated with the vertices of the graph G . Then by the definition of reducible matrices, $V(G)$ can be partitioned into two non-empty subsets V_1 and V_2 such that $a_{ij} = 0$ if $i \in V_1$ and $j \in V_2$ (or vice versa). It then follows that there is no edge connecting the vertices in V_1 to those in V_2 hence G has two disjoint components, which contradicts our assumption that G is connected. \square

By definition and Proposition 3.1.1, the adjacency matrix satisfies the conditions of the Perron-Frobenius Theorem hence we can deduce that its spectral radius $\rho(G)$ is actually the largest positive eigenvalue, i.e., the index of G . Suppose we let λ be an eigenvalue of A_G and \mathbf{x} its corresponding eigenvector. Then by definition we have

$$\lambda x_u = \sum_{uv \in E(G)} x_v,$$

where x_v is the component of the non-zero vector \mathbf{x} corresponding to the vertex v .

Proposition 3.1.2 ([13], p. 2). *Let Δ_G be the maximum degree of a simple graph G . Then $|\lambda| \leq \Delta_G$ for every eigenvalue λ of A_G .*

Proof. Let \mathbf{x} be an eigenvector corresponding to an eigenvalue λ of the adjacency matrix of a graph G and x_u be the component of \mathbf{x} corresponding to

a vertex u . If we let u be the vertex in G for which $|x_u|$ is maximal, then by the definition of an eigenvalue, we have

$$\begin{aligned}\lambda x_u &= \sum_{uv \in E(G)} x_v \\ |\lambda||x_u| &\leq \sum_{uv \in E(G)} |x_v| \leq |\Delta_G||x_u|.\end{aligned}$$

Since $|x_u| \neq 0$, this implies that $|\lambda| \leq \Delta_G$. \square

Proposition 3.1.3 ([2], p. 32). *Let δ_G and Δ_G be the minimum and maximum degrees of a simple graph G , then $\delta_G \leq \rho(G) \leq \Delta_G$.*

Proof. The upper bound follows immediately from Proposition 3.1.2. Now, we need to prove the lower bound. Let λ_1 be the largest eigenvalue of A_G . Then by Theorem 2.1.15 we have

$$\lambda_1 \geq \frac{\mathbf{1}^T A_G \mathbf{1}}{\mathbf{1}^T \mathbf{1}} = \frac{2m}{n},$$

where m and n are the size and order of G . We can easily see from Theorem 2.2.1 that $2m \geq n\delta_G$ hence $\rho(G) = \lambda_1 \geq \delta_G$. Therefore, by the Perron-Frobenius Theorem the result holds. \square

Remark 3.1.4. *It is important to note that when the degrees of all the vertices of G are the same, then*

$$\rho(G) = \delta_G = \Delta_G.$$

Such graphs are called regular graphs.

Later in this section, we shall discuss more about regular graphs and also introduce some further bounds on $\rho(G)$ for any simple graph G . Meanwhile, we will use the above noted facts to determine the spectral radii of some classes of simple graphs.

Note that if two graphs are isomorphic then they have the same spectrum since by definition of isomorphic graphs adjacency is preserved. However, the converse does not hold. That is, there are some non-isomorphic graphs with the same spectrum (see [13, p. 4]). Graphs with the same spectrum are called cospectral graphs.

Theorem 3.1.5. *Let H be a subgraph of a graph G . Then*

$$\rho(H) \leq \rho(G).$$

Proof. Let h_{ij} and g_{ij} denote the ij -th entry of the adjacency matrices A_H and A_G of the graphs G and H respectively. Suppose $|V(H)| = k$ and $|V(G)| = n$. By the definition of a subgraph, we get two cases.

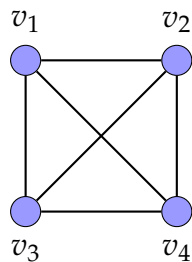
The first case is when $V(H) = V(G)$ and $E(H) \subseteq E(G)$. For this case, we have $n = k$ and $h_{ij} \leq g_{ij}$, for all $i, j = 1, \dots, n$. Then the result follows from Theorem 2.1.20.

The second case is when $V(H) \subset V(G)$ and $E(H) \subseteq E(G)$, implying that $k < n$. We form a graph H' from H by adding $n - k$ isolated vertices to H . This will not affect the property we want to prove. This is because the columns (and rows) of $A_{H'}$ associated to the isolated vertices are entirely zeros. So the spectrum of $A_{H'}$ is equal to the spectrum of A_H plus a set of $n - k$ zeros. Hence they have the same spectral radius. Now, we have $h'_{ij} \leq g_{ij}$, for all $i, j = 1, \dots, n$. The result then follows from Theorem 2.1.20. \square

3.2 Spectral radii of some classes of graphs

3.2.1 Complete graphs

A complete graph, denoted by K_n , is a graph of order n with each vertex adjacent to all other vertices. Hence each vertex has degree $n - 1$. An example of a complete graph and its adjacency matrix A_{K_n} is shown in Figure 3.2.



$$A_{K_4} = \begin{matrix} & \begin{matrix} v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \end{matrix}.$$

(a) The complete graph K_4 .

(b) Adjacency matrix A_{K_4} .

Figure 3.2: A complete graph and its adjacency matrix.

Theorem 3.2.1 ([2], p. 26). *The eigenvalues of A_{K_n} are $n - 1$ with multiplicity 1 and -1 with multiplicity $n - 1$.*

Proof. It can be observed that the adjacency matrix of a complete graph K_n is of the form $A_{K_n} = J - I$, where I is an identity matrix and J is a matrix

whose entries are all equal to one. From this we get $A_{K_n} + I = J$. This implies that -1 is an eigenvalue with multiplicity $n - 1$ since the rank of $A_{K_n} + I$ is 1.

Let α be the other eigenvalue of A_{K_n} . We can obtain α by considering the fact that the sum of the eigenvalues of A_{K_n} is equal to the trace, which is equal to zero. Thus

$$\begin{aligned} \alpha + \sum_{i=1}^{n-1} (-1) &= 0 \\ \alpha - (n - 1) &= 0 \\ \alpha &= n - 1. \end{aligned}$$

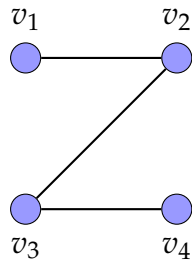
□

Corollary 3.2.2. *The spectral radius of a complete graph K_n of order n is given by $n - 1$.*

The proof of Corollary 3.2.2 follows directly from the results in Theorem 3.2.1 since one can easily notice that the largest eigenvalue of A_{K_n} is $n - 1$.

3.2.2 Paths

Let A_{P_n} denote the adjacency matrix of a path P_n of order n . Figure 3.3 gives an example of a path and its adjacency matrix.



(a) A path P_4 .

$$A_{P_4} = \begin{matrix} & \begin{matrix} v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{matrix}.$$

(b) Adjacency matrix A_{P_4} .

Figure 3.3: A path and its adjacency matrix.

Definition 3.2.3. *Orthogonal polynomials are sets of polynomials such that a certain inner product of any two of them is always equal to zero. Chebyshev polynomials are sequences of orthogonal polynomials which can be expressed in recursive form. They also satisfy some identities related to the De Moivre's formula, $(\cos \theta + i \sin \theta)^n = \cos n\theta + i \sin n\theta$. There are two main kinds, namely*

1. the Chebyshev polynomials of the first kind $P_n(x)$ which satisfy the recursive relation

$$P_0(x) = 1,$$

$$P_1(x) = x,$$

$$P_n(x) = 2xP_{n-1}(x) - P_{n-2}(x) \quad \text{for } n \geq 2.$$

2. the Chebyshev polynomials of the second kind $Q_n(x)$ which satisfy the recursive relation

$$Q_0(x) = 1,$$

$$Q_1(x) = 2x,$$

$$Q_n(x) = 2xQ_{n-1}(x) - Q_{n-2}(x) \quad \text{for } n \geq 2.$$

Our interest is in the Chebyshev polynomials of the second kind $Q_n(x)$ which we shall relate to the characteristic polynomial of the adjacency matrix of a path.

Theorem 3.2.4 ([28], p. 23). *The Chebyshev polynomials of the second kind $Q_n(x)$ satisfy the relation*

$$Q_n(\cos(t)) = \frac{\sin((n+1)t)}{\sin(t)}.$$

Proof. We shall prove this Theorem using the definition of the Chebyshev polynomials of the second kind $Q_n(x)$ and the principle of mathematical induction. For the base cases, we shall consider $n = 0$, where

$$Q_0(\cos(t)) = \frac{\sin(t)}{\sin(t)} = 1,$$

and $n = 1$, where

$$\begin{aligned} Q_1(\cos(t)) &= \frac{\sin(2t)}{\sin(t)} \\ &= \frac{2 \sin t \cos t}{\sin(t)} \\ &= 2 \cos t. \end{aligned}$$

It can be observed that in both cases the expressions agree with the definition of the Chebyshev polynomials of the second kind $Q_n(x)$. Now for our

inductive hypothesis we assume the identity holds for positive integers less than or equal to $n - 1$ and use the assumption to prove that it also holds for n . We know that

$$Q_n(\cos(t)) = 2 \cos(t)Q_{n-1}(\cos(t)) - Q_{n-2}(\cos(t)),$$

so by our induction hypothesis, we get

$$\begin{aligned} Q_n(\cos(t)) &= 2 \cos(t) \frac{\sin(nt)}{\sin(t)} - \frac{\sin((n-1)t)}{\sin(t)} \\ &= \frac{2 \cos(t) \sin(nt) - \sin((n-1)t)}{\sin(t)} \\ &= \frac{2 \cos(t) \sin(nt) - \sin(nt) \cos(t) + \sin(t) \cos(nt)}{\sin(t)} \\ &= \frac{\sin(nt) \cos(t) + \sin(t) \cos(nt)}{\sin(t)} \\ &= \frac{\sin((n+1)t)}{\sin(t)}. \end{aligned}$$

□

Theorem 3.2.5 ([2], p. 27). *The eigenvalues of the adjacency matrix A_{P_n} of a path P_n are given by $2 \cos\left(\frac{\pi k}{n+1}\right)$ where $k = 1, 2, \dots, n$.*

Proof. We want to find the eigenvalues of A_{P_n} ; so if we let λ be an eigenvalue then the characteristic polynomial of A_{P_n} is given by

$$\begin{aligned} \phi_{P_n}(\lambda) &= \det(\lambda I - A_{P_n}) \\ &= \begin{vmatrix} \lambda & -1 & 0 & 0 & \cdots & 0 \\ -1 & \lambda & -1 & 0 & \cdots & 0 \\ 0 & -1 & \lambda & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & \cdots & 0 & -1 & \lambda \end{vmatrix}. \end{aligned}$$

Therefore, if we set $\lambda = 2 \cos t$ and compute $\det((2 \cos t)I - A_{P_n})$ by expansion with respect to its first row and further compute the minor of -1 in the first row by expansion along the first column we obtain a recurrence

$$\begin{aligned} \phi_{P_0}(2 \cos t) &= 1, \quad \phi_{P_1}(2 \cos t) = 2 \cos t, \\ \phi_{P_n}(2 \cos t) &= 2 \cos t \phi_{P_{n-1}}(2 \cos t) - \phi_{P_{n-2}}(2 \cos t) \quad \text{for } n \geq 2. \end{aligned}$$

It can be observed that $\phi_{P_n}(2 \cos t) = Q_n(\cos t)$ so by Theorem 3.2.4 we get

$$\phi_{P_n}(2 \cos t) = \frac{\sin((n+1)t)}{\sin(t)}. \quad (3.1)$$

We determine the roots of $\phi_{P_n}(2 \cos t)$ by solving

$$\begin{aligned} \frac{\sin((n+1)t)}{\sin(t)} &= 0 \\ \sin((n+1)t) &= 0. \end{aligned} \quad (3.2)$$

The possible values of t that satisfy (3.2) are $t = \frac{k\pi}{(n+1)}$ for an integer k . However, for $k = 0$ we have $t = 0$. We get around this case by taking the limit as t approaches zero on both sides of equation 3.1 to obtain

$$\lim_{t \rightarrow 0} \phi_{P_n}(2 \cos t) = \lim_{t \rightarrow 0} \frac{\sin((n+1)t)}{\sin(t)},$$

which by L'Hopital's rule yields

$$\begin{aligned} \lim_{t \rightarrow 0} \phi_{P_n}(2 \cos t) &= \lim_{t \rightarrow 0} \frac{(n+1) \cos((n+1)t)}{\cos(t)} \\ &= n+1 \\ &\neq 0. \end{aligned}$$

This implies that $2 \cos t$ is not an eigenvalue when $t = 0$. The same reasoning applies for $k = n+1$, where we have $t = \pi$. Since we know that the cosine function is periodic and $\cos(-\theta) = \cos(\theta)$, it suffices for us to choose $k = \{1, 2, \dots, n\}$. Hence the eigenvalues of A_{P_n} are given by

$$\lambda = 2 \cos \left(\frac{k\pi}{n+1} \right), \quad \text{for } k = 1, 2, \dots, n.$$

□

Corollary 3.2.6. *The spectral radius of a path P_n is $2 \cos \left(\frac{\pi}{n+1} \right)$.*

Proof. Using the cosine identity

$$\cos \left(\frac{(n+1-k)\pi}{n+1} \right) = -\cos \left(\frac{k\pi}{n+1} \right) \quad \text{for all } k,$$

and Theorem 3.2.5 we deduce that the eigenvalues of A_{P_n} are

$$\begin{aligned} &2 \cos \left(\frac{\pi}{n+1} \right), 2 \cos \left(\frac{2\pi}{n+1} \right), \dots, 2 \cos \left(\frac{n\pi}{2(n+1)} \right), \\ &-2 \cos \left(\frac{n\pi}{2(n+1)} \right), \dots, -2 \cos \left(\frac{2\pi}{n+1} \right), -2 \cos \left(\frac{\pi}{n+1} \right), \end{aligned}$$

when n is even and

$$2 \cos \left(\frac{\pi}{n+1} \right), 2 \cos \left(\frac{2\pi}{n+1} \right), \dots, 2 \cos \left(\frac{(n-1)\pi}{2(n+1)} \right), 2 \cos \left(\frac{(n+1)\pi}{2(n+1)} \right) = 0,$$

$$-2 \cos \left(\frac{(n-1)\pi}{2(n+1)} \right), \dots, -2 \cos \left(\frac{2\pi}{n+1} \right), -2 \cos \left(\frac{\pi}{n+1} \right),$$

when n is odd.

We know that $\cos(\theta)$ decreases for an increasing θ within the interval $[0, \frac{\pi}{2}]$.

Thus as

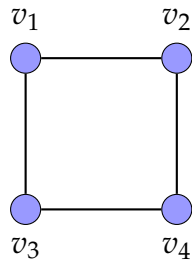
$$0 < \frac{\pi}{n+1} < \frac{2\pi}{n+1} < \frac{3\pi}{n+1} < \dots < \frac{n\pi}{2(n+1)} < \frac{\pi}{2},$$

$$1 = \cos(0) > \cos \left(\frac{\pi}{n+1} \right) > \dots > \cos \left(\frac{n\pi}{2(n+1)} \right) > \cos \left(\frac{\pi}{2} \right) = 0.$$

Hence we conclude that the largest eigenvalue in terms of absolute values of A_{P_n} is $2 \cos \left(\frac{\pi}{n+1} \right)$. □

3.2.3 Cycles

Suppose C_n is a cycle of order n . Its adjacency matrix will be denoted by A_{C_n} . An example of an n -cycle and its adjacency matrix A_{C_n} is shown in Figure 3.4.



(a) A 4-cycle C_4 .

$$A_{C_4} = \begin{matrix} & \begin{matrix} v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \end{matrix}.$$

(b) Adjacency matrix A_{C_4} .

Figure 3.4: A 4-cycle and its adjacency matrix.

Our aim here is to determine the eigenvalues of A_{C_n} and hence deduce its spectral radius. We shall therefore review circulant matrices since A_{C_n} is an example and their eigenvalues and eigenvectors are known.

Definition 3.2.7. A circulant matrix C is a matrix in which each row vector is obtained from the previous row vector by a cyclic shift. It is of the form

$$C = \begin{pmatrix} a_1 & a_2 & a_3 & \dots & a_n \\ a_n & a_1 & a_2 & \dots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \dots & a_{n-2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ a_2 & \dots & a_{n-1} & a_n & a_1 \end{pmatrix}.$$

We define some vectors of the form $\mathbf{x}_k = (1, \rho_k, \rho_k^2, \dots, \rho_k^{n-1})^T$, where ρ_k is the n -th root of unity given by $\rho_k = e^{\frac{2i\pi k}{n}}$, where $k = 0, 1, \dots, n-1$. Now, if we compute $C\mathbf{x}_k$ for each k we get

$$\begin{aligned} C\mathbf{x}_k &= \begin{pmatrix} a_1 & a_2 & a_3 & \dots & a_n \\ a_n & a_1 & a_2 & \dots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \dots & a_{n-2} \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ a_2 & \dots & a_{n-1} & a_n & a_1 \end{pmatrix} \begin{pmatrix} 1 \\ \rho_k \\ \rho_k^2 \\ \vdots \\ \rho_k^{n-1} \end{pmatrix} \\ &= \begin{pmatrix} a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1} \\ a_n + a_1\rho_k + a_2\rho_k^2 + \dots + a_{n-1}\rho_k^{n-1} \\ a_{n-1} + a_n\rho_k + a_1\rho_k^2 + \dots + a_{n-2}\rho_k^{n-1} \\ \vdots \\ a_2 + \dots + a_{n-1} + a_n\rho_k^{n-2} + a_1\rho_k^{n-1} \end{pmatrix} \\ &= \begin{pmatrix} a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1} \\ \rho_k(a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1}) \\ \rho_k^2(a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1}) \\ \vdots \\ \rho_k^{n-1}(a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1}) \end{pmatrix} \\ &= \lambda_k \mathbf{x}_k, \end{aligned}$$

where $\lambda_k = a_1 + a_2\rho_k + a_3\rho_k^2 + \dots + a_n\rho_k^{n-1}$. It then follows that the λ_k are eigenvalues of C and \mathbf{x}_k their respective eigenvectors. Note that some of the eigenvalues λ_k might be the same so we need to show that the corresponding eigenvectors \mathbf{x}_k span the eigenspace. To do this, we compute the determinant of E , which is an $n \times n$ matrix whose rows are the eigenvectors \mathbf{x}_k . The idea is that if some of the eigenvectors \mathbf{x}_k were linearly dependent

then the determinant of E would be zero. Now

$$\det(E) = \begin{vmatrix} 1 & \rho_0 & \rho_0^2 & \cdots & \rho_0^{n-1} \\ 1 & \rho_1 & \rho_1^2 & \cdots & \rho_1^{n-1} \\ 1 & \rho_2 & \rho_2^2 & \cdots & \rho_2^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \rho_{n-1} & \rho_{n-1}^2 & \cdots & \rho_{n-1}^{n-1} \end{vmatrix}.$$

Subtracting the first row from all the other rows we get

$$\det(E) = \begin{vmatrix} 1 & \rho_0 & \rho_0^2 & \cdots & \rho_0^{n-1} \\ 0 & \rho_1 - \rho_0 & \rho_1^2 - \rho_0^2 & \cdots & \rho_1^{n-1} - \rho_0^{n-1} \\ 0 & \rho_2 - \rho_0 & \rho_2^2 - \rho_0^2 & \cdots & \rho_2^{n-1} - \rho_0^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \rho_{n-1} - \rho_0 & \rho_{n-1}^2 - \rho_0^2 & \cdots & \rho_{n-1}^{n-1} - \rho_0^{n-1} \end{vmatrix}.$$

We compute column $n - i$ minus $\rho_0 \times$ column $n - 1 - i$ for all $0 \leq i \leq n - 2$ to obtain

$$\det(E) = \begin{vmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \rho_1 - \rho_0 & \rho_1(\rho_1 - \rho_0) & \cdots & \rho_1^{n-2}(\rho_1 - \rho_0) \\ 0 & \rho_2 - \rho_0 & \rho_2(\rho_2 - \rho_0) & \cdots & \rho_2^{n-2}(\rho_2 - \rho_0) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \rho_{n-1} - \rho_0 & \rho_{n-1}(\rho_{n-1} - \rho_0) & \cdots & \rho_{n-1}^{n-2}(\rho_{n-1} - \rho_0) \end{vmatrix}.$$

Expanding with respect to the first column we get

$$\det(E) = \begin{vmatrix} \rho_1 - \rho_0 & \rho_1(\rho_1 - \rho_0) & \cdots & \rho_1^{n-2}(\rho_1 - \rho_0) \\ \rho_2 - \rho_0 & \rho_2(\rho_2 - \rho_0) & \cdots & \rho_2^{n-2}(\rho_2 - \rho_0) \\ \vdots & \vdots & \vdots & \vdots \\ \rho_{n-1} - \rho_0 & \rho_{n-1}(\rho_{n-1} - \rho_0) & \cdots & \rho_{n-1}^{n-2}(\rho_{n-1} - \rho_0) \end{vmatrix}$$

It can be observed that from each row r we can factor out $\rho_r - \rho_0$, where $1 \leq r \leq n - 1$. Therefore we get

$$\begin{aligned} \det(E) &= \prod_{r=1}^{n-1} (\rho_r - \rho_0) \begin{vmatrix} 1 & \rho_1 & \rho_1^2 & \cdots & \rho_1^{n-1} \\ 1 & \rho_2 & \rho_2^2 & \cdots & \rho_2^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \rho_{n-1} & \rho_{n-1}^2 & \cdots & \rho_{n-1}^{n-1} \end{vmatrix} \\ &= \prod_{r=1}^{n-1} (\rho_r - \rho_0) \det(E_{n-1}). \end{aligned}$$

We iterate to obtain

$$\begin{aligned}\det(E) &= \prod_{r_1=1}^{n-1} (\rho_{r_1} - \rho_0) \prod_{r_2=2}^{n-1} (\rho_{r_2} - \rho_1) \prod_{r_3=3}^{n-1} (\rho_{r_3} - \rho_2) \cdots (\rho_n - \rho_{n-1}) \\ &= \prod_{0 \leq i < j \leq n-1} (\rho_j - \rho_i).\end{aligned}$$

Since the determinant of E is not zero, the eigenvectors \mathbf{x}_k are linearly independent and hence span the eigenspaces.

Remark 3.2.8. *The matrix E is called the Vandermonde matrix so its determinant is normally called the Vandermonde determinant.*

Note that $\rho_0 = 1$, so $x_0 = 1$. Therefore, by Theorem 2.1.19 we have x_0 as the Perron vector of C and its corresponding eigenvalue, $\lambda_0 = \sum_{i=1}^n a_i$, is the spectral radius of C .

With this, we can deduce the eigenvalues and the spectral radius of the adjacency matrix of an n -cycle which is captured in the following theorem.

Theorem 3.2.9 ([2], p. 27). *The eigenvalues of the adjacency matrix A_{C_n} of an n -cycle are given by $2 \cos\left(\frac{2\pi k}{n}\right)$, where $k = 0, 1, \dots, n-1$. The spectral radius is 2.*

Proof. If we let the row entries of the $n \times n$ circulant matrix C be given by

$$a_i = \begin{cases} 1 & \text{if } i = 2, n, \\ 0 & \text{otherwise,} \end{cases}$$

then we obtain the adjacency matrix A_{C_n} of an n -cycle. So the eigenvalues of A_{C_n} are given by

$$\begin{aligned}\lambda_k &= \rho_k + \rho_k^{n-1} \\ &= e^{\frac{2i\pi k}{n}} + e^{\frac{2i\pi(n-1)k}{n}} \\ &= e^{\frac{2i\pi k}{n}} + e^{2i\pi k} \cdot e^{\frac{-2i\pi k}{n}} \\ &= e^{\frac{2i\pi k}{n}} + e^{\frac{-2i\pi k}{n}} \\ &= 2 \cos\left(\frac{2\pi k}{n}\right), \quad \text{for } k = 0, 1, \dots, n-1.\end{aligned}$$

Note that $e^{i\theta} = \cos \theta + i \sin \theta$ and hence $e^{2i\pi k} = 1$ for all k . We know that

$$-1 \leq \cos\left(\frac{2\pi k}{n}\right) \leq 1$$

for all k and $n > 0$. Hence the spectral radius is 2, which is attained when $k = 0$. In the case when n is even, C_n is bipartite so we can also get -2 as an eigenvalue, which is attained when $k = \frac{n}{2}$. \square

Remark 3.2.10. *It is important to note that the characteristic polynomial of a cycle is the Chebyshev polynomial of the first kind (see [30], p. 8).*

3.2.4 Bipartite graphs

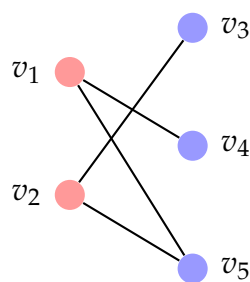
A bipartite graph G is a graph whose vertex set $V(G)$ can be divided into two disjoint subsets V_1 and V_2 such that every edge joins a vertex in V_1 to a vertex in V_2 . The adjacency matrix A_G of a bipartite graph G of order n is of the form

$$A_G = \begin{matrix} & \begin{matrix} v_1, \dots, v_k & v_{k+1}, \dots, v_n \end{matrix} \\ \begin{matrix} v_1, \dots, v_k \\ v_{k+1}, \dots, v_n \end{matrix} & \begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \end{matrix},$$

where $V_1 = \{v_1, \dots, v_k\}$, $V_2 = \{v_{k+1}, \dots, v_n\}$, O is a matrix with all its entries equal to zero and B is a matrix with entries

$$b_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

An example of a bipartite graph and its adjacency matrix is shown in Figure 3.5.



$$A_{S_{2,4}} = \begin{matrix} & \begin{matrix} v_1 & v_2 & v_3 & v_4 & v_5 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix} \end{matrix}.$$

(a) A bipartite graph G .

(b) Adjacency matrix A_G .

Figure 3.5: A bipartite graph and its adjacency matrix.

Theorem 3.2.11 ([2], p. 30). *Let G be a bipartite graph of order n . If λ is an eigenvalue of its adjacency matrix A_G with multiplicity k then $-\lambda$ is also an eigenvalue of A_G with multiplicity k .*

Proof. Let λ be an eigenvalue of A_G corresponding to the eigenvector \mathbf{x} . We let

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix},$$

where \mathbf{x}_1 is a vector whose entries are the components of \mathbf{x} corresponding to the vertices in V_1 . The vector \mathbf{x}_2 is defined similarly. Then by definition of an eigenvalue and the decomposition of A_G , we have

$$\begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}.$$

This yields the following equations:

$$\begin{aligned} B^T \mathbf{x}_2 &= \lambda \mathbf{x}_1 \\ B \mathbf{x}_1 &= \lambda \mathbf{x}_2. \end{aligned}$$

Now, we want to check if $-\lambda$ is also an eigenvalue. So we consider the equation

$$\begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ -\mathbf{x}_2 \end{pmatrix} = -\lambda \begin{pmatrix} \mathbf{x}_1 \\ -\mathbf{x}_2 \end{pmatrix},$$

which is equivalent to

$$\begin{aligned} B^T \mathbf{x}_2 &= \lambda \mathbf{x}_1 \\ B \mathbf{x}_1 &= \lambda \mathbf{x}_2. \end{aligned}$$

This shows that $-\lambda$ is also an eigenvalue, with eigenvector $\begin{pmatrix} \mathbf{x}_1 \\ -\mathbf{x}_2 \end{pmatrix}$. Now, if the eigenspace of λ consists of k linearly independent eigenvectors then this construction gives us k linearly independent eigenvectors in the eigenspace of $-\lambda$. \square

3.2.5 Regular graphs

As defined earlier, a graph G is regular if all its vertices have the same degree. Therefore, we say a graph is r -regular if each vertex has degree r . Examples of regular graphs include complete graphs K_n , cycles C_n , completely bipartite graphs $K_{n,n}$, the Petersen graph (see Figure 3.6) etc.

Theorem 3.2.12 ([13], p. 2). *The spectral radius of the adjacency matrix A_G of an r -regular graph G is r and its corresponding eigenvector is $\mathbf{1}$.*

Proof. If we let $\mathbf{x} = \mathbf{1}$ then for each vertex u we get

$$\begin{aligned} \sum_{uv \in E(G)} x_v &= \sum_{uv \in E(G)} 1 = r, \\ \Rightarrow A_G \cdot \mathbf{1} &= r \cdot \mathbf{1}. \end{aligned}$$

Therefore r is an eigenvalue of A_G and it corresponds to the unique positive eigenvector $\mathbf{1}$. So by Theorem 2.1.19, r is the spectral radius of A_G . \square

It follows immediately that the spectral radius of the adjacency matrix of a complete graph of order n is $n - 1$ and that of a cycle is 2 (as determined earlier). Moreover, all cubic graphs, such as the Petersen graph, the Wagner graph(see Figure 3.6), etc., have spectral radius 3.

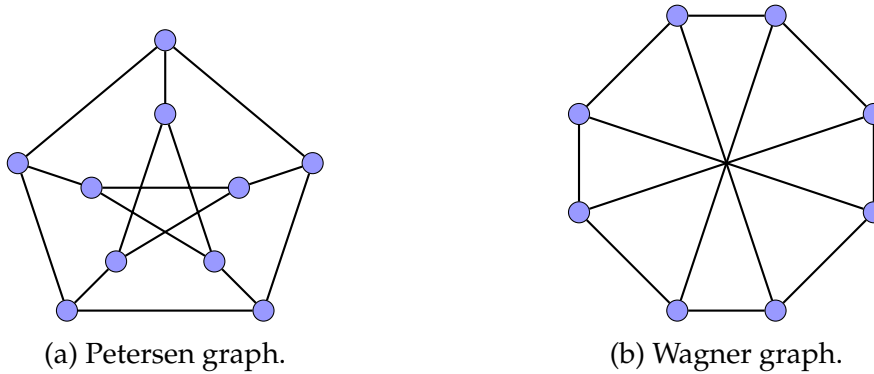


Figure 3.6: The Petersen graph and the Wagner graph.

Definition 3.2.13. *An k -partite graph G is a graph whose vertex set G can be divided into k disjoint subsets, V_1, V_2, \dots, V_k , such that every edge joins a vertex in one partite set to another. Therefore, an k -partite graph in which every pair of vertices from two different partite sets are adjacent is called a complete k -partite graph, denoted by K_{m_1, \dots, m_k} where $m_i = |V_i|, i = 1, \dots, k$.*

Suppose K_{m_1, \dots, m_k} is a complete k -partite graph such that $m_1 = \dots = m_k = r$. By the definition a complete k -partite graph, we know that for each vertex in partite set, say V_1 , is adjacent to all the vertices in the remaining $k - 1$ partite sets, each of size r . Therefore, K_{m_1, \dots, m_k} is an $r(k - 1)$ -regular graph. By Theorem 3.2.12, we have that such graphs have spectral radius $r(k - 1)$. So the complete bipartite graph K_{nn} the spectral radius is n .

3.2.6 Semi-regular graphs

A semi-regular graph G is a bipartite graph with partite vertex sets V_1 and V_2 such that each vertex $u \in V_1$ and $v \in V_2$ has degree d_1 and d_2 respectively. Each edge in G has one end $u \in V_1$ and another end $v \in V_2$. So counting the number of edges in G is equivalent to computing $|V_1|d_1$ or $|V_2|d_2$, where $|V_1|$ and $|V_2|$ are the respective cardinalities of V_1 and V_2 . This implies that $|V_1|d_1 = |V_2|d_2 = |E(G)|$. An example of a semi-regular graph and its adjacency matrix $A_{S_{m,n}}$ are shown in Figure 3.7.

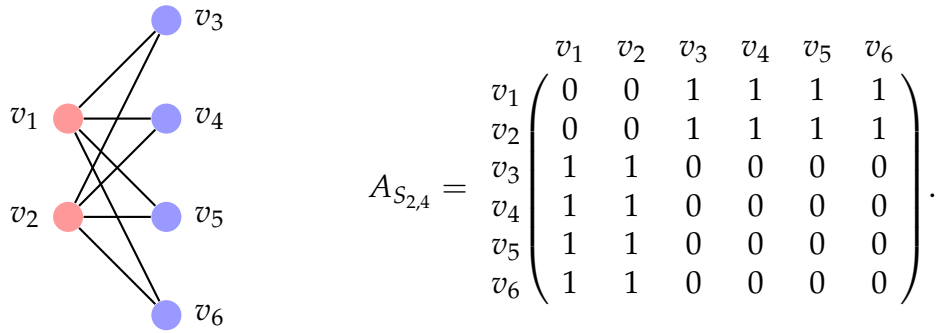
(a) A semi-regular graph G .(b) Adjacency matrix A_G .

Figure 3.7: A semi-regular graph and its adjacency matrix.

In general, the adjacency matrix of G is given by

$$A_G = \begin{pmatrix} O & C^T \\ \begin{matrix} m \times m \\ C \end{matrix} & \begin{matrix} m \times n \\ O \end{matrix} \\ \begin{matrix} n \times m \\ C \end{matrix} & \begin{matrix} n \times n \\ O \end{matrix} \end{pmatrix},$$

where O is a matrix with all its entries equal to zero and C is an $n \times m$ matrix with entries

$$c_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, the sum of each row is d_2 in C and d_1 in C^T .

Theorem 3.2.14. *Let d_1, d_2 be the respective degrees of each vertex in the vertex sets V_1, V_2 of a semi-regular graph G . Then the spectral radius of its adjacency matrix is $\sqrt{d_1 d_2}$.*

Proof. We let λ be a real number and \mathbf{x} a non-zero vector. Suppose we let x_u denote the component of \mathbf{x} corresponding to a vertex u in G . Then we

define the entries of our vector \mathbf{x} as $x_u = a$ for all $u \in V_1$ and $x_v = b$ for all $v \in V_2$. So if the following equations,

$$\begin{aligned}d_1 b &= \lambda a, \\d_2 a &= \lambda b,\end{aligned}$$

hold then we get $A_G \mathbf{x} = \lambda \mathbf{x}$ implying λ is an eigenvalue and it corresponds to the eigenvector \mathbf{x} . Now, multiplying both equations and simplifying yields

$$\begin{aligned}\lambda^2 ab &= d_1 d_2 ab \\ \lambda &= \pm \sqrt{d_1 d_2}.\end{aligned}$$

If a and b are taken to be positive (e.g. $a = 1$ and $b = \sqrt{\frac{d_2}{d_1}}$), then \mathbf{x} is a positive vector, so by the Perron-Frobenius theorem $\sqrt{d_1 d_2}$ is the spectral radius of A_G . \square

Definition 3.2.15. A bipartite graph in which each vertex u in the vertex subset V_1 is adjacent to all vertices in the vertex subset V_2 is called a complete bipartite graph, denoted by $K_{m,n}$, where m and n are the sizes of V_1 and V_2 respectively. A complete bipartite graph is also semi-regular graph since each vertex $u \in V_1$ and $v \in V_2$ has degree n and m respectively.

Corollary 3.2.16 ([2], p. 26). The spectral radius of the adjacency matrix of a complete bipartite graph $K_{m,n}$ is given by \sqrt{mn} .

Proof. The proof follows directly from Theorem 3.2.14 by substituting m for d_1 and n for d_2 . \square

Corollary 3.2.17. If G is a bipartite graph then

$$\rho(G) \leq \sqrt{pq},$$

where $p = |V_1|$ and $q = |V_2|$. Equality holds when G is a complete bipartite graph $K_{p,q}$.

Proof. Let G be a bipartite graph whose vertex set $V(G)$ is divided into two disjoint subsets V_1 and V_2 such that $|V_1| = p$ and $|V_2| = q$. It is clear that G is a subgraph of $K_{p,q}$. Hence by Theorem 3.1.5 and Corollary 3.2.16, the theorem holds. \square

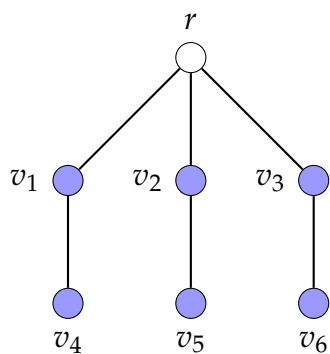
Definition 3.2.18. A star graph is a tree of order n with $n - 1$ leaves and one central vertex adjacent to all of them. It is also a complete bipartite graph denoted by $K_{1,n-1}$.

Corollary 3.2.19. The spectral radius of a star graph of order n is $\sqrt{n - 1}$.

Proof. The proof of Corollary 3.2.19 follows directly from the result in Theorem 3.2.16 by substituting 1 for m and $n - 1$ for n . \square

3.2.7 Extended star graph

An extended star graph $E_{k,d}$ is a rooted tree of order $kd + 1$ with root r and d paths of length k attached to it. Note that $E_{k,1}$ and $E_{k,2}$ are paths of order $k + 1$ and $2k + 1$ respectively. Also, $E_{1,d}$ is a star graph (or a complete bipartite graph $K_{1,d}$) of order $d + 1$. An example of the adjacency matrix $A_{E_{k,d}}$ of an extended star graph $E_{k,d}$ is shown in Figure 3.8.



(a) An extended star graph $E_{2,3}$.

$$A_{E_{2,3}} = \begin{matrix} & r & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \\ \begin{matrix} r \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{matrix} & \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} & \end{matrix}.$$

(b) Adjacency matrix $A_{E_{2,3}}$.

Figure 3.8: An extended star graph and its adjacency matrix.

As noted earlier, in a tree there is only one path between any two vertices. Using this fact, we can group the vertices of an extended star graph $E_{k,d}$ into levels with respect to their heights. That is we shall call all vertices of $E_{k,d}$ which have distance j from the root vertex r as vertices on the j -th level. For instance, vertices v_1, v_2 and v_3 in Figure 3.8 are on the first level since their distance from the root r is 1. Our first goal in this section is to determine the spectral radius of $A_{E_{k,d}}$ for fixed $k = 2, 3$ and any value of d . Secondly, we fix d and also investigate the spectral radius of $A_{E_{k,d}}$ for any value of k .

Theorem 3.2.20. For $k=2$, the eigenvalues of the adjacency matrix of an extended star graph $E_{2,d}$ are 0 with multiplicity 1, ± 1 , each with multiplicity $d - 1$, and $\pm\sqrt{d + 1}$, each with multiplicity 1. Hence its spectral radius is $\sqrt{d + 1}$.

Proof. Let us label the root of $E_{2,d}$ as r , and the vertices on the j -th level as $v_{d(j-1)+l}$, where $l = \{1, 2, \dots, d\}$. So vertices on the first level will be v_l , ($l = \{1, 2, \dots, d\}$) and those on the second level will be v_{d+l} , ($l = \{1, 2, \dots, d\}$). With this labelling, the adjacency matrix $A_{E_{2,d}}$ of an extended star graph $E_{2,d}$ will be of the form

$$A_{E_{2,d}} = \begin{matrix} & r & v_1 & v_2 & \dots & v_d & v_{d+1} & v_{d+2} & \dots & v_{2d} \\ \begin{matrix} r \\ v_1 \\ v_2 \\ \vdots \\ v_d \\ v_{d+1} \\ v_{d+2} \\ \vdots \\ v_{2d} \end{matrix} & \begin{pmatrix} 0 & 1 & 1 & \dots & 1 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 & 1 & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{matrix}.$$

It can be observed that the sum of the columns associated to the vertices v_{d+1} to v_{2d} is equal to the first column. So the first column can be expressed as a linear combination of those columns. Hence the rank of $A_{E_{2,d}}$ is at most $2d$. With this, we see that its determinant is zero and also that it has zero as an eigenvalue with multiplicity at least 1.

Also, if we consider the matrix $A_{E_{2,d}} + I$, we can express each of the columns associated to the vertices v_1 to v_d as a linear combination of some other columns. If we let C_{v_i} denote the column associated to vertex v_i , then we get

$$C_{v_j} = C_{v_1} + C_{v_{j+d}} - C_{v_{d+1}}, \quad \text{for } j = \{2, 3, \dots, d\}.$$

With this, we have that the rank of the matrix $A_{E_{2,d}} + I$ is at most $d + 2$ implying that its determinant is zero and hence -1 is an eigenvalue of $A_{E_{2,d}}$ with multiplicity at least $d - 1$.

Similarly, if we consider the matrix $A_{E_{2,d}} - I$, then we have

$$C_{v_j} = C_{v_1} + C_{v_{d+1}} - C_{v_{j+d}}, \quad \text{for } j = \{2, 3, \dots, d\}.$$

So we also have the rank of the matrix $A_{E_{2,d}} - I$ to be at most $d + 2$ implying that 1 is an eigenvalue of $A_{E_{2,d}}$ with multiplicity at least $d - 1$.

Now to determine the remaining eigenvalues we let λ be any real number and \mathbf{x} a non-zero vector. Suppose we let the entries of \mathbf{x} be x_0, x_1 and x_2 where x_0 corresponds to the root r , x_1 corresponds to each vertex on the first level and similarly x_2 is assigned to each vertex on the second level. Now, if the following equations,

$$dx_1 = \lambda x_0, \quad (3.3)$$

$$x_0 + x_2 = \lambda x_1, \quad (3.4)$$

$$x_1 = \lambda x_2, \quad (3.5)$$

are satisfied then we have $A_{E_{2,d}}\mathbf{x} = \lambda\mathbf{x}$ implying that λ is an eigenvalue and \mathbf{x} an eigenvector of $A_{E_{2,d}}$. Now, adding equations (3.3) and (3.5) and substituting (3.4) we get

$$(d + 1)x_1 = \lambda(x_0 + x_2)$$

$$(d + 1)x_1 = \lambda(\lambda x_1)$$

$$\lambda = \pm\sqrt{d + 1}.$$

Therefore, we get $\pm\sqrt{d + 1}$ as eigenvalues of $A_{E_{2,d}}$ each with multiplicity at least 1. Since the algebraic multiplicities of all the eigenvalues we have found sum up to $2d + 1$, we can change all the "at least" to "exactly". Furthermore, if \mathbf{x} above is positive then it is the Perron vector which implies that $\sqrt{d + 1}$ is the spectral radius of $A_{E_{2,d}}$. \square

Theorem 3.2.21. *Let $A_{E_{3,d}}$ be the adjacency matrix of an extended star graph $E_{3,d}$. Then its spectral radius is $\sqrt{\frac{(d+2)+\sqrt{d^2+4}}{2}}$.*

Proof. Suppose we let the vertices of $E_{3,d}$ be labelled as described in the proof of Theorem 3.2.20. We obtain a similar adjacency matrix as $A_{E_{2,d}}$. Therefore, we define the entries of a non-zero vector \mathbf{x} as x_0 corresponding to the root r and x_j corresponding to each vertex on the j -th level, where $j = \{1, 2, 3\}$. Note that each x_j (except x_0) occurs d times in \mathbf{x} so the dimen-

sion of x is $3d + 1$. Now if the following equations,

$$\begin{aligned} dx_1 &= \lambda x_0, \\ x_0 + x_2 &= \lambda x_1, \\ x_1 + x_3 &= \lambda x_2, \\ x_2 &= \lambda x_3, \end{aligned}$$

are satisfied for some real number λ , then we have $A_{E_{3,d}}x = \lambda x$ implying that λ is an eigenvalue and its associate eigenvector is x . From these equations, we obtain the following equation:

$$\begin{aligned} A'x' &= \lambda x' \\ \begin{pmatrix} 0 & d & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} &= \lambda \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix}. \end{aligned} \quad (3.6)$$

This shows that λ is also an eigenvalue of A' so we can determine its value by solving the following equation:

$$\begin{aligned} \det(\lambda I - A') &= 0 \\ \begin{vmatrix} \lambda & -d & 0 & 0 \\ -1 & \lambda & -1 & 0 \\ 0 & -1 & \lambda & -1 \\ 0 & 0 & -1 & \lambda \end{vmatrix} &= 0. \end{aligned}$$

Expanding along the first row, we obtain

$$\begin{aligned} \lambda \begin{vmatrix} \lambda & -1 & 0 \\ -1 & \lambda & -1 \\ 0 & -1 & \lambda \end{vmatrix} + d \begin{vmatrix} -1 & -1 & 0 \\ 0 & \lambda & -1 \\ 0 & -1 & \lambda \end{vmatrix} &= 0 \\ \lambda [\lambda(\lambda^2 - 1) - \lambda] + d [-1(\lambda^2 - 1)] &= 0 \\ \lambda^4 - 2\lambda^2 - d\lambda^2 + d &= 0 \\ \lambda^4 - \lambda^2(d + 2) + d &= 0. \end{aligned}$$

We let $\lambda^2 = a$ to get

$$\begin{aligned} a^2 - a(d+2) + d &= 0 \\ a &= \frac{(d+2) \pm \sqrt{d^2+4}}{2} \\ \therefore \lambda &= \pm \sqrt{\frac{(d+2) \pm \sqrt{d^2+4}}{2}}. \end{aligned}$$

We obtain all the four eigenvalues of A' which are also eigenvalues of $A_{E_{3,d}}$. If we let the entries of \mathbf{x} to be positive then by the Perron-Frobenius Theorem we have $\sqrt{\frac{(d+2)+\sqrt{d^2+4}}{2}}$ as the spectral radius of $A_{E_{3,d}}$. \square

Following from these results it can be observed that as d , the degree of the root vertex, increases then the spectral radius also increases for a fixed k . Note that this result is also a consequence of Theorem 3.1.5. Also, when we increased k from 2 to 3 for a fixed d then the spectral radius also increased, that is $\sqrt{d+1} < \sqrt{\frac{(d+2)+\sqrt{d^2+4}}{2}}$. However, when k gets larger for a fixed d then we obtain the following result.

Theorem 3.2.22. *For large values of k and a fixed d , the spectral radius $\rho(E_{k,d})$ is bounded above by*

$$\rho(E_{k,d}) \leq \begin{cases} 2 & \text{if } d = 1, 2, \\ \frac{d}{\sqrt{d-1}} & \text{if } d > 2. \end{cases}$$

Equality only holds in the limit.

To prove Theorem 3.2.22, we state the following Lemma and apply the technique used in Example 2.3 and 2.4 of [30].

Lemma 3.2.23 ([30], Lemma 2.2). *Let $\rho(G_\infty) > 2$ be the spectral radius of an infinite graph G_∞ with bounded vertex degrees. If $\rho(G_\infty)$ is an eigenvalue, then the components of its positive eigenvector \mathbf{x} satisfies*

$$x_i = x_0 t^{-i}$$

along any infinite pendent path of G_∞ . Here, x_0 is associated to the vertex to which the infinite path is attached and t is given by

$$t = \frac{\rho(G_\infty) + \sqrt{\rho(G_\infty)^2 - 4}}{2}.$$

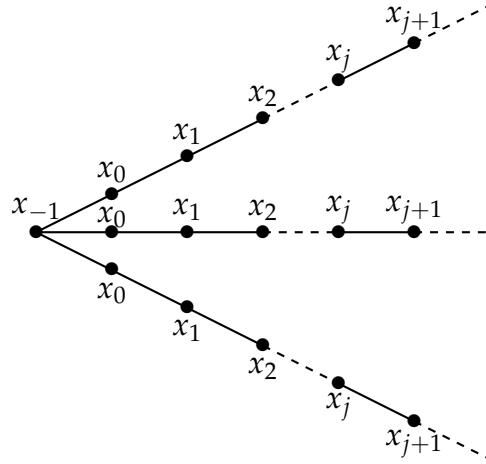


Figure 3.9: An infinite extended star graph $E_{\infty,3}$

Proof of Theorem 3.2.22. As noted earlier, $E_{k,1}$ and $E_{k,2}$ are paths. So by Corollary 3.2.6, their spectral radii are bounded above by 2.

Now, we consider the case when $d > 2$. To prove this case, we turn all the pendent paths of $E_{k,d}$ into infinite paths to obtain an infinite extended star graph $E_{\infty,d}$. We let λ be the spectral radius of $E_{\infty,d}$ and \mathbf{x} its Perron vector. We define the entries of \mathbf{x} as x_{-1} corresponding to the root r and $x_i, i \geq 0$, corresponding to the vertices on the $i + 1$ -th level as depicted in Figure 3.9. Without loss of generality, we set $x_0 = 1$. So by Lemma 3.2.23 we get

$$x_i = t^{-i}, i \geq 0,$$

where $t = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}$, from which we obtain $\lambda = t + \frac{1}{t}$.

Note that x_{-1} satisfies the following eigenvalue equations

$$\lambda x_{-1} = dx_0, \tag{3.7}$$

$$\lambda x_0 = x_{-1} + x_1. \tag{3.8}$$

By Lemma 3.2.23 and equations 3.7 and 3.8 we get

$$\begin{aligned}
 x_{-1} &= \frac{d}{\lambda}, \\
 x_{-1} &= \lambda - \frac{1}{t} = t, \\
 \Rightarrow \frac{d}{\lambda} &= t \\
 t\lambda &= d \\
 t \left(t + \frac{1}{t} \right) &= d \\
 t^2 + 1 &= d \\
 t &= \sqrt{d-1}.
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \lambda &= \sqrt{d-1} + \frac{1}{\sqrt{d-1}} \\
 &= \frac{d}{\sqrt{d-1}}.
 \end{aligned}$$

Note that, since λ increases with k we get

$$\rho(E_{k,d}) \leq \frac{d}{\sqrt{d-1}}.$$

□

3.3 The spectral radius and some graph parameters

Definition 3.3.1. A walk w of length l in a graph G is a finite alternating sequence of vertices and edges in G which is of the form

$$v_{i_0}, e_{k_1}, v_{i_1}, e_{k_2}, v_{i_2}, \dots, v_{i_{l-1}}, e_{k_l}, v_{i_l},$$

where v_{i_0} is the start vertex, v_{i_l} is the end vertex and $e_{k_p} = v_{i_p}v_{i_{p+1}}$, $p = 0, \dots, l-1$.

Theorem 3.3.2 ([13], p. 14). For $l \geq 1$, we let a_{ij}^l denote the ij -th entry of the l -th power A_G^l of the adjacency matrix A_G of a graph G . Then, a_{ij}^l counts the number of walks of length l from vertex v_i to v_j in G .

Proof. We shall prove this theorem using matrix multiplication and the principle of mathematical induction.

We first consider the base case where $l = 1$. By definition we know that if $a_{ij} = 1$, then the vertex v_i is adjacent to the vertex v_j and this is a walk of length 1 from v_i to v_j . Conversely, if $a_{ij} = 0$, then v_i is not adjacent to v_j and there is no walk of length 1 from v_i to v_j .

For our induction hypothesis, we assume that the number of walks of length k (where $k < l$) from vertex v_i to vertex v_j is equal to a_{ij}^k .

Now we use this induction hypothesis to prove our theorem. By the definition of matrix multiplication, the ij -th entry of $A_G^l = A_G^{l-1}A_G$ is given by

$$a_{ij}^l = \sum_{m=1}^n a_{im}^{l-1} a_{mj}.$$

On the other hand, a walk of length l from vertex v_i to vertex v_j is actually a walk of length $l - 1$ from v_i to a neighbour of v_j plus one more edge. Therefore, summing over all such walks gives us the total number of walks of length l from vertex v_i to vertex v_j , which is equal to a_{ij}^l . \square

Remark 3.3.3. *Theorem 3.3.2 is true for the adjacency matrix of non-simple graphs, i.e. graphs with loops or multiple edges, with an analogous proof.*

Following from Theorem 3.3.2, we can easily compute the total number of walks of length l in a graph G by simply summing all the entries of A_G^l , thus by computing $\mathbf{1}^T A_G^l \mathbf{1}$. Recall that $\mathbf{1}^T A_G \mathbf{1}$ gives us twice the number of edges in the graph G . For simplicity, the total number of walks of length l in a graph G will be denoted by $w_l(G)$.

Now we proceed to show that the total number of walks of length l in a graph G can be estimated by the eigenvalues of the adjacency matrix A_G . Recall that the eigenvectors of the symmetric matrix A_G are orthogonal hence we can construct orthonormal eigenvectors. Let $\mathbf{q}_i, i = 1, \dots, n$, be the orthonormal eigenvectors corresponding to the eigenvalues λ_i of A_G . So we form an orthogonal matrix Q whose columns are the \mathbf{q}_i 's and let \mathbf{c} be a vector of real constants $c_i = \mathbf{q}_i^T \mathbf{1}, i = 1, \dots, n$. Then, we have

$$\sum_{i=1}^n c_i \mathbf{q}_i = \mathbf{1}. \quad (3.9)$$

Note that Q is an orthogonal matrix so if we let $\mathbf{c} = Q^T \mathbf{1}$ then we obtain the above result.

Now substituting equation (3.9) into the equation for computing the total number of walks of length l in a graph G we get

$$\begin{aligned} \mathbf{1}^T A_G^l \mathbf{1} &= \left(\sum_{i=1}^n c_i \mathbf{q}_i \right)^T A_G^l \left(\sum_{i=1}^n c_i \mathbf{q}_i \right) \\ &= \left(\sum_{i=1}^n c_i \mathbf{q}_i^T \right) \left(\sum_{i=1}^n c_i \lambda_i^l \mathbf{q}_i \right) \\ &= \sum_{i=1}^n c_i^2 \lambda_i^l. \end{aligned} \quad (3.10)$$

We can deduce from equation (3.10) that

$$\mathbf{1}^T A_G^0 \mathbf{1} = \sum_{i=1}^n c_i^2 = n. \quad (3.11)$$

This is simply counting the number of vertices of the graph G .

Proposition 3.3.4. *Let G be a r -regular graph of order n . Then the number of walks of length l is*

$$w_l(G) = r^l w_0(G) = nr^l.$$

Proof. Let us consider a walk of length l in an r -regular graph G starting from a vertex u . For each step in such a walk, there are always r possible vertices to visit. Hence there are r^l of such walks. Since G is of order n , the results follows directly. \square

This result give us the idea about the contribution of the spectral radius to the growth of the number of walks in a graph. This concept is also captured in the following theorem for non-bipartite graphs.

Theorem 3.3.5 ([10], p. 5). *Suppose G is a connected non-bipartite graph of order n and A_G the adjacency matrix. Then the total number of walks of length l (for large values of l) is asymptotically $c_1^2 \lambda_1^l$, where λ_1 is the spectral radius of A_G and c_1 is a constant obtained by summing the entries of the unit eigenvector associated to the spectral radius.*

Proof. Let G be a connected non-bipartite graph of order n and A_G the adjacency matrix. We let $\lambda_i, (i = 1, \dots, n)$ be the eigenvalues of A_G with λ_1 as

the spectral radius. By the Perron-Frobenius Theorem, we know that $\lambda_1 > 0$ and also by the definition of spectral radius we have $|\lambda_i| \leq \lambda_1, (i \neq 1)$ with equality holding only for bipartite graphs.

From equation (3.10) we get that the total number of walks of length l in G is given by

$$\begin{aligned} \mathbf{1}^T A_G^l \mathbf{1} &= \sum_{i=1}^n c_i^2 \lambda_i^l \\ \frac{\mathbf{1}^T A_G^l \mathbf{1}}{\lambda_1^l} &= \left(c_1^2 + \sum_{i=2}^n c_i^2 \frac{\lambda_i^l}{\lambda_1^l} \right). \end{aligned} \quad (3.12)$$

Taking the limit as $l \rightarrow \infty$ on both sides of equation 3.12 gives us

$$\begin{aligned} \lim_{l \rightarrow \infty} \frac{\mathbf{1}^T A_G^l \mathbf{1}}{\lambda_1^l} &= \lim_{l \rightarrow \infty} \left[c_1^2 + \sum_{i=2}^n c_i^2 \left(\frac{\lambda_i}{\lambda_1} \right)^l \right] \\ &= c_1^2. \end{aligned}$$

Note that $\frac{|\lambda_i|}{\lambda_1} < 1$ for $i \neq 1$, hence $\left(\frac{\lambda_i}{\lambda_1} \right)^l \rightarrow 0$ for large values of l . \square

Remark 3.3.6. *Theorem 3.3.5 tells us that the spectral radii of non-bipartite graphs give information about the growth of the total number of walks in such graphs.*

Remark 3.3.7. *For the case of a bipartite graph, we know that its spectrum is symmetric about the origin. So we have*

$$\lim_{l \rightarrow \infty} \frac{\mathbf{1}^T A_G^l \mathbf{1}}{\lambda_1^l} = \lim_{l \rightarrow \infty} \left[c_1^2 + c_n^2 (-1)^l + \sum_{i=2}^{n-1} c_i^2 \left(\frac{\lambda_i}{\lambda_1} \right)^l \right].$$

The limit does not exist since it keeps on alternating between $c_1^2 - c_n^2$ and $c_1^2 + c_n^2$ for large values of l .

Another result we can deduce from Theorem 3.3.2 concerns the number of closed walks of length l , which is a walk of length l from a vertex back to itself, in a graph G . In particular, these closed walks are counted by the diagonal entries of A_G^l . Hence the trace of A_G^l gives us the total number of closed walks of length l in a graph G , which we shall denote by ${}_c w_l(G)$. We know that the sum of the eigenvalues of A_G is equal to its trace so this gives us an idea of an application of the spectral radius of A_G . There is a relation between the spectral radius of A_G and the number of closed walks in a graph G . This relation will be captured in our next theorem.

Theorem 3.3.8. *Suppose we let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of the adjacency matrix A_G of a graph G of order n and λ_1 its spectral radius. Then the total number of closed walks of length l is given by*

$${}_c w_l(G) = \lambda_1^l \left[1 + \sum_{i=2}^n \left(\frac{\lambda_i}{\lambda_1} \right)^l \right].$$

Proof. From Theorem 3.3.2, we know that the total number of closed walks of length l in a graph G , denoted by ${}_c w_l(G)$, is given by $\text{tr}(A_G^l)$, which we know is equal to the sum of the eigenvalues of A_G^l . Therefore, from Theorem 2.1.13 we have that

$$\begin{aligned} {}_c w_l(G) &= \text{tr}(A_G^l) \\ &= \lambda_1^l + \lambda_2^l + \dots + \lambda_n^l \\ &= \lambda_1^l \left[1 + \sum_{i=2}^n \left(\frac{\lambda_i}{\lambda_1} \right)^l \right]. \end{aligned}$$

□

There are several corollaries we can obtain from Theorem 3.3.8 and we shall state and prove some of them.

Corollary 3.3.9. *The total number of closed walks of length l in a complete graph K_n of order n is given by*

$${}_c w_l(K_n) = \begin{cases} (n-1)^l + (n-1) & \text{if } l \text{ is even,} \\ (n-1)^l - (n-1) & \text{if } l \text{ is odd,} \end{cases}$$

where $(n-1)$ is the spectral radius of A_{K_n} .

Proof. We know from Theorem 3.2.1 and Corollary 3.2.19 the eigenvalues and the spectral radius of A_{K_n} . So from Theorem 3.3.8 we get

$$\begin{aligned} {}_c w_l(K_n) &= \lambda_1^l \left[1 + \sum_{i=2}^n \left(\frac{\lambda_i}{\lambda_1} \right)^l \right] \\ &= (n-1)^l \left[1 + \sum_{i=2}^n \left(\frac{-1}{n-1} \right)^l \right] \\ &= (n-1)^l \left[1 + \frac{(-1)^l}{(n-1)^{l-1}} \right] \\ &= (n-1)^l + (-1)^l (n-1). \end{aligned}$$

□

Corollary 3.3.10. *For a complete bipartite graph $K_{m,n}$, the total number of closed walks of even length l is given by $2(\sqrt{mn})^l$, where \sqrt{mn} is the spectral radius of $A_{K_{m,n}}$. Also, there is no closed walk of odd length in $K_{m,n}$.*

Proof. From Theorems 3.2.16 and 3.3.8, we get

$$\begin{aligned} {}_c w_l(K_{m,n}) &= \lambda_1^l \left[1 + \sum_{i=2}^n \left(\frac{\lambda_i}{\lambda_1} \right)^l \right] \\ &= (\sqrt{mn})^l \left[1 + \left(\frac{-\sqrt{mn}}{\sqrt{mn}} \right)^l \right] \\ &= (\sqrt{mn})^l (1 + (-1)^l) \\ &= \begin{cases} 2(\sqrt{mn})^l & \text{if } l \text{ is even,} \\ 0 & \text{if } l \text{ is odd.} \end{cases} \end{aligned}$$

□

Corollary 3.3.11. *Let λ_i , for $1 \leq i \leq n$, be the eigenvalues of the adjacency matrix A_G of a graph G of order n and size m . Then*

$$\sum_{i=1}^n \lambda_i^2 = 2m.$$

Proof. Let a_{ii}^2 be the diagonal entry of A_G^2 associated with the vertex v_i . Then we know from Theorem 3.3.2 that a_{ii}^2 counts closed walks of length 2 from v_i . In particular, a_{ii}^2 is equal to the degree of v_i since it is just count walks to its neighbours and back to v_i itself. Therefore, the trace of A_G^2 is the sum of all the degrees of the vertices of G which we know to be equal to twice the size of G . Hence the results follows. □

Remark 3.3.12. *One can easily deduce from Corollary 3.3.11 that the number of closed walks of length 2 in a graph G is equal to the total number of walks of length 1 in the graph since both of them give us twice the size of G . It then follows immediately from this aforementioned fact and Proposition 3.3.4 that if a graph G of order n and size m is regular then it satisfies*

$$\lambda_1 = \frac{\sum_{i=1}^n \lambda_i^2}{n} = \frac{2m}{n} = \mathcal{D},$$

where $\lambda_i, 1 \leq i \leq n$, are the eigenvalues of the adjacency matrix A_G with λ_1 as the spectral radius and \mathcal{D} as its average degree. This gives evidence of how the spectrum of a graph can be used (to some extent) as a characterization of the graph.

Motivated by the result in Theorem 3.3.5, we obtain the following result relating the number of closed walks in a graph to its spectral radius.

Theorem 3.3.13 ([30], p.40). *Let G be a non-bipartite graph of order n . Then the number of closed walks of length l (for large values of l) is asymptotically λ_1^l , where λ_1 is the spectral radius of G .*

Proof. The proof is analogous to the proof of Theorem 3.3.5. □

Remark 3.3.14. *For the case of a bipartite graph G , we have*

$$\lim_{l \rightarrow \infty} \frac{c w_l(G)}{\lambda_1^l} = \lim_{l \rightarrow \infty} \left[1 + (-1)^l + \sum_{i=2}^{n-1} \left(\frac{\lambda_i}{\lambda_1} \right)^l \right].$$

The limit does not exist since it approaches 2 when l is even and 0 when l is odd.

Let us now discuss the relationship between the spectral radius of a graph and its chromatic number.

Definition 3.3.15. *The chromatic number $\chi(G)$ of a graph G is the minimum number of colours required to colour the vertices of G such that no adjacent vertices share the same colour.*

Examples of some graphs with their chromatic number are shown in Figure 3.10.

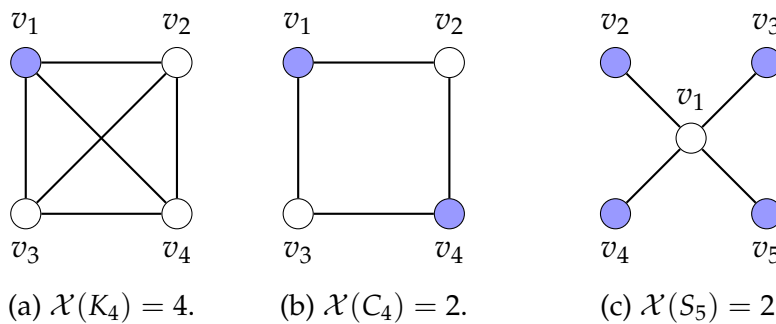


Figure 3.10: Graphs and their chromatic numbers.

Theorem 3.3.16 ([2], p. 31). *Let G be a simple graph and $\chi(G)$ its chromatic number. Then the chromatic number is bounded above by $\rho(G) + 1$. That is*

$$\chi(G) \leq \rho(G) + 1.$$

Equality holds when G is a complete graph.

Proof. Let $\mathcal{X}(G) = k$ such that $k \geq 1$. For the case when $k = 1$, the theorem holds trivially by the definition of the spectral radius. Let H be a subgraph of G such that $\mathcal{X}(H) = k$ and that H is minimal with respect to the number of vertices. That is, $\mathcal{X}(H \setminus v_i) < k$ for $v_i \in V(H)$.

Let $\delta(H)$ be the smallest degree of H . To prove the theorem, we show that $\delta(H) \geq k - 1$. We assume that there exist a vertex $v_i \in V(H)$ such that the degree, denoted by d_{v_i} , is less than $k - 1$. We know that $\mathcal{X}(H \setminus v_i) < k$ so we can colour $H \setminus v_i$ with $k - 1$ distinct colours. By our assumption, we can also colour H with $k - 1$ distinct colours since $d_{v_i} < k - 1$. We have a contradiction since $\mathcal{X}(H) = k$. It implies that $\delta(H) \geq k - 1$.

From Theorem 3.1.3, we have $\rho(H) \geq \delta(H)$ and also from Theorem 3.1.5 we have $\rho(H) \leq \rho(G)$. Therefore, we get

$$k - 1 \leq \delta(H) \leq \rho(H) \leq \rho(G).$$

For a complete graph K_n of order n , its chromatic number is equal n . This completes the proof. \square

3.4 Bounds on the spectral radius

The relationship between graph parameters and the spectral radius has been established in the previous section. However, it would be more interesting if one can bound the spectral radius using these graph parameters since determining the spectral radii of graphs is sometimes difficult. In light of this, a lot of research has been conducted to find upper and lower bounds on the spectral radii of graphs (see [26, 18, 17, 19, 34, 24, 6]). In this section we present some of these bounds in terms of graph parameters such as the number of vertices and edges, the number of walks and the degree sequence.

Let us first consider upper bounds in terms of the number of vertices and edges.

Theorem 3.4.1. *Let A_G be the adjacency matrix of a graph G . Then*

$$\rho(A_G) \leq \sqrt{2nm},$$

where n and m are the order and size of G respectively.

Proof. Let A_G be the adjacency matrix of a graph G of order n and size m . Then by Theorem 2.1.17 we know that

$$\rho(A_G) \leq \sqrt{n \cdot \text{tr}(A_G^2)}$$

and by Corollary 3.3.11 we have

$$\text{tr}(A_G^2) = \sum_{i=1}^n \lambda_i^2 = 2m.$$

Hence the result follows. □

Remark 3.4.2. Suppose $\lambda_i, 1 \leq i \leq n$, are the eigenvalues of a graph G of order n . We define its energy \mathbb{E}_G as

$$\mathbb{E}_G = \sum_{i=1}^n |\lambda_i|.$$

It is clear that the spectral of a graph G is always less than or equal to its energy, i.e. $\rho(A_G) \leq \mathbb{E}_G$. From the proof of Theorem 2.1.17 and by Corollary 3.3.11, we get

$$\mathbb{E}_G \leq \sqrt{2nm}.$$

Theorem 3.4.3 ([2], p. 31). Let A_G be the adjacency matrix of a graph G of order n and size m . Then the spectral radius satisfies

$$\rho(G) \leq \sqrt{\frac{2m(n-1)}{n}}.$$

Proof. Let the eigenvalues of G be given by $\rho(G) = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. If we let $\mathbf{x} = \{\lambda_2, \dots, \lambda_n\}$ and $\mathbf{y} = \{1, \dots, 1\}$ then by the Cauchy-Schwarz inequality we get

$$\left[\sum_{i=2}^n |\lambda_i| \right]^2 \leq (n-1) \sum_{i=2}^n \lambda_i^2. \quad (3.13)$$

But we know that

$$\lambda_1 = - \sum_{i=2}^n \lambda_i \leq \sum_{i=2}^n |\lambda_i|$$

and

$$2m - \lambda_1^2 = \sum_{i=2}^n \lambda_i^2,$$

so the inequality (3.13) becomes

$$\begin{aligned}\lambda_1^2 &\leq (n-1)(2m - \lambda_1^2) \\ \lambda_1^2 + (n-1)\lambda_1^2 &\leq 2m(n-1) \\ \lambda_1^2 &\leq \frac{2m(n-1)}{n} \\ \lambda_1 &\leq \sqrt{\frac{2m(n-1)}{n}}.\end{aligned}$$

□

Corollary 3.4.4. *Let A_G be the adjacency matrix of a graph G of order n . Then*

$$\rho(G) \leq n - 1.$$

Proof. We know that $m \leq \frac{n(n-1)}{2}$, so with this fact and Theorem 3.4.3 we have that

$$\begin{aligned}\rho(G) &\leq \sqrt{\frac{2m(n-1)}{n}} \\ &\leq \sqrt{\left(\frac{2(n-1)}{n}\right) \left(\frac{n(n-1)}{2}\right)} \\ &= n - 1.\end{aligned}$$

□

We therefore obtain an upper bound for the spectral radius in terms of only the number of vertices. Note that equality holds for complete graphs. It then follows that the complete graph K_n has the maximum spectral radius among all simple graphs of order n .

Now, let us consider some bounds in terms of the number of walks in graph. One important result that can easily be deduced from our discussion on the number of walks in graph (in Section 3.3) is captured in the following theorem. Note that Nikiforov in [26] proved a generalised version of our result and also introduced more upper bounds in terms of the number of walks and the clique number of a graph.

Theorem 3.4.5. *Let $\rho(G)$ be the spectral radius of a graph G of order n . Then for $k \geq 1$,*

$$\rho^k(G) \geq \frac{w_k(G)}{w_0(G)}.$$

Equality holds when G is a regular graph.

Proof. From Theorem 2.1.15, if we let $\mathbf{x} = \mathbf{1}$ then we have

$$\rho^k(A_G) \geq \frac{\mathbf{1}^T A_G^k \mathbf{1}}{\mathbf{1}^T \mathbf{1}} = \frac{w_k(G)}{w_0(G)}.$$

We know that equality holds when $\mathbf{1}$ is an eigenvector. So by Theorem 3.2.12 we have equality for regular graphs. \square

We obtain the following corollaries where we introduce some lower bounds in terms of the average degree and the degree sequence of a graph.

Corollary 3.4.6. *Let $\rho(G)$ be the spectral radius of a graph G of order n and \mathcal{D} its average degree. Then $\rho(G) \geq \mathcal{D}$. Equality holds for regular graphs.*

Proof. The proof is analogous to the proof of Theorem 3.4.5 by setting $k = 1$. \square

Corollary 3.4.7 ([17, 18, 34, 6]). *Let $\rho(G)$ be the spectral radius of a graph G of order n and $(d(v_1), \dots, d(v_n))$ its degree sequence. Then*

$$\rho(G) \geq \sqrt{\frac{1}{n} \sum_{i=1}^n d^2(v_i)}.$$

Equality holds for regular and semi-regular graphs.

Proof. We set $k = 2$ in Theorem 3.4.5 to obtain

$$\rho(G) \geq \sqrt{\frac{w_2(G)}{n}}.$$

Now we need to show that $w_2(G) = \sum_{i=1}^n d^2(v_i)$. To do this, we let a_{ij} be the ij -th entry of the adjacency matrix A_G . Then by the definition of an adjacency matrix, we know that the degree of the vertex $v_i \in V(G)$ is given by $d(v_i) = \sum_{j=1}^n a_{ij}$. Now considering the equation $w_2(G) = \mathbf{1}^T A^2 \mathbf{1}$ and applying matrix multiplication we get

$$\begin{aligned} \mathbf{1}^T A^2 \mathbf{1} &= \sum_{k=1}^n \sum_{j=1}^n \sum_{i=1}^n a_{jk} a_{ki} \\ &= \sum_{k=1}^n \sum_{j=1}^n a_{kj} \sum_{i=1}^n a_{ki} \\ &= \sum_{k=1}^n d^2(v_k). \end{aligned}$$

For equality holding for regular graphs we use the same argument from the proof of Theorem 3.4.5. Now let us show why equality also holds for semi-regular graphs. Let d_1, d_2 be the respective degrees of each vertex in the partite sets V_1, V_2 of a semi-regular graph H of order n . If we let $|V_1| = a$ then we know that $ad_1 = (n - a)d_2$. We have

$$\begin{aligned} \sum_{k=1}^n d^2(v_k) &= ad_1^2 + (n - a)d_2^2 \\ &= ad_1^2 + ad_1d_2 - ad_1d_2 + (n - a)d_2^2 \\ &= ad_1(d_1 + d_2) - d_2(ad_1 - (n - a)d_2) \end{aligned}$$

From the equation $ad_1 = (n - a)d_2$, we obtain $d_1 + d_2 = \frac{nd_2}{a}$. So we get

$$\sum_{k=1}^n d^2(v_k) = nd_1d_2.$$

Therefore, by Theorem 3.2.14 the result holds. \square

The following result is as a consequence of Theorem 3.1.5.

Theorem 3.4.8. *Let G be a graph with an r -regular graph as a subgraph. Then*

$$r \leq \rho(A_G)$$

with equality when G is r -regular.

Proof. This Theorem follows directly from Theorem 3.1.5 and Theorem 3.2.12. \square

It follows from Theorem 3.4.8 that if a graph G contains a cycle then its spectral radius $\rho(G) \geq 2$.

Corollary 3.4.9. *If the spectral radius $\rho(G)$ of a connected graph G is less than 2, then G is a tree.*

Proof. Trees contain no cycles so they are the only connected graphs with possible spectral radius less than 2. \square

Remark 3.4.10. *This does not imply that all trees have spectral radii less than 2. For instance, star graphs of order $n \geq 5$ all have spectral radii greater than or equal to 2. However, paths are examples of trees that satisfy Corollary 3.4.9. This is as a consequence of Corollary 3.2.6. This shows that knowing the spectral radius of a graph can (to some extent) imply the structure of the graph.*

Corollary 3.4.11. *The path P_n has the minimum spectral radius among all graphs of order n with 2 pendant vertices.*

Proof. The proof follows from the well known fact that a path P_n is the only tree with two pendant vertices. Moreover, if such a graph is not a tree then obviously it contains a cycle and hence by Theorem 3.4.8 the result holds. \square

3.5 Extremal trees

In this section, we focus on extremal trees among all trees with a prescribed order, degree sequence, number of leaves and maximum degree.

Definition 3.5.1 ([33]). *The greedy tree $G(\alpha)$, also known as BFD-tree [5], is a rooted tree obtained from a degree sequence α by the following "greedy algorithm":*

- (i) *assign the largest degree to the root r ;*
- (ii) *label the neighbours of r as $v_1, v_2, \dots, v_{d(r)}$, from left to right or vice versa, and assign the largest degrees available to them such that $d(v_1) \geq d(v_2) \geq \dots \geq d(v_{d(r)})$;*
- (iii) *label the neighbours of v_1 (except r) as $v_{11}, v_{12}, \dots, v_{1d(v_1)}$ and assign degrees as in (ii);*
- (iv) *Repeat (iii) for $v_2, v_3, \dots, v_{d(r)}$ and all the newly labelled vertices. The neighbours of the labelled vertex with the largest degrees whose neighbours are not yet labelled should be considered first.*

Example 3.5.2. *We construct a greedy tree for the degree sequence:*

$$\alpha = (4, 3, 3, 2, 2, 2, 1, 1, 1, 1, 1, 1).$$

The degree of the root r is 4, and it has the neighbours v_1, v_2, v_3, v_4 . We therefore assign the next largest available degree, which is 3, to v_1 and repeat the procedure for the other vertices. Following the algorithm yields Figure 3.11.

The following lemma gives a characterisation of a greedy tree.

Lemma 3.5.3 ([33]). *A rooted tree T with a given degree sequence is a greedy tree if*

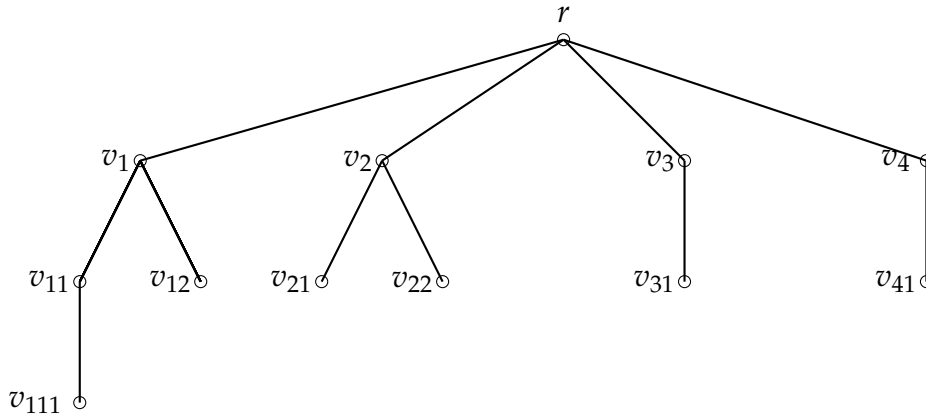


Figure 3.11: A greedy tree $G(\alpha)$.

- (i) the root r has the largest degree;
- (ii) the heights of any two leaves differ by at most 1. Recall that the height $h_T(v)$ of a vertex v is the distance from v to the root r ;
- (iii) for any two vertices v and w , if $h_T(v) < h_T(w)$, then $d(v) \geq d(w)$;
- (iv) for any two vertices v and w of the same height, if $d(v) > d(w)$, then $d(v') \geq d(w')$ for any successors v' of v and w' of w of the same height;
- (v) for any two vertices v and w of the same height, if $d(v) > d(w)$, then $d(v') \geq d(w')$ and $d(v'') \geq d(w'')$ for any siblings v' of v and w' of w or successors v'' of v' and w'' of w' of w of the same height.

Theorem 3.5.4 ([5]). *The optimal tree T_{\max} that maximizes the spectral radius among all trees with the same degree sequence α is the greedy tree $G(\alpha)$.*

We use the same technique used by Biyikoğlu and Leydold in [5] to prove Theorem 3.5.4. That is, investigating the change in the spectral radius of a tree T resulting from rearranging its edges. We therefore state some definitions and lemmas which will help us to prove this theorem.

The Rayleigh quotient of the adjacency matrix of an n -vertex tree T on a unit vector \mathbf{f} is given by

$$R_T(\mathbf{f}) = 2 \sum_{uv \in E(T)} f(u)f(v), \quad (3.14)$$

where $f(u)$ is the component of \mathbf{f} corresponding to the vertex u . By Theorem 2.1.15, we get

$$\rho(T) \geq R_T(\mathbf{f}),$$

with equality if \mathbf{f} is an eigenvector corresponding to $\rho(T)$.

Lemma 3.5.5 ([5]). *For any two vertices u and v in an optimal tree T_{\max} , if $d(u) > d(v)$ then $f(u) > f(v)$, where \mathbf{f} is the Perron vector of T_{\max} .*

Proof. We assume (for contradiction) that $d(u) > d(v)$ such that $d(u) - d(v) = k$ but $f(u) \leq f(v)$. Let $w_i, 1 \leq i \leq k$, be neighbours of u such that the path from u to v is contained in the path from w_i to v . We then increase the degree of v by deleting the edges of the form $uw_i, 1 \leq i \leq k$, in T_{\max} and adding the edges of the form $vw_i, 1 \leq i \leq k$. We obtain a new tree T' from T_{\max} with the same degree sequence. We let the edge sets of T' and T_{\max} be denoted by E' and E respectively. By rearranging the edges we obtain

$$\begin{aligned} R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f}) &= 2 \left(\sum_{x'y' \in E' \setminus E} f(x')f(y') - \sum_{xy \in E \setminus E'} f(x)f(y) \right) \\ &= 2 \left(\sum_{i=1}^k f(v)f(w_i) - \sum_{i=1}^k f(u)f(w_i) \right) \\ &= 2 \left(\sum_{i=1}^k [f(v) - f(u)]f(w_i) \right) \\ &\geq 0. \end{aligned}$$

It then follows that $R_{T'}(\mathbf{f}) \geq R_{T_{\max}}(\mathbf{f})$, which by Theorem 2.1.15 implies that

$$\rho(T') \geq R_{T'}(\mathbf{f}) \geq R_{T_{\max}}(\mathbf{f}) = \rho(T_{\max}).$$

Equality, i.e. $\rho(T') = \rho(T_{\max})$, holds if and only if \mathbf{f} is also a Perron vector for T' . So from the equation $A_{T'}\mathbf{f} = \rho(T')\mathbf{f}$ we obtain

$$\rho(T')f(v) = \sum_{i=1}^k f(w_i) + \sum_{xv \in E} f(x) > \sum_{xv \in E} f(x) = \rho(T_{\max})f(v). \quad (3.15)$$

Hence a contradiction occurs here. This forces $\rho(T') > \rho(T_{\max})$ and this also contradicts the fact that T_{\max} is the optimal tree. \square

Remark 3.5.6. *For the case when $f(u) = f(v)$ in T_{\max} , one can easily deduce from equation 3.15 that $d(u) = d(v)$.*

Lemma 3.5.7 ([5]). *Let \mathbf{f} be the Perron vector of an optimal tree T_{\max} . Suppose $f(u) \geq f(v)$ for $u, v \in V(T_{\max})$. If u', v' are the successors of u, v respectively with $P(u', v') \subset P(u, v)$ (or vice versa) such that $f(u) \geq f(u')$ and $f(v) \geq f(v')$, then $f(u') \geq f(v')$.*

Proof. The proof is analogous to the proof of Lemma 3.5.5. We assume $f(u') < f(v')$ and form another tree T' with the same degree sequence as T_{\max} by deleting the edges uu' and vv' and adding the edges uv' and vu' . We obtain

$$R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f}) = 2[(f(u) - f(v))(f(v') - f(u'))] \geq 0.$$

It follows from Theorem 2.1.15 that $\rho(T') \geq R_{T'}(\mathbf{f}) \geq R_{T_{\max}}(\mathbf{f}) = \rho(T_{\max})$ with equality if and only if \mathbf{f} is also a Perron vector for T' . So from the equations $A_{T_{\max}}\mathbf{f} = \rho(T_{\max})\mathbf{f}$ and $A_{T'}\mathbf{f} = \rho(T')\mathbf{f}$ we obtain

$$\begin{aligned} \rho(T_{\max})f(u) &= \sum_{ux \in E} f(x) = f(u') + \sum_{ux \in E \cap E'} f(x), \\ \rho(T')f(u) &= \sum_{ux \in E'} f(x) = f(v') + \sum_{ux \in E \cap E'} f(x). \end{aligned}$$

This implies that $f(u') = f(v')$, hence a contradiction. Moreover, $\rho(T') > \rho(T_{\max})$ also contradicts the fact that T_{\max} is the optimal tree. \square

Now we present the proof of Theorem 3.5.4 by showing that the construction of the optimal tree follows the greedy algorithm.

Proof of Theorem 3.5.4. Let T_{\max} be an optimal tree among all trees with the same degree sequence and \mathbf{f} its Perron vector. We let the root $r \in V(T_{\max})$ be the vertex corresponding to the maximum component of \mathbf{f} . Then by Lemma 3.5.5 we get $d(r) \geq d(u)$, for any other vertex $u \in V(T_{\max})$. We shall call all the vertices of T_{\max} which have distance j from the root r vertices on the j -th level. So for the vertices on the first level, we have the neighbours of r denoted by $v_1, v_2, \dots, v_{d(r)}$. By Lemma 3.5.7, we know that the entries of \mathbf{f} corresponding to the neighbours of r are larger than those of any other vertex. We can without loss of generality assume that $f(v_1) \geq f(v_2) \geq \dots \geq f(v_{d(r)})$. So by Lemma 3.5.5 we get $d(v_1) \geq d(v_2) \geq \dots \geq d(v_{d(r)})$. Now we consider those vertices on the second level. If we let $v_{i1}, v_{i2}, \dots, v_{id(v_i)}$ be the neighbours of v_i for $1 \leq i \leq d(r)$, then for each v_i , we can assume that $f(v_{i1}) \geq f(v_{i2}) \geq \dots \geq f(v_{id(v_i)})$, which by Lemma 3.5.5 implies $d(v_{i1}) \geq d(v_{i2}) \geq \dots \geq d(v_{id(v_i)})$. Now if we let v'_i and v'_j be neighbours of v_i and v_j respectively where $i > j$, then applying Lemma 3.5.7 we get $f(v'_i) \geq f(v'_j)$, which again by Lemma 3.5.5 implies that $d(v'_i) \geq d(v'_j)$. Continuous application of Lemma 3.5.5 and Lemma 3.5.7 to the vertices at

higher levels reveals that in the optimal tree the larger the distance of a vertex from the root the smaller its degree. Also, vertices on the same level are ordered with respect to non-increasing degrees. This construction of the optimal tree corresponds to the greedy algorithm. Hence T_{\max} is the greedy tree. \square

Our next goal is to find the extremal tree among all trees with prescribed maximum degree and number of leaves. We begin by introducing the concept of majorization which will help us compare trees with different degree sequences.

Definition 3.5.8. Let $X = (x_1, \dots, x_n)$ and $Y = (y_1, \dots, y_n)$ be sequences of non-negative numbers. If for all $1 \leq k \leq n$ we have

$$\sum_{i=1}^k x_i \leq \sum_{i=1}^k y_i$$

then Y majorizes X . Suppose S_n is the set of all permutation of $\{1, \dots, n\}$. If for any $\sigma \in S_n$ the sequence Y still majorizes $(x_{\sigma(1)}, \dots, x_{\sigma(n)})$, then we write $X \preceq Y$.

The set S_n consists of $n!$ permutations. However, one does not need to check for all of them in order to show that $X \preceq Y$. This is because, if we let $\sigma \in S_n$ be the permutation corresponding to the sequence satisfying $x_{\sigma(1)} \geq \dots \geq x_{\sigma(n)}$, then we can see that $(x_{\sigma'(1)}, \dots, x_{\sigma'(n)}) \preceq (x_{\sigma(1)}, \dots, x_{\sigma(n)})$ for all other $\sigma' \in S_n$. So proving that $X \preceq Y$ is equivalent to showing that $(x_{\sigma(1)}, \dots, x_{\sigma(n)}) \preceq Y$.

Remark 3.5.9. It is important to note that majorization is transitive. That is, if $X \preceq Y$ and $Y \preceq Z$ then it implies that $X \preceq Z$.

Remark 3.5.10. Let X and Y be two degree sequences of two n -vertex trees. It then follows from Proposition 2.2.10 that

$$\sum_{i=1}^n x_i = \sum_{i=1}^n y_i = 2(n-1),$$

even if $X \preceq Y$ or vice versa.

Theorem 3.5.11 ([5]). Let X and Y be the degree sequences of n -vertex trees. Suppose $X \preceq Y$; then

$$\rho(G(X)) \leq \rho(G(Y)).$$

Equality holds if and only if $X = Y$.

We state and prove the following Lemma which will help us to prove Theorem 3.5.11.

Lemma 3.5.12 ([5, 35]). *Let $X = (x_1, \dots, x_n)$ and $X' = (x'_1, \dots, x'_n)$ be two non-increasing degree sequences of trees. If $X \preceq X'$, then there exists a sequence of k trees with degree sequences X_1, \dots, X_k such that $X \preceq X_1 \preceq \dots \preceq X_k \preceq X'$, where exactly two entries of X_i and X_{i+1} differ by 1, i.e. $x_p(x'_p)$ and $x_q(x'_q)$ of $X_i(X_{i+1})$, are such that $x'_p = x_p - 1, x'_q = x_q + 1$, where $p > q$.*

Proof. Suppose $X \preceq X'$ and $X \neq X'$. Now, we let j be the first index from 1 to n such that $x_j > x'_j$ and let i be the first index from j to 1 such that $x_i < x'_i$, where $x_p = x'_p$ for all $i < p < j$. Note that by the definition of majorization such positions exist. Now we construct the sequence X_k from X' by replacing x'_i by $x'_i - 1$ and x'_j by $x'_j + 1$. So we get $X_k = (x'_1, \dots, x'_i - 1, \dots, x'_j + 1, \dots, x'_n)$ which by Proposition 2.2.10 is still a degree sequence of a tree. It can be observed that $x'_i - 1 \geq x_i$ and $x'_j + 1 \leq x_j$, so we get $X \preceq X_k \preceq X'$. Now, we can apply the same procedure to X and X_k to obtain X_{k-1} . Continuous repetition of this process yields the result. \square

Proof of Theorem 3.5.11. If $X \preceq Y$ and $X \neq Y$, then we know from Lemma 3.5.12 that there exists a degree sequence X_1 such that $X \preceq X_1 \preceq Y$, where X and X_1 differ in exactly two positions. So we get the two non-increasing sequences to be

$$\begin{aligned} X &= (x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_n), \\ X_1 &= (x_1, x_2, \dots, x_i + 1, \dots, x_j - 1, \dots, x_n). \end{aligned}$$

By the definition of majorization, we can assume that $x_i \geq x_j \geq 2$. Let u and v be vertices in the greedy tree $G(X)$ such that $d(u) = x_i$ and $d(v) = x_j$. Let w be a neighbour of v . If we remove the edge vw and add the edge uw to $G(X)$ then clearly we obtain a new tree T' with degree sequence X_1 . If we let \mathbf{f} be the Perron vector for $G(X)$ then it follows from Lemma 3.5.5 that $f(u) \geq f(v)$. We let E and E' denote the edge sets of $G(X)$ and T' respectively. So

$$\begin{aligned} R_{T'}(\mathbf{f}) - R_{G(X)}(\mathbf{f}) &= 2 \left(\sum_{x'y' \in E' \setminus E} f(x')f(y') - \sum_{xy \in E \setminus E'} f(x)f(y) \right) \\ &= 2f(w)(f(u) - f(v)) \geq 0. \end{aligned}$$

We get that $\rho(T') \geq \rho(G(X))$. Equality holds if and only if f is also a Perron vector for T' . So we obtain

$$\rho(T')f(u) = f(w) + \sum_{xu \in E} f(x) > \sum_{xu \in E} f(x) = \rho(G(X))f(u),$$

which is impossible. It follows from Theorem 3.5.4 that $\rho(T') \leq \rho(G(X_1))$. So we get $\rho(G(X)) \leq \rho(G(X_1))$. We iterate this process to obtain the result. \square

Definition 3.5.13. A *Volkman tree* $V_{n,\Delta}$ is a greedy tree of order n with degree sequence $\alpha = (\Delta, \dots, \Delta, r, 1, \dots, 1)$, where Δ is the maximum degree and $0 < r < \Delta$.

Example 3.5.14. The figure below is a Volkman tree with the degree sequence: $\alpha = (3, 3, 3, 3, 3, 3, 3, 3, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$.

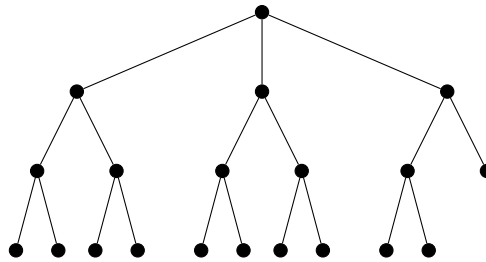


Figure 3.12: A Volkman tree $V_{20,3}$.

The key feature of Theorem 3.5.11 is to allow us to compare the spectral radius of two trees of the same order but with different degree sequence. With this, we obtain the following corollaries.

Corollary 3.5.15. Among all trees of order n with maximum degree Δ , the Volkman tree maximizes the spectral radius.

Proof. Let $\mathbb{T}_{n,\Delta}$ denote the set of all trees of order n with maximum degree Δ . Let $X = (x_1, x_2, \dots, x_n)$ be the degree sequence of a tree $T \in \mathbb{T}_{n,\Delta}$. By Theorem 3.5.4, we know that $\rho(G(X)) \geq \rho(T)$. Obviously,

$$(x_1, x_2, \dots, x_n) \preceq (\Delta, \dots, \Delta, r, 1, \dots, 1).$$

It then follows from Theorem 3.5.11 that $\rho(G(X)) \leq \rho(V_{n,\Delta})$. This completes the proof. \square

Corollary 3.5.16. *Among all trees of order n with k leaves, the tree corresponding to the degree sequence $\alpha = (k, 2, \dots, 2, 1, \dots, 1)$ maximizes the spectral radius.*

Proof. Let $\mathbb{T}_{n,k}$ denote the set of all trees of order n with k leaves. Let $X = (x_1, x_2, \dots, x_n)$ be the degree sequence of a tree $T \in \mathbb{T}_{n,k}$. Then we have $x_i > 1$ for $1 \leq i \leq (n - k)$ and $x_j = 1$ for $(n - k + 1) \leq j \leq n$. Moreover, it is clear that

$$(x_1, x_2, \dots, x_n) \preceq (k, 2, \dots, 2, 1, \dots, 1).$$

The result then follows from Theorems 3.5.4 and 3.5.11. \square

In particular, the greedy tree with k leaves corresponding to the degree sequence $\alpha = (k, 2, \dots, 2, 1, \dots, 1)$ is either an extended star graph or a subgraph of an extended star graph as defined in Section 3.2.7. With this, we obtain an upper bound of the spectral radius in terms of the number of leaves. This result is captured in the following corollary.

Corollary 3.5.17. *Let $l(T)$ be the number of leaves in a tree T of order n . Then the spectral radius $\rho(T)$ satisfies the inequality*

$$\rho(T) < \frac{l(T)}{\sqrt{l(T) - 1}}.$$

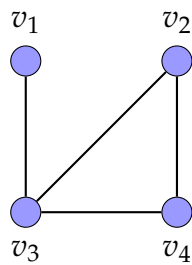
Proof. In an extended star graph $E_{k,d}$, we know that the number of leaves $l(E_{k,d})$ is equal to the degree d of the root. The result then follows from Corollary 3.5.16 and Theorem 3.2.22. \square

Chapter 4

The Distance Matrix

4.1 Introduction

Let G be a graph with n vertices. The distance matrix of G , denoted by D_G , is the symmetric matrix whose ij -th entry is the length of the shortest path from vertex v_i to vertex v_j . The eigenvalues of D_G are real and they sum up to 0, since the trace is equal to 0. The spectral radius of the distance matrix of a graph G will be denoted by $\mu(G)$. For simplicity, we will call $\mu(G)$ the distance spectral radius of G . Relabelling of the vertices does not affect the distance spectral radius by the same reasoning as for the spectral radius of the adjacency matrix. An example of the distance matrix D_G of a graph G is shown in Figure 4.1.



(a) The graph G .

$$D_G = \begin{matrix} & \begin{matrix} v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} & \begin{pmatrix} 0 & 2 & 1 & 2 \\ 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 2 & 1 & 1 & 0 \end{pmatrix} \end{matrix}.$$

(b) Distance matrix D_G .

Figure 4.1: A graph and its distance matrix.

Proposition 4.1.1. *The distance matrix D_G of a graph G is irreducible if G is connected.*

Proof. The proof is analogous to the proof of Proposition 3.1.1. □

By definition and Proposition 4.1.1, the distance matrix D_G of a connected graph satisfies the conditions of the Perron-Frobenius Theorem hence its spectral radius is equal to the largest positive eigenvalue.

Let λ be an eigenvalue of the distance matrix D_G of a graph G and x its corresponding eigenvector. Then by the definition of an eigenvalue, we get

$$\lambda x_u = \sum_{v \neq u} d_G(u, v) x_v,$$

where $d_G(u, v)$ is the distance between the vertices u and v , and x_v the component of the non-zero vector x corresponding to the vertex v .

4.2 Distance spectral radii of some classes of graphs

4.2.1 Vertex-Transitive graphs

We define an automorphism of a graph G as an isomorphism from G to itself, i.e. an automorphism $f : V(G) \rightarrow V(G)$. Two vertices v_1 and v_2 are said to be similar if there is an automorphism f such that $f(v_1) = v_2$. A vertex-transitive graph G is a graph in which any pair of its vertices are similar.

A graph is symmetric if any pair of adjacent vertices can be mapped to any other pair by an automorphism. Note that every symmetric graph without isolated vertices is vertex-transitive but not all vertex-transitive graphs are symmetric.

Every vertex-transitive graph is regular but not all regular graphs are vertex-transitive. Examples of vertex-transitive graphs are the complete graph K_n , the n -cycle C_n , the complete bipartite graph $K_{n,n}$ etc.

If we consider the distance matrix of a vertex-transitive graph G , then it can be observed that for each vertex u

$$\sum_{v \in V(G)} d_G(u, v) = r, \tag{4.1}$$

is a constant that is independent of u . It follows that the sum of each row in D_G is equal to r . This idea leads us to the following theorem.

Theorem 4.2.1. *A vertex-transitive graph G has r (as defined in equation 4.1) as the spectral radius of the distance matrix D_G and $\mathbf{1}$ as its corresponding eigenvector (Perron vector).*

Proof. If we let $x = \mathbf{1}$, then we have

$$\begin{aligned} \sum_{v \neq u} d_G(u, v)x_v &= \sum_{v \neq u} d_G(u, v) = r, \\ \Rightarrow D_G \cdot \mathbf{1} &= r \cdot \mathbf{1}. \end{aligned}$$

It follows that r is an eigenvalue of the distance matrix D_G of a vertex-transitive graph G and it corresponds to a positive eigenvector $\mathbf{1}$. So by Theorem 2.1.19, r is the spectral radius. \square

Corollary 4.2.2. *The spectral radius of the distance matrix of the complete graph K_n of order n is $n - 1$.*

Proof. For a complete graph K_n , each vertex is adjacent to all other vertices and $d_{K_n}(u, u) = 0$ so we have

$$r = \sum_v d_{K_n}(u, v) = \sum_v 1 = n - 1$$

for all $u \in V(K_n)$. \square

Corollary 4.2.3 ([23]). *The spectral radius of the distance matrix of a cycle of order n is $\frac{n^2}{4}$ if n is even and $\frac{n^2-1}{4}$ if n is odd.*

Proof. We label the vertices of the cycle such that v_i is adjacent to v_{i+1} , where $i = 1, 2, \dots, n - 1$, and v_n is adjacent to v_1 . Therefore, if n is even then each row of D_{C_n} has the entries $\{1, 2, 3, \dots, \frac{n}{2}, \frac{n}{2} - 1, \frac{n}{2} - 2, \dots, 2, 1\}$. Now, the spectral radius r is by Theorem 4.2.1 equal to the sum of the entries of each row in D_{C_n} which is given by

$$\begin{aligned} r &= \sum_{k=1}^{\frac{n}{2}} k + \sum_{k=1}^{\frac{n}{2}-1} k \\ &= \frac{\frac{n}{2}(\frac{n}{2} + 1)}{2} + \frac{\frac{n}{2}(\frac{n}{2} - 1)}{2} \\ &= \frac{n^2}{4}. \end{aligned}$$

Also, if n is odd then each row of D_{C_n} has the entries $\{1, 2, 3, \dots, \frac{n-1}{2}, \frac{n-1}{2}, \frac{n-1}{2} - 1, \dots, 2, 1\}$. Then we get

$$\begin{aligned} r &= 2 \sum_{k=1}^{\frac{n-1}{2}} k \\ &= \frac{n^2 - 1}{4}. \end{aligned}$$

□

Corollary 4.2.4 ([7]). *Let $K_{n,n}$ be a complete bipartite graph of order $2n$. Then the spectral radius of its distance matrix is $3n - 2$.*

Proof. Let the vertex set of $K_{n,n}$ consist of the partite sets $V_1 = \{v_1, v_2, \dots, v_n\}$ and $V_2 = \{v_{n+1}, \dots, v_{2n}\}$. By the definition of complete bipartite graphs and the distance matrix of a graph, we have $d_{K_{n,n}}(v_i, v_j) = 2$ if $v_i, v_j \in V_1$ or $v_i, v_j \in V_2$ and $d_{K_{n,n}}(v_i, v_j) = 1$ if v_i and v_j are in different vertex sets, i.e., $v_i \in V_1$ and $v_j \in V_2$ or vice versa. Hence each row in $D_{K_{n,n}}$ has $n - 1$ 2s and n 1s, it follows that $r = 2(n - 1) + n = 3n - 2$. □

4.2.2 Complete bipartite graphs

Suppose $K_{m,n}$ is a complete bipartite graph with partite vertex sets $V_1 = \{v_1, \dots, v_m\}$ and $V_2 = \{v_{m+1}, \dots, v_{m+n}\}$. Its distance matrix $D_{K_{m,n}}$ is of the form

$$D_{K_{m,n}} = \begin{matrix} & \begin{matrix} v_1 & v_2 & \cdots & v_m & v_{m+1} & v_{m+2} & \cdots & v_{m+n} \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ \vdots \\ v_m \\ v_{m+1} \\ v_{m+2} \\ \vdots \\ v_{m+n} \end{matrix} & \begin{pmatrix} 0 & 2 & \cdots & 2 & 1 & 1 & \cdots & 1 \\ 2 & 0 & \ddots & \vdots & 1 & 1 & \cdots & 1 \\ \vdots & \ddots & \ddots & 2 & \vdots & \vdots & \vdots & \vdots \\ 2 & \cdots & 2 & 0 & 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 & 0 & 2 & \cdots & 2 \\ 1 & 1 & \cdots & 1 & 2 & 0 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 2 \\ 1 & 1 & \cdots & 1 & 2 & \cdots & 2 & 0 \end{pmatrix} \end{matrix}.$$

Theorem 4.2.5 ([7]). *The eigenvalues of the distance matrix of a complete bipartite graph $K_{m,n}$ are -2 with multiplicity $m + n - 2$, $(m + n - 2) + \sqrt{(m + n)^2 - 3mn}$ and $(m + n - 2) - \sqrt{(m + n)^2 - 3mn}$. Therefore, the distance spectral radius $\mu(D_{K_{m,n}})$ is given by $(m + n - 2) + \sqrt{(m + n)^2 - 3mn}$.*

Proof. Let $D_{K_{m,n}}$ be of the form as noted above. Now, we shall consider the matrix $-2I - D_{K_{m,n}}$. It can be observed that the columns (or rows) associated with vertices from the same partite sets are the same and those associated with vertices from different partite sets are linearly independent. Hence the matrix $-2I - D_{K_{m,n}}$ has rank 2. This implies that -2 is an eigenvalue of $D_{K_{m,n}}$ with multiplicity $m + n - 2$.

To find the other eigenvalues, we let λ be a real number and \mathbf{x} a non-zero vector, whose entries are defined in a similar way as in the proof of Theorem 3.2.16. If the following set of equations,

$$2(m-1)a + nb = \lambda a, \quad (4.2)$$

$$2(n-1)b + ma = \lambda b, \quad (4.3)$$

is satisfied, then we can deduce that $D_{K_{m,n}}\mathbf{x} = \lambda\mathbf{x}$ which implies that λ is an eigenvalue and its corresponding eigenvector is \mathbf{x} . Now, we solve the equations simultaneously for λ . From equation (4.2) we get

$$a = \frac{-nb}{2(m-1) - \lambda}$$

and substituting into equation (4.3) gives us

$$2(n-1)b + \frac{-nmb}{2(m-1) - \lambda} = \lambda b$$

$$4(m-1)(n-1) - 2\lambda(n-1) - mn = 2\lambda(m-1) - \lambda^2$$

$$\lambda^2 - 2\lambda(m+n-2) + 4mn - 4m - 4n + 4 - mn = 0$$

$$\lambda^2 - 2\lambda(m+n-2) + 3mn - 4(m+n-1) = 0.$$

Therefore, we get

$$\begin{aligned} \lambda &= \frac{2(m+n-2) \pm \sqrt{4(m+n-2)^2 - 12mn + 16(m+n-1)}}{2} \\ &= m+n-2 \pm \sqrt{(m+n-2)^2 - 3mn + 4(m+n-1)} \\ &= m+n-2 \pm \sqrt{(m+n)^2 - 4(m+n) + 4 - 3mn + 4(m+n-1)} \\ &= m+n-2 \pm \sqrt{(m+n)^2 - 3mn}. \end{aligned}$$

If \mathbf{x} is positive then it is the Perron vector and hence we have $m+n-2 + \sqrt{(m+n)^2 - 3mn}$ as the distance spectral radius of a complete bipartite graph. \square

Corollary 4.2.6. *The eigenvalues of the distance matrix of a star graph of order n are -2 with multiplicity $n - 2$, $(n - 2) + \sqrt{n^2 - 3(n - 1)}$ and $(n - 2) - \sqrt{n^2 - 3(n - 1)}$. Its distance spectral radius is given by $(n - 2) + \sqrt{n^2 - 3(n - 1)}$.*

Proof. The proof follows directly from the results in Theorem 4.2.5 by substituting 1 for m and $n - 1$ for n . \square

4.3 Bounds on the distance spectral radius

In this section, we present some bounds on the distance spectral radii of graphs.

Definition 4.3.1. *The Wiener index $WI(G)$ of a graph G is defined as the sum of the distances between all unordered pairs of vertices in G . That is*

$$WI(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v).$$

It can also be defined as half the sum of all the entries of the distance matrix D_G . That is

$$WI(G) = \frac{1}{2} \mathbf{1}^T D_G \mathbf{1}.$$

The following results present some lower bounds on the distance spectral radii of graphs in terms of the Wiener index and the number of vertices.

Theorem 4.3.2 ([22]). *Let $\mu(G)$ be the distance spectral radius of a graph G of order n . Then*

$$\mu(G) \geq \frac{2WI(G)}{n}.$$

Equality holds when G is a vertex-transitive graph.

Proof. This result follows from Theorem 2.1.15 by setting $\mathbf{x} = \mathbf{1}$. That is

$$\mu(G) \geq \frac{\mathbf{1}^T D_G \mathbf{1}}{\mathbf{1}^T \mathbf{1}} = \frac{2WI(G)}{n}.$$

We know that equality holds if and only if $\mathbf{1}$ is the Perron vector of G . So by Theorem 4.2.1 equality holds for vertex-transitive graphs. \square

Corollary 4.3.3. *Let $\mu(G)$ be the distance spectral radius of a graph G of order n . Then*

$$\mu(G) \geq n - 1.$$

Equality holds when G is a complete graph.

Proof. Let G be a graph of order n . We know that the distance between any two vertices, say u and v , in G is greater than or equal to 1. If we set $d_G(u, v) = 1$ for all $u, v \in V(G)$ and $u \neq v$, then we get

$$WI(G) = \sum_{i=1}^{n-1} i = \frac{n(n-1)}{2}.$$

Therefore, by Theorem 4.3.2 we obtain the result. Note that the graph with distance 1 among all pairs of vertices is the complete graph. \square

Remark 4.3.4. *It follows from Corollary 4.3.3 that the complete graph minimises the distance spectral radius among all graphs with a prescribed order.*

4.4 Extremal trees

In this section, we deal with the trees that maximise the distance spectral radii analogous to the results in Section 3.5. Stevanović and Ilić in [31] proved that the broom, which is a star graph with a path attached to one of its leaves, has the maximum distance spectral radius among all trees with a given maximum degree. Surya, Milan and Somnath also in [8] determined extremal graphs among all graphs with fixed number of pendant vertices. Several other results of this kind can be found in [27, 9, 29, 21]. Motivated by these results, we focus on trees with given degree sequence. For this result, we shall consider the distance matrix and a matrix $M(T)$ (related to the distance matrix). This section is based on joint work with Valisoa Razanajatovo Misanantenaina and Stephan Wagner [14].

Definition 4.4.1. *A caterpillar is a tree with the property that removing its leaves results in a path graph. We call the resulting path graph the backbone of the caterpillar.*

Example 4.4.2. *Figure 4.2 is an example of a caterpillar with degree sequence: $\alpha = (5, 4, 3, 1, 1, 1, 1, 1, 1, 1)$.*

Theorem 4.4.3. *Let T_{max} be a tree that maximizes the distance spectral radius among all trees with a given degree sequence. Then T_{max} is a caterpillar.*

Before we begin the proof of Theorem 4.4.3, let us recall a few definitions.

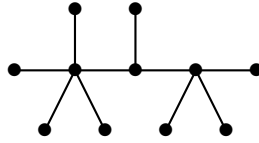


Figure 4.2: A caterpillar.

Definition 4.4.4. A caterpillar branch of a tree T is a maximal induced subgraph B of T that is a non-trivial caterpillar (i.e. with more than one vertex) and has the property that $T \setminus B$ is still a tree.

The Rayleigh quotient of the distance matrix D_G of a graph G on a unit vector \mathbf{f} is

$$R_G(\mathbf{f}) = 2 \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) f(u) f(v),$$

where $f(u)$ is the entry \mathbf{f} associated with the vertex u . Note that if \mathbf{f} is the Perron vector of G then $\mu(D_G) = R_G(\mathbf{f})$. Let S be a subset of vertices in the graph G . We set

$$|S|_f = \sum_{u \in S} f(u).$$

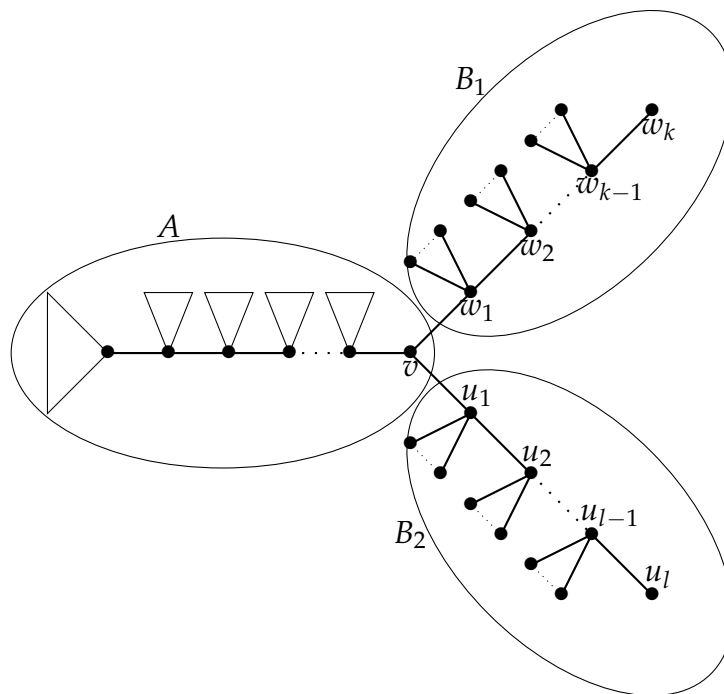


Figure 4.3: B_1, B_2 and A in an optimal tree T_{\max} that is not a caterpillar.

Proof of Theorem 4.4.3. Let T_{\max} be an optimal tree among all trees with some prescribed degree sequence. Suppose that T_{\max} is not a caterpillar. We consider pairs B_1, B_2 of caterpillar branches in T_{\max} that are attached to the same vertex v . Among all such pairs we choose the pair B_1, B_2 for which $|B_1|_f + |B_2|_f$ is minimal, where f is the Perron vector of T_{\max} . Let $P = vw_1w_2 \cdots w_k$, for $k > 1$, and $P' = vu_1u_2 \cdots u_l$, for $l > 1$, be the longest paths (backbones) of the caterpillar branches B_1 and B_2 respectively. Furthermore, we denote $T_{\max} \setminus \{B_1 \cup B_2\}$ by A . This is shown in Figure 4.3. Without loss of generality, we can assume that $|B_2|_f \geq |B_1|_f$. Note that $|A|_f > |B_2|_f$, for otherwise one could find a pair of caterpillar branches inside A with smaller weight than $|B_1|_f + |B_2|_f$ or if $A \setminus \{v\}$ is a caterpillar branch by itself, then we can replace B_2 by it.

We form a new tree T' from T_{\max} by interchanging B_2 and w_k . That is, we remove the edges $w_{k-1}w_k$ and vu_1 , and add the edges $w_{k-1}u_1$ and vw_k . Clearly, this does not change the degree sequence. Note that the distance between two vertices x and y will only change after the interchange if $x \in B_2$ or $x = w_k$ and $y \in A$ or $y \in B_1 \setminus \{w_k\}$ (or vice versa). We then compute

$$R_{T'}(f) - R_{T_{\max}}(f) = 2 \left(\sum_{\{x,y\} \subseteq V(T_{\max})} [d_{T'}(x,y) - d_{T_{\max}}(x,y)] f(x)f(y) \right).$$

This yields the following cases:

Case 1: One end is in A and the other is in B_2 . The contribution of this case to $R_{T'}(f) - R_{T_{\max}}(f)$ is

$$\begin{aligned} &= 2 \sum_{\substack{x \in A \\ y \in B_2}} [d_{T'}(x,y) - d_{T_{\max}}(x,y)] f(x)f(y) \\ &= 2 \sum_{\substack{x \in A \\ y \in B_2}} [d_{T_{\max}}(x,v) + d_{T_{\max}}(v,w_k) + d_{T_{\max}}(u_1,y) - d_{T_{\max}}(x,v) \\ &\quad - d_{T_{\max}}(v,u_1) - d_{T_{\max}}(u_1,y)] f(x)f(y) \\ &= 2 \sum_{\substack{x \in A \\ y \in B_2}} [d_{T_{\max}}(v,w_k) - 1] f(x)f(y) \\ &= 2[d_{T_{\max}}(v,w_k) - 1]|A|_f|B_2|_f. \end{aligned}$$

Case 2: One end is in A and the other is w_k . The contribution of this case to

$R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$ is

$$\begin{aligned}
&= 2 \sum_{\substack{x \in A \\ y = w_k}} [d_{T'}(x, w_k) - d_{T_{\max}}(x, w_k)] f(x) f(w_k) \\
&= 2 \sum_{\substack{x \in A \\ y = w_k}} [d_{T_{\max}}(x, v) + 1 - d_{T_{\max}}(x, v) - d_{T_{\max}}(v, w_k)] f(x) f(w_k) \\
&= 2f(w_k)[1 - d_{T_{\max}}(v, w_k)]|A|_f.
\end{aligned}$$

Case 3: One end is in $B_1 \setminus \{w_k\}$ and the other is in B_2 . The contribution of this case to $R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$ is

$$\begin{aligned}
&= 2 \sum_{\substack{x \in B_1 \setminus \{w_k\} \\ y \in B_2}} [d_{T'}(x, y) - d_{T_{\max}}(x, y)] f(x) f(y) \\
&= 2 \sum_{\substack{x \in B_1 \setminus \{w_{k-1}, w_k\} \\ y \in B_2}} [d_{T_{\max}}(x, w_k) + d_{T_{\max}}(u_1, y) - d_{T_{\max}}(x, v) - 1 - d_{T_{\max}}(u_1, y)] f(x) f(y) \\
&\quad + 2 \sum_{y \in B_2} [1 + d_{T_{\max}}(u_1, y) - d_{T_{\max}}(v, w_{k-1}) - 1 - d_{T_{\max}}(u_1, y)] f(y) f(w_{k-1}) \\
&= 2 \sum_{x \in B_1 \setminus \{w_{k-1}, w_k\}} [d_{T_{\max}}(x, w_k) - d_{T_{\max}}(x, v) - 1] |B_2|_f f(x) \\
&\quad + 2[1 - d_{T_{\max}}(v, w_k)] |B_2|_f f(w_{k-1}).
\end{aligned}$$

Case 4: One end is in $B_1 \setminus \{w_k\}$ and the other is w_k . The contribution of this case to $R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$ is

$$\begin{aligned}
&= 2 \sum_{\substack{x \in B_1 \setminus \{w_k\} \\ y = w_k}} [d_{T'}(x, w_k) - d_{T_{\max}}(x, w_k)] f(x) f(w_k) \\
&= 2 \sum_{\substack{x \in B_1 \setminus \{w_{k-1}, w_k\} \\ y = w_k}} [d_{T_{\max}}(x, v) + 1 - d_{T_{\max}}(x, w_k)] f(x) f(w_k) \\
&\quad + 2[d_{T_{\max}}(v, w_{k-1}) + 1 - 1] f(w_{k-1}) f(w_k) \\
&= 2 \sum_{x \in B_1 \setminus \{w_{k-1}, w_k\}} [d_{T_{\max}}(x, v) + 1 - d_{T_{\max}}(x, w_k)] f(x) f(w_k) \\
&\quad + 2[d_{T_{\max}}(v, w_k) - 1] f(w_{k-1}) f(w_k)
\end{aligned}$$

Combining the cases 3 and 4, we obtain that their contribution to $R_{T'}(\mathbf{f}) -$

$R_{T_{\max}}(\mathbf{f})$ is

$$\begin{aligned} &= 2 \sum_{x \in B_1 \setminus \{w_{k-1}, w_k\}} f(x) [d_{T_{\max}}(x, w_k) - d_{T_{\max}}(x, v) - 1] (|B_2|_f - f(w_k)) \\ &\quad + 2f(w_{k-1}) [1 - d_{T_{\max}}(v, w_k)] (|B_2|_f - f(w_k)). \end{aligned}$$

Considering the longest path P in B_1 , it can be observed that $d_{T_{\max}}(w_{k-1}, w_k) = 1$, so $d_{T_{\max}}(x, w_k) \geq 2$ for all $x \in B_1 \setminus \{w_{k-1}, w_k\}$. Also, we have that $d_{T_{\max}}(v, x) \leq d_{T_{\max}}(v, w_k)$ for all $x \in B_1 \setminus \{w_k\}$. Using these facts, we obtain that the contribution of these cases to $R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$ is at least

$$\begin{aligned} &\geq 2 \sum_{x \in B_1 \setminus \{w_{k-1}, w_k\}} f(x) [2 - 1 - d_{T_{\max}}(v, w_k)] (|B_2|_f - f(w_k)) \\ &\quad + 2f(w_{k-1}) [1 - d_{T_{\max}}(v, w_k)] (|B_2|_f - f(w_k)) \\ &= 2[1 - d_{T_{\max}}(v, w_k)] |B_1 \setminus \{w_k\}|_f (|B_2|_f - f(w_k)). \end{aligned}$$

Now summing all the cases we get that $R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$ is

$$\begin{aligned} &\geq 2(d_{T_{\max}}(v, w_k) - 1) [|A|_f (|B_2|_f - f(w_k)) - |B_1 \setminus \{w_k\}|_f (|B_2|_f - f(w_k))] \\ &= 2(d_{T_{\max}}(v, w_k) - 1) (|A|_f - |B_1 \setminus \{w_k\}|_f) (|B_2|_f - f(w_k)) \\ &> 0 \end{aligned}$$

since $|A|_f > |B_2|_f \geq |B_1|_f > f(w_k)$. Therefore we obtain

$$\mu(T') \geq R_{T'}(\mathbf{f}) > R_{T_{\max}}(\mathbf{f}) = \mu(T_{\max}).$$

This contradicts the optimality of T_{\max} . □

Example 4.4.5. Figure 4.4 shows the respective extremal trees for the degree sequences

$$\begin{aligned} \alpha_1 &= (5, 4, 3, 2, 1, 1, 1, 1, 1, 1, 1), \\ \alpha_2 &= (8, 5, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1), \\ \alpha_3 &= (10, 4, 3, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1), \\ \alpha_4 &= (8, 4, 4, 4, 3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1). \end{aligned}$$

Note that the characterization of the caterpillar T_{\max} is still an open problem. The problem seems to be difficult since the analogous problem for the Wiener index, which is a simpler invariant, is already difficult.

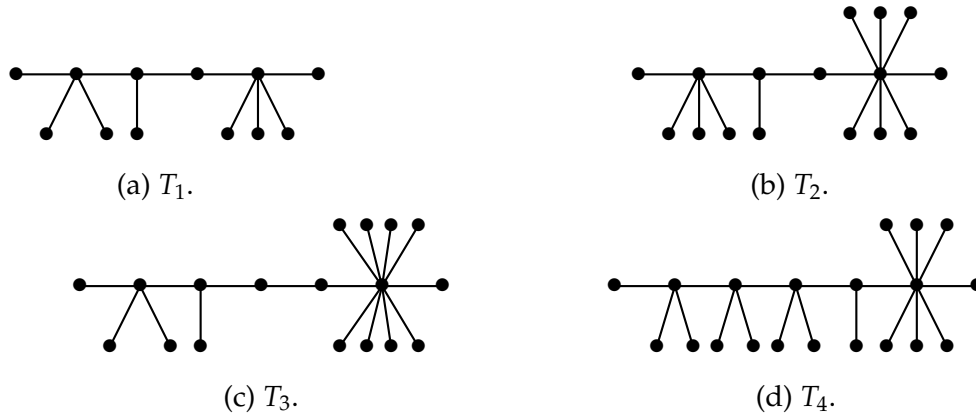


Figure 4.4: Extremal trees T_1, T_2, T_3 and T_4 .

Let us now define a new matrix $M(T)$ and state the motivation behind considering it. Graham and Pollak in [15] proved that for a tree T on n vertices, the determinant of its distance matrix is given by

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

It can be observed that the determinant depends only on the number of vertices of the tree, but not its structure. Bapat in [1] and Collins in [11] extended this results to a weighted tree T_w on n vertices with edge weights α_i , for $i = 1, \dots, n - 1$. They proved that the determinant of its distance matrix D is given by

$$\det(D(T_w)) = (-1)^{n-1}2^{n-2} \left(\prod_{i=1}^{n-1} \alpha_i \right) \left(\sum_{i=1}^{n-1} \alpha_i \right),$$

which is independent of the tree structure but depends on the edge weights and the number of vertices.

Furthermore, Bapat, Kirkland and Neumann in [4] proved that for a weighted tree T_w on n vertices with edge weights α_i , for $i = 1, \dots, n - 1$, and any real number x , the determinant of the matrix $M_x(T_w) = D(T_w) + xJ$, where J is a matrix with all entries equal to one, is

$$\det(M_x(T_w)) = (-1)^{n-1}2^{n-2} \left(\prod_{i=1}^{n-1} \alpha_i \right) \left(2x + \sum_{i=1}^{n-1} \alpha_i \right),$$

which again is independent of the structure of the tree. In the following, we shall discuss the spectral radius of a matrix similar to $M(T_w)$.

A conjecture of Stevanović and Ilić in [31] states that among all trees with order n and given maximum degree, the Volkmann tree minimises the spectral radius of the distance matrix. We shall discuss the reverse version of this conjecture by proving that the greedy tree maximizes the spectral radius of a family of matrices (related to the distance matrix) among all trees with the same degree sequence. Our result provides further evidence for the correctness of the Stevanović-Ilić conjecture.

Theorem 4.4.6. *Let c be any constant greater than or equal to one plus the number of non-leaves of a tree with degree sequence α . Then the optimal tree T that maximizes the spectral radius of the matrix $M(T) = cJ - D(T)$ among all trees with the same degree sequence α is the greedy tree $G(\alpha)$. Here, J is a matrix with all entries equal to one and $D(T)$ the distance matrix of T .*

Remark 4.4.7. *The maximum diameter (obtained for a caterpillar) of trees with degree sequence α is equal to the minimum value of c , implying that the matrix $M(T)$ has only nonnegative entries.*

From the formula for the determinant of the matrix $M_x(T_w)$ by Bapat, Kirkland and Neumann in [4], we obtain the determinant of $M(T)$ as

$$\begin{aligned} \det(cJ - D(T)) &= (-1)^n \det(D(T) - cJ) \\ &= (-1)^n \left[(-1)^{n-1} 2^{n-2} (-2c + (n-1)) \right] \\ &= 2^{n-2} (2c - n + 1) \end{aligned}$$

which is also independent of the structure of the tree but depends on c and the number of vertices n .

In order to prove Theorem 4.4.6, we need some definitions and lemmas, most of which we will state and prove in this section. We will basically investigate the behaviour of the spectral radius of $M(T)$ as we rearrange the edges of the tree (swapping the vertices). Our ideas are based on similar results for the Wiener index by Wang in [33].

Let T be a tree of order n with vertex set V and edge set E . Let $M(T) = cJ - D(T)$ as described in Theorem 4.4.6 and \mathbf{f} an $n \times 1$ unit vector. The Rayleigh quotient of $M(T)$ (which we will write as M for the sake of simplicity) on the vector \mathbf{f} is defined as

$$R_T(\mathbf{f}) = \frac{\mathbf{f}^T M \mathbf{f}}{\mathbf{f}^T \mathbf{f}} = 2 \sum_{\{u,v\} \subseteq V(T)} [c - d_T(u,v)] f(u) f(v),$$

where $d_T(u, v)$ is the distance between vertices u and v , and $f(u)$ is the component of f associated with the vertex $u \in V$. By Theorem 2.1.15 we have

$$\mu(T) \geq R_T(f),$$

with equality if f is an eigenvector corresponding to $\mu(T)$.

Now, we describe a decomposition of a tree T taken from [33] which will aid us in the proof of some lemmas and Theorem 4.4.6. Consider two vertices x and y in the tree T . Let the path $P_T(x, y)$ from the vertex x to the vertex y be given by

$$P_T(x, y) = x_k x_{k-1} \dots x_2 x_1 y_1 y_2 y_3 \dots y_{k-1} y_k$$

when its length is odd, or

$$P_T(x, y) = x_k x_{k-1} \dots x_2 x_1 z y_1 y_2 \dots y_{k-1} y_k$$

when its length is even, where $x_k = x, y_k = y$. Furthermore, we let X_i, Y_i and Z denote the subtrees of the tree T that contain x_i, y_i and z respectively, where $i = 1, \dots, k$. Also, we let $X_{>k}$ (resp. $Y_{>k}$) be the subtree of the tree induced by the vertices in $X_{k+1} \cup X_{k+2} \cup \dots$ (resp. $Y_{k+1} \cup Y_{k+2} \cup \dots$). This decomposition described is shown in Figure 4.5 for an odd path length. We set

$$|X_i|_f = \sum_{u \in X_i} f(u),$$

where f is the Perron vector of the matrix $M(T) = cJ - D(T)$. Furthermore, we let \mathbb{T}_α denote the set of all trees with the same degree sequence α and T_{max} the optimal tree, the tree with the maximum distance spectral radius.

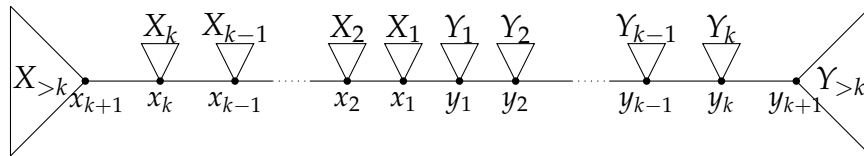


Figure 4.5: Labeling of a path and the components.

Lemma 4.4.8 (cf.[33]). *Let T_{max} be decomposed as depicted in Figure 4.5. If $|X_i|_f \geq |Y_i|_f$ for $i = 1, 2, \dots, k - 1$ and $|X_{>k-1}|_f \geq |Y_{>k-1}|_f$, then $d(x_k) \geq d(y_k)$.*

Proof. We assume (for contradiction) that $d(x_k) < d(y_k)$ such that $d(y_k) - d(x_k) = a > 0$. We let u_i ($i = 1, \dots, a$) be the neighbours of y_k other than y_{k-1} and y_{k+1} . Then we increase the degree of x_k by removing all the edges of the form $y_k u_i$ ($i = 1, \dots, a$) and adding all edges of the form $x_k u_i$ ($i = 1, \dots, a$) instead. Note that this operation does not change the degree sequence, and we want to show that it increases the Rayleigh quotient $R_{T_{\max}}(\mathbf{f})$ of $M(T_{\max})$ on its Perron vector \mathbf{f} . Let T' be the new tree obtained after performing this operation and A be the set of vertices in the components of $T_{\max} \setminus y_k u_i$ ($i = 1, \dots, a$) that contain u_1, u_2, \dots, u_a .

We compute: $R_{T'}(\mathbf{f}) - R_{T_{\max}}(\mathbf{f})$

$$\begin{aligned} &= 2 \sum_{\{u,v\} \subseteq V} [c - d_{T'}(u,v)] f(u)f(v) - 2 \sum_{\{u,v\} \subseteq V} [c - d_{T_{\max}}(u,v)] f(u)f(v) \\ &= 2 \sum_{\{u,v\} \subseteq V} [d_{T_{\max}}(u,v) - d_{T'}(u,v)] f(u)f(v). \end{aligned}$$

It can be observed that in this operation, the distance between two vertices w and v will only change if $w \in A$ and $v \in T_{\max} \setminus A$ (or vice versa). We will consider the case when the path shown in Figure 4.5 has odd length, and otherwise it follows in a similar way. We will therefore obtain the following four possible cases:

Case 1: If one end is in X_i ($i = 1, \dots, k-1$) and the other end is in A , then the distance between the vertices decreases by $2i - 1$. Therefore

$$\begin{aligned} 2 \sum_{\substack{w \in A \\ u \in X_i}} [d_{T_{\max}}(w,u) - d_{T'}(w,u)] f(w)f(u) &= 2 \sum_{w \in A} f(w) \left[\sum_{i=1}^{k-1} (2i-1) |X_i|_f \right] \\ &= 2 \sum_{i=1}^{k-1} (2i-1) |X_i|_f |A|_f. \end{aligned}$$

Case 2: If one end is in Y_i ($i = 1, \dots, k-1$) and the other end is in A , then the distance between the vertices increases by $2i - 1$. Therefore

$$\begin{aligned} 2 \sum_{\substack{w \in A \\ u \in Y_i}} [d_{T_{\max}}(w,u) - d_{T'}(w,u)] f(w)f(u) &= 2 \sum_{w \in A} f(w) \left[\sum_{i=1}^{k-1} -(2i-1) |Y_i|_f \right] \\ &= -2 \sum_{i=1}^{k-1} (2i-1) |Y_i|_f |A|_f. \end{aligned}$$

Case 3: If one end is in $X_{>k-1}$ and the other end is in A , then the distance between the vertices decreases by $2k - 1$. Therefore

$$\begin{aligned} 2 \sum_{\substack{w \in A \\ u \in X_{>k-1}}} [d_{T_{\max}}(w, u) - d_{T'}(w, u)] f(w) f(u) &= 2 \sum_{w \in A} f(w) (2k - 1) |X_{>k-1}|_f \\ &= 2(2k - 1) |X_{>k-1}|_f |A|_f. \end{aligned}$$

Case 4: If one end is in $Y_{>k-1} \setminus A$ and the other end is in A , then the distance between the vertices increases by $2k - 1$. Therefore

$$\begin{aligned} 2 \sum_{\substack{w \in A \\ u \in Y_{>k-1} \setminus A}} [d_{T_{\max}}(w, u) - d_{T'}(w, u)] f(w) f(u) \\ &= 2 \sum_{w \in A} f(w) [-(2k - 1)] [|Y_{>k-1}|_f - |A|_f] \\ &= -2(2k - 1) |A|_f (|Y_{>k-1}|_f - |A|_f). \end{aligned}$$

Hence, for odd path length we have $R_{T'}(f) - R_{T_{\max}}(f)$ equal to

$$2|A|_f \left[\sum_{i=1}^{k-1} (2i - 1) (|X_i|_f - |Y_i|_f) + (2k - 1) (|X_{>k-1}|_f - |Y_{>k-1}|_f + |A|_f) \right]$$

and for even path length we have

$$2|A|_f \left[\sum_{i=1}^{k-1} (2i) (|X_i|_f - |Y_i|_f) + (2k) (|X_{>k-1}|_f - |Y_{>k-1}|_f + |A|_f) \right].$$

But we assumed that $|X_i|_f \geq |Y_i|_f$ and $|X_{>k-1}|_f \geq |Y_{>k-1}|_f$, so $R_{T'}(f) - R_{T_{\max}}(f) > 0$. It follows that

$$\mu(T') \geq R_{T'}(f) > R_{T_{\max}}(f) = \mu(T_{\max}).$$

However, $\mu(T') > \mu(T_{\max})$ is a contradiction since we assumed T_{\max} to be the optimal tree. \square

Lemma 4.4.9 (cf.[33]). *Let P be a path of an optimal tree T_{\max} whose end vertices are leaves.*

For odd path length $(2l - 1)$, we label the vertices of P as $u_1 u_{l-1} \dots u_1 w_1 w_2 \dots w_l$ and U_i, W_i are the subtrees that contain u_i, w_i respectively, for $i = 1, \dots, l$. If we assume without loss of generality that $|U_1|_f \geq |W_1|_f$, then we get

$$|U_1|_f \geq |W_1|_f \geq |U_2|_f \geq |W_2|_f \geq \dots \geq |U_l|_f = |W_l|_f.$$

Note that for the case when $|U_1|_f = |W_1|_f$, if we assume without loss of generality that for the first index j for which $|U_j|_f \neq |W_j|_f$, we have

$$|U_1|_f = |W_1|_f = \dots = |U_j|_f > |W_j|_f \geq \dots \geq |U_l|_f = |W_l|_f.$$

For even path length ($2l$), we label the vertices as $u_{l+1}u_lu_{l-1}\dots u_1w_1w_2\dots w_l$, and we get

$$|U_1|_f \geq |W_1|_f \geq |U_2|_f \geq |W_2|_f \geq \dots \geq |W_l|_f = |U_{l+1}|_f.$$

In order to prove Lemma 4.4.9, we propose an equivalent definition for the Rayleigh quotient of $M(T)$ on its Perron vector \mathbf{f} .

Proposition 4.4.10. *We can write*

$$\sum_{\{u,v\} \subseteq V} d_T(u,v) f(u) f(v) = \sum_{uv \in E} \sum_{w \in C(u,v)} f(w) \sum_{w \in C(v,u)} f(w), \quad (4.4)$$

where $C(u,v)$ is the set of all vertices closer to the vertex u than to the vertex v .

Therefore the Rayleigh quotient of $M(T)$ on its Perron vector \mathbf{f} can be written as

$$\begin{aligned} R_T(\mathbf{f}) &= 2 \sum_{\{u,v\} \subseteq V} c f(u) f(v) - 2 \sum_{\{u,v\} \subseteq V} d_T(u,v) f(u) f(v) \\ &= 2 \sum_{\{u,v\} \subseteq V} c f(u) f(v) - 2 \sum_{uv \in E} \sum_{w \in C(u,v)} f(w) \sum_{w \in C(v,u)} f(w). \end{aligned}$$

Proof. To prove this proposition we prove the equation (4.4). Firstly, the right hand side of the equation counts the number of unordered pairs of vertices $\{u', v'\}$ with their weights $f(u')f(v')$ such that $P(u', v')$ contains the edge uv where u' and v' are the vertices closer to u and v respectively. Now, if we consider such a path $P(u', v')$, then the number of edges it contains is $d(u', v')$. Hence considering the weights $f(u')f(v')$ of these unordered pairs of vertices $\{u', v'\}$ gives the left hand side of the equation. Note that there is only one unique path between any pair of vertices in a tree. \square

We use a theorem by Hardy, Littlewood and Pólya ([16]). For a sequence s of the form

$$s_{-l}, s_{-l+1}, \dots, s_{-1}, s_0, s_1, \dots, s_{l-1}, s_l,$$

we obtain the sequence s^+ by rearranging the elements so that

$$s_0^+ \geq s_1^+ \geq s_{-1}^+ \geq s_2^+ \geq s_{-2}^+ \geq \dots \geq s_l^+ \geq s_{-l}^+.$$

Theorem 4.4.11 ([16], Theorem 371). *Let p, q , and r be nonnegative sequences. Suppose the sequence r is symmetrically increasing, that is*

$$r_0 \leq r_1 = r_{-1} \leq r_2 = r_{-2} \leq \dots \leq r_{2k} = r_{-2k},$$

and the sequences p and q have no prescribed order. Then the bilinear form

$$\sum_{a=-k}^k \sum_{b=-k}^k r_{a-b} p_a q_b$$

is minimum when p is p^+ and q is q^+ .

Proof of Lemma 4.4.9. We will prove the statement for odd path length and note that it is similar for even path length. As described in the Lemma, $P = u_1 u_{l-1} \dots u_1 w_1 w_2 \dots w_l$. Let S be the sequence $S_{-l+1}, \dots, S_0, \dots, S_l$. We set

$$\begin{aligned} S_{-l+1} &= |U_l|_f, S_{-l+2} = |U_{l-1}|_f, \dots, S_0 = |U_1|_f, \\ S_1 &= |W_1|_f, S_2 = |W_2|_f, \dots, S_l = |W_l|_f. \end{aligned}$$

We now consider the contribution C of edges of the path P to the Rayleigh quotient $R_T(\mathbf{f})$ as described in our Proposition 4.4.10 because the contribution of all other edges other than those described in our proposition remains the same when the order of the branches $U_1, \dots, U_l, W_1, \dots, W_l$ is changed. Then we get

$$\begin{aligned} C &= S_{-l+1}(S_{-l+2} + \dots + S_l) \\ &\quad + (S_{-l+1} + S_{-l+2})(S_{-l+3} + \dots + S_l) \\ &\quad \vdots \\ &\quad + (S_{-l+1} + S_{-l+2} + \dots + S_{l-1})S_l. \end{aligned}$$

It can be seen that the summands of C can be expressed as $S_a S_b$, hence we can count them. To obtain a product $S_a S_b$, we must have S_a and S_b occurring in different parentheses, which occurs $k = a - b$ times. We notice that $S_a S_b = S_b S_a$, so we set their coefficient $r_{a-b} = r_{b-a} = \frac{k}{2}$. We have

$$C = \sum_{a=-l+1}^l \sum_{b=-l+1}^l r_{a-b} S_a S_b$$

where r is symmetrically increasing, namely

$$r_0 = 0 \leq r_1 = r_{-1} = \frac{1}{2} \leq \dots \leq c_{2l-1} = c_{-2l+1} = \frac{2l-1}{2}.$$

Therefore, by Theorem 4.4.11, C attains its minimum if S is S^+ hence

$$S_0^+ \geq S_1^+ \geq S_{-1}^+ \geq S_2^+ \geq S_{-2}^+ \geq \dots \geq S_{-l+1}^+ \geq S_l^+$$

implying

$$|U_1|_f \geq |W_1|_f \geq |U_2|_f \geq |W_2|_f \geq \dots \geq |U_l|_f \geq |W_l|_f.$$

Note that when C is minimum it implies that the right hands side of equation (4.4) is also minimum. Hence the Rayleigh quotient $R_T(\mathbf{f})$ as described in Proposition 4.4.10 attain its maximum value. Therefore, the optimal tree has to have this property. \square

Lemma 4.4.12 (cf.[33]). *Let T_{\max} be the optimal tree. For a path P with labelling as described in Lemma 4.4.9, we have*

$$d(u_1) \geq d(w_1) \geq d(u_2) \geq d(w_2) \geq \dots \geq d(u_l) = d(w_l) = 1$$

if the path length is odd and

$$d(u_1) \geq d(w_1) \geq d(u_2) \geq d(w_2) \geq \dots \geq d(u_l) \geq d(w_l) = d(u_{l+1}) = 1$$

if the path length is even.

Proof. Again we will show the proof for odd path length, and otherwise it follows in a similar manner. From Lemma 4.4.9 we have

$$|U_1|_f \geq |W_1|_f \geq |U_2|_f \geq |W_2|_f \geq \dots \geq |U_l|_f \geq |W_l|_f.$$

We will then apply Lemma 4.4.8 by choosing appropriate y_i and x_i to obtain the following:

Case 1: Let $x_i = u_i$ and $y_i = w_i$ for $i = 1, 2, \dots, l$; then we obtain $d(u_i) \geq d(w_i)$ by Lemma 4.4.8.

Case 2: Let $y_1 = u_{i+1}, y_2 = u_{i+2}, \dots$ and $x_1 = u_i, x_2 = u_{i-1}, \dots, x_i = u_1, x_{i+1} = w_1, \dots$. Then we get

$$|Y_{>1}|_f = \sum_{k=i+2}^l |U_k|_f \quad \text{and} \quad |X_{>1}|_f = \sum_{k=1}^l |W_k|_f + \sum_{k=1}^{i-1} |U_k|_f$$

implying $|X_{>1}|_f > |Y_{>1}|$, so by Lemma 4.4.8 we get $d(x_1) = d(u_i) \geq d(y_1) = d(u_{i+1})$. That is, we have

$$d(u_1) \geq d(u_2) \geq d(u_3) \geq \dots \geq d(u_l).$$

Case 3: Let $y_1 = w_i, y_2 = w_{i-1}, \dots, y_{i+1} = u_1, \dots$ and $x_1 = w_{i+1}, x_2 = w_{i+2}, \dots$. Then we get

$$|X_{>1}|_f = \sum_{k=i+2}^l |W_k|_f \quad \text{and} \quad |Y_{>1}|_f = \sum_{k=1}^l |U_k|_f + \sum_{k=1}^{i-1} |W_k|_f$$

implying $|X_{>1}|_f < |Y_{>1}|$, so by Lemma 4.4.8 we get $d(y_1) = d(w_i) \geq d(x_1) = d(w_{i+1})$. That is, we have

$$d(w_1) \geq d(w_2) \geq d(w_3) \geq \dots \geq d(w_l).$$

Case 4: Let $z = u_1, y_i = u_{i+1}, x_i = w_i$ to get $d(w_i) \geq d(u_{i+1})$ for $i = 1, 2, \dots, l$. Since

$$|X_{>i}|_f = \sum_{k=i+1}^l |W_k|_f \quad \text{and} \quad |Y_{>i}|_f = \sum_{k=i+2}^l |U_k|_f$$

we have $|X_{>i}|_f > |Y_{>i}|$ and $d(x_i) \geq d(y_i)$ by Lemma 4.4.8. Now, combining all the results from all these cases we get

$$d(u_1) \geq d(w_1) \geq d(u_2) \geq d(w_2) \geq \dots \geq d(u_l) = d(w_l) = 1.$$

□

Definition 4.4.13. We say that a function g defined on the vertices of a path $x_i x_{i+1} \dots x_j$ is concave if $g(x_{k+1}) - g(x_k) < g(x_k) - g(x_{k-1})$ for all k .

Lemma 4.4.14. We set

$$N_f(u) = \sum_{v \in V} [c - d_T(u, v)] f(v),$$

which is the coordinate corresponding to u in $M\mathbf{f}$, thus equal to $\mu(M)f(u)$ since \mathbf{f} is the Perron vector of M . This expression is concave along paths. It follows that the maximum of N_f is attained either at one or two adjacent points (vertices) in the tree T .

Proof of Lemma 4.4.14. Let $P_1 = x_1x_2 \cdots x_l$ be a path in a tree T and let $A_{<i}$ and $B_{>i+1}$ be the components of $T \setminus x_ix_{i+1}$ that contain the vertices $x_1 \dots x_i$ and $x_{i+1} \dots x_l$ respectively. We have

$$\begin{aligned} N_f(x_{i+1}) - N_f(x_i) &= \sum_{v \in V} [d_T(x_i, v) - d_T(x_{i+1}, v)]f(v) \\ &= \sum_{v \in A_{<i}} (-1)f(v) + \sum_{v \in B_{>i+1}} f(v) \\ &= -|A_{<i}|_f + |B_{>i+1}|_f. \end{aligned}$$

It can be observed that when i increases, $|A_{<i}|_f$ increases and $|B_{>i+1}|_f$ decreases and hence $N_f(x_{i+1}) - N_f(x_i)$ decreases. Conversely, $N_f(x_{i+1}) - N_f(x_i)$ increases as i decreases. So N_f is concave, thus reaches maximum at either at one vertex, x_k , or two adjacent vertices, x_k, x_{k+1} , along the path P_1 . Now, let y, z be two vertices in the tree T such that $N_f(y)$ and $N_f(z)$ are maximum. We know that N_f is concave along the path that passes through the two vertices y and z , so they have to be adjacent. It is important to note that there cannot be more than two vertices where the maximum of N_f is attained since they would form a triangle which is impossible in a tree. Therefore we obtain that the maximum of N_f is attained either at one or two adjacent vertices in the tree T . \square

Now, using all the auxiliary results, we prove Theorem 4.4.6 by showing that the optimal tree satisfies all the properties of the greedy tree as in Lemma 3.5.3.

Proof of Theorem 4.4.6. Consider a path labelled as described in Lemma 4.4.9. We have

$$\begin{aligned} N_f(u_1) - N_f(u_2) &= \sum_{v \in V} [d_T(u_2, v) - d_T(u_1, v)]f(v) \\ &= \sum_{v \in U_{>1}} (-1)f(v) + \sum_{v \in W_{\geq 1} \cup U_1} f(v) \\ &= -|U_{>1}|_f + |W_{\geq 1} \cup U_1|_f, \end{aligned}$$

which is greater than zero by Lemma 4.4.9. It follows that $N_f(u_1) > N_f(u_2)$.

Also,

$$\begin{aligned}
 N_f(u_1) - N_f(w_1) &= \sum_{v \in V} [d_T(w_1, v) - d_T(u_1, v)]f(v) \\
 &= \sum_{v \in U_{\geq 1}} f(v) + \sum_{v \in W_{\geq 1}} (-1)f(v) \\
 &= |U_{\geq 1}|_f - |W_{\geq 1}|_f,
 \end{aligned}$$

which is greater than (or equal to) zero by Lemma 4.4.9. Thus $N_f(u_1) \geq N_f(w_1)$.

From Lemma 4.4.9 and Lemma 4.4.12, we know that for an optimal tree labelled as in those lemmas, $d(u_1)$ and $|U_1|_f$ are the respective maxima among all vertices along the path. We also know that the function N_f is concave along the path, $N_f(u_1) > N_f(u_2)$ and $N_f(u_1) \geq N_f(w_1)$, so $N_f(u_1)$ is the maximum along the path.

We recall from Lemma 4.4.14 that N_f is maximal at either only one vertex, which we then label as r , or two adjacent vertices in the tree T_{\max} , which we label r and v_1 .

We will show the proof for the case when N_f is maximal at only one vertex r , and otherwise it follows in a similar manner.

Now we consider the optimal tree T_{\max} to be a rooted tree with root r , so since $N_f(r) \geq N_f(z)$ for every vertex z in T_{\max} by assumption, r must be the vertex u_1 in any path containing it, and thus have the largest degree by Lemma 4.4.12. Thus (i) in Lemma 3.5.3 is satisfied.

Suppose we have a path from a leaf u passing through r (root) to another leaf v in T_{\max} such that the only ancestor of u and v is r . By Lemma 4.4.9 we have $|d_T(u, r) - d_T(v, r)| = 0$ if the path length is even and $|d_T(u, r) - d_T(v, r)| = 1$ if the path length is odd. Hence the heights of any two leaves differ by at most 1, which yields (ii) in Lemma 3.5.3.

Let $h_{T_{\max}}(y)$ and $h_{T_{\max}}(z)$ be the heights of the vertices y and z respectively such that $h_{T_{\max}}(y) < h_{T_{\max}}(z)$. These heights are with respect to the root vertex r of the optimal tree. If z is a successor of y and we consider the path from the leaf u to the leaf v passing through y, z , then we get $d(y) \geq d(z)$ by Lemma 4.4.12. Now, suppose z is not a successor of y . We consider a path from a leaf y' to a leaf z' passing through the vertices y, s, z such that s is the first common ancestor of y, z . We can set $s = u_1$ in Lemma 4.4.9. Also, we let $i = h_{T_{\max}}(y) - h_{T_{\max}}(s)$ and $j = h_{T_{\max}}(z) - h_{T_{\max}}(s)$ be the height of y and z with respect to the vertex s . So, we get two possible labellings of the

path, that is either $y = u_{i+1}, z = w_j$ or $y = w_i, z = u_{j+1}$. If we consider the first labelling then we get $i + 1 \leq j$, which by Lemma 4.4.12 implies that $d(y) \geq d(z)$. Note that this is also true for the second labelling. Thus (iii) in Lemma 3.5.3 is also satisfied.

Furthermore, let y, z be on the same level, thus $h_{T_{\max}}(y) = h_{T_{\max}}(z)$, such that $d(y) > d(z)$, and let y', z' be their respective successors such that $h_{T_{\max}}(y') = h_{T_{\max}}(z')$. Consider the longest path that passes through y', y, s, z, z' , where z is the first ancestor of y and z' . Again we let $s = u_1$ in Lemma 4.4.9 with $y = w_i, y' = w_j, z = u_{i+1}, z' = u_{j+1}$ where $i = h_{T_{\max}}(y) - h_{T_{\max}}(s), j = h_{T_{\max}}(y') - h_{T_{\max}}(s)$. Then by Lemma 4.4.12, we see that $d(y) > d(z)$ implies $d(y') \geq d(z')$. This yields (iv) in Lemma 3.5.3.

Finally, let y_1, z_1 be the respective parents of y, z and y', z' their respective siblings and y'', z'' successors of y', z' . We let Y denote the subtree induced by the vertices $v \in V(T_{\max})$ for which $P_{T_{\max}}(v, r)$ contains y and $h_{T_{\max}}(v) \geq h_{T_{\max}}(y)$; Y_1, Z, Z_1 are defined in an analogous way. If we let $d(y) > d(z)$ then by (iv) in Lemma 3.5.3, we have

$$|Y_1 \setminus Y'|_f > |Z_1 \setminus Z'|_f \quad (4.5)$$

since $|Y|_f > |Z|_f$. Now, consider the path passing through y'', y', s, z', z'' , where s is the common ancestor of y, z that is on the path $P_{T_{\max}}(y', z')$. We can set $u = u_1$ in Lemma 4.4.9 with $y' = w_i, y'' = w_j, z' = u_{i+1}, z'' = u_{j+1}$ where $i = h_{T_{\max}}(y') - h_{T_{\max}}(s), j = h_{T_{\max}}(y'') - h_{T_{\max}}(s)$. By the inequality (4.5) and Lemma 4.4.12, we have $d(y') \geq d(z')$ and $d(y'') \geq d(z'')$. Thus (v) in Lemma 3.5.3 is also satisfied. In conclusion, we have proven the optimal tree T_{\max} to be the greedy tree. \square

Now, let us compare trees with different degree sequences.

Lemma 4.4.15 (cf.[35]). *Let $G(\alpha)$ be the greedy tree for the degree sequence α . Let x and y be two vertices in $V(G(\alpha))$ satisfying the inequality $d_{G(\alpha)}(x) \geq d_{G(\alpha)}(y) \geq 2$. Note that if $d_{G(\alpha)}(x) = d_{G(\alpha)}(y)$, we assume that y comes after x in the ordering of vertices in the greedy tree. Let s be a successor of y and let T' be the tree obtained from $G(\alpha)$ by deleting the edge ys and adding the edge xs . Then*

- (i) $\alpha \preceq \alpha'$, where α' is the degree sequence of T' .
- (ii) $\mu(G(\alpha)) < \mu(T')$.

Proof. For the first part (i), we know that $d_{T'}(x) = d_{G(\alpha)}(x) + 1, d_{T'}(y) = d_{G(\alpha)}(y) - 1$ and the degrees of other vertices remain the same. From the fact that $d_{G(\alpha)}(x) \geq d_{G(\alpha)}(y)$, it follows that $\alpha \preceq \alpha'$.

For the second part (ii), we consider a longest path that contains the vertices x, y, z such that z is the common ancestor of x and y . We will show the proof for odd path length, and otherwise it follows in a similar way. Let $z = u_1$ in the labelling described in Lemma 4.4.9. We know that $d(x) \geq d(y)$ so we set $x = u_p, y = w_q$, where $p \leq q$. Let S be the subtree induced by the vertex s and its successors. Let \mathbf{f} be the Perron vector of $G(\alpha)$. It can be observed that the distance between two vertices v and w will only change after switching (described in the Lemma) if $v \in S$ and $w \in G(\alpha) \setminus S$ (or vice versa). We compute $R_{T'}(\mathbf{f}) - R_{G(\alpha)}(\mathbf{f})$ and we obtain the following cases.

Case 1: The contribution to the difference between $R_{G(\alpha)}(\mathbf{f})$ and $R_{T'}(\mathbf{f})$ of vertex pairs where one vertex is in S and the other in some U_i is

$$\begin{aligned}
&= 2 \sum_{i=1}^l \sum_{\substack{s \in S \\ v \in U_i}} [(c - d_{T'}(s, v)) - (c - d_{G(\alpha)}(s, v))] f(s) f(v) \\
&= 2 \sum_{i=1}^l \sum_{\substack{s \in S \\ v \in U_i}} [d_{G(\alpha)}(s, v) - d_{T'}(s, v)] f(s) f(v) \\
&= 2 \sum_{i=1}^l \sum_{\substack{s \in S \\ v \in U_i}} [d_{G(\alpha)}(u_i, u_1) - d_{G(\alpha)}(u_i, u_p) + q] f(s) f(v) \\
&= 2 \sum_{i=1}^l |S|_f \sum_{v \in U_i} [d_{G(\alpha)}(u_i, u_1) - d_{G(\alpha)}(u_i, u_p) + q] f(v) \\
&= 2 \sum_{i=1}^p (2i - 1 + q - p) |S|_f \sum_{v \in U_i} f(v) + 2 \sum_{i=p+1}^l (p + q - 1) |S|_f \sum_{v \in U_i} f(v) \\
&= 2 \sum_{i=1}^p (2i - 1 + q - p) |U_i|_f |S|_f + 2 \sum_{i=p+1}^l (p + q - 1) |U_i|_f |S|_f.
\end{aligned}$$

Case 2: The contribution to the difference between $R_{G(\alpha)}(\mathbf{f})$ and $R_{T'}(\mathbf{f})$ of vertex pairs where one vertex is in S and the other in some $W_i \setminus S$ is

$$\begin{aligned}
&= 2 \sum_{i=1}^l \sum_{\substack{s \in S \\ v \in W_i \setminus S}} [d_{G(\alpha)}(s, v) - d_{T'}(s, v)] f(s) f(v) \\
&= 2 \sum_{i=1}^{q-1} (-2i + 1 + q - p) |W_i|_f |S|_f \\
&\quad - 2(p + q - 1) (|W_q|_f - |S|_f) |S|_f - 2 \sum_{i=q+1}^l (p + q - 1) |W_i|_f |S|_f.
\end{aligned}$$

Summing the case we get $R_{T'}(f) - R_{G(\alpha)}(f)$

$$\begin{aligned}
&= 2 \sum_{i=1}^p (2i-1)(|U_i|_f - |W_i|_f)|S|_f + 2 \sum_{i=1}^p (q-p)(|W_i|_f + |U_i|_f)|S|_f \\
&+ 2 \sum_{i=p+1}^{q-1} (p+q-1)(|U_i|_f - |W_i|_f)|S|_f + 2 \sum_{i=p+1}^{q-1} (2q-2i)|W_i|_f|S|_f \\
&+ 2 \sum_{i=q+1}^l (p+q-1)(|U_i|_f - |W_i|_f)|S|_f \\
&+ 2(p+q-1)(|U_q|_f - |W_q|_f + |S|_f)|S|_f.
\end{aligned}$$

By Lemma 4.4.15, we have $|U_i|_f \geq |W_i|_f$, besides $q \geq p$ and $2q \geq 2i$ for $i \leq q-1$. Therefore, each term in the summation is non-negative. Also, we know that $|S|_f > 0$, so $R_{T'}(f) - R_{G(\alpha)}(f) > 0$ because of the term $(p+q-1)|S|_f^2$. Therefore,

$$\mu(G(\alpha)) = R_{G(\alpha)}(f) < R_{T'}(f) \leq \mu(T').$$

□

Theorem 4.4.16 (cf.[35]). *Let X and Y be the degree sequences of n -vertex trees. Suppose $X \preceq Y$; then*

$$\mu(G(X)) \leq \mu(G(Y)).$$

Proof. We know from Lemma 3.5.12 that there exists a tree with degree sequence X_1 such that $X \preceq X_1 \preceq Y$, where X and X_1 only differ in exactly two places. So we get the two non-increasing sequences to be $X = (x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_n)$ and $X_1 = (x_1, x_2, \dots, x_i + 1, \dots, x_j - 1, \dots, x_n)$ with $i < j$. Let v, w be two vertices in the greedy tree $G(X)$ such that $d_{G(X)}(v) = x_i$ and $d_{G(X)}(w) = x_j$. By the definition of majorization, we can assume that $x_i \geq x_j \geq 2$. Let s be a neighbour of w . If we remove the edge ws and add the edge to $G(X)$ then we obtain a new tree T' with degrees sequence X_1 . Therefore, from Lemma 4.4.15 we get $\mu(T') > \mu(G(X))$. Also, by Theorem 4.4.6, we have $\mu(T') \leq \mu(G(X_1))$. So

$$\mu(G(X_1)) \geq \mu(T') > \mu(G(X)).$$

Continuous repetition of this process yields the result. □

We obtain the following corollaries using the Theorems 4.4.16 and 4.4.6 as a the main tools.

Corollary 4.4.17. *Among trees of order n with maximum degree Δ , the Volkmann tree $V_{n,\Delta}$ maximizes the spectral radius of $M(T)$.*

Proof. The proof is similar to the proof of Corollary 3.5.15 but using Theorems 4.4.6 and 4.4.16. \square

Corollary 4.4.18. *Among all trees of order n with k leaves, the greedy tree corresponding to the degree sequence $\alpha = (k, 2, \dots, 2, 1, \dots, 1)$ maximizes the spectral radius of $M(T)$.*

Proof. The proof is similar to the proof of Corollary 3.5.16 but using Theorems 4.4.6 and 4.4.16. \square

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