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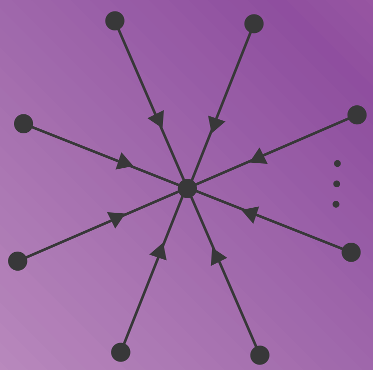

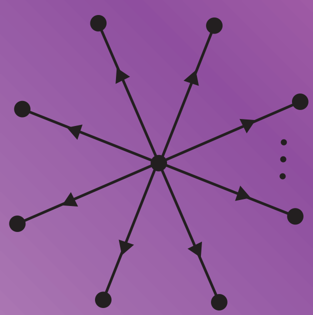

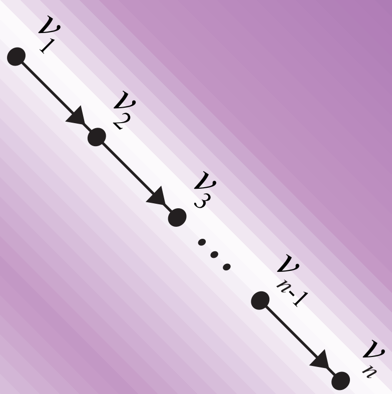

Spectral properties of digraphs with a fixed dichromatic number

Xiuwen Yang

SPECTRAL PROPERTIES OF DIGRAPHS WITH A FIXED DICHROMATIC NUMBER

DISSERTATION

to obtain
the degree of doctor at the University of Twente,
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on account of the decision of the Doctorate Board,
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Preface

This thesis focuses on the study of the spectral properties of directed graphs (digraphs for short) with a fixed dichromatic number. This study involves different types of matrices associated with the digraph, such as the Laplacian matrix, the A_α matrix and the eccentricity matrix. The content of the thesis is based on the research that the author performed when she was working as a joint PhD student at Northwestern Polytechnical University (NPU) and the University of Twente (UT).

After the introductory chapter (Chapter 1), the reader will find four closely related technical chapters (Chapters 2–5), each of which has the structure of a journal paper. Chapters 2 and 3 focus on the spectral moments of digraphs with a fixed dichromatic number, involving the Laplacian matrix and the A_α matrix. Chapters 4 and 5 focus on the spectral radius of digraphs with a fixed dichromatic number, involving the A_α matrix and the eccentricity matrix.

In Chapter 2, our main purpose is to characterize the digraphs which attain the minimal and maximal Laplacian energy within classes of digraphs with a fixed dichromatic number. In Chapter 3, we extend the results about Laplacian spectral moments we obtained in Chapter 2 to A_α spectral moments. In our main result of Chapter 4, we characterize the digraph which has the maximal A_α spectral radius among all digraphs with a fixed dichromatic number, by using the equitable quotient matrix. In Chapter 5, we mainly obtain lower bounds for the eccentricity spectral radius among all join digraphs with a fixed dichromatic number.

Papers underlying this thesis

[1] Sharp bounds for Laplacian spectral moments of digraphs with a fixed dichromatic number, *Discrete Mathematics* **347** (2024), 113659 (with H.J. Broersma and L. Wang). (Chapter 2)

[2] The A_α spectral moments of digraphs with a given dichromatic number, accepted by *Linear Algebra and Its Applications* (with H.J. Broersma and L. Wang). (Chapter 3)

[3] Colorings and A_α spectral radius of (join) digraphs, submitted (with L. Wang and J. Li). (Chapter 4)

[4] The bounds for eccentricity spectral radius of join digraphs with a fixed dichromatic number, submitted (with H.J. Broersma and L. Wang). (Chapter 5)

Other papers by the author

[1] Ordering of bicyclic signed digraphs by energy, *Filomat* **34** (2020), 4297–4309 (with L. Wang).

[2] Iota energy orderings of bicyclic signed digraphs, *Transactions on Combinatorics* **10** (2021), 187–200 (with L. Wang).

[3] The eccentricity matrix of a digraph, *Discrete Applied Mathematics* **322** (2022), 61–73 (with L. Wang).

[4] On the sum of the k largest absolute values of Laplacian eigenvalues of digraphs, *Electronic Journal of Linear Algebra* **39** (2023), 409–422 (with X. Liu and L. Wang).

Contents

Chapter 1

Introduction

Before giving some essential terminology and notation related to (di)graphs in Section 1.1 and related to matrices and spectral properties in Section 1.2, we start with a brief introduction, including some background and motivation for the presented results.

Graphs are used in many application areas to model and analyze pairwise relationships between objects. For symmetric relationships this is done by introducing edges, i.e., unordered pairs of vertices, for any pair of related objects each of which is represented by a separate vertex. For asymmetric relationships the model is based on arcs, i.e., ordered pairs of vertices, to represent the direction of the relationship between the represented objects. This leads to the mathematical concepts of undirected graphs (or graphs for short) and directed graphs (or digraphs for short), respectively. We will introduce digraphs and the relevant terminology more formally in Section 1.1.

Given a graph or digraph, one can define several different types of matrices associated with the (di)graph, as we will see in Section 1.2. Several important structural properties of the (di)graph are captured by the spectral properties of such matrices, i.e., the value of certain concepts involving the eigenvalues of these matrices. The study of the spectral properties of these matrices and its consequences for the structural properties of the associated graphs is usually referred to as spectral graph theory.

Spectral graph theory is a very important research topic in algebraic graph theory and combinatorial matrix theory. It is one of the fourteen topics on the development of mathematics listed in "Fueling Innovation and Discovery: The Mathematical Sciences in the 21st Century". Since the publication of the monograph "Spectra of Graphs" by Cvetković et al. [26] back in 1980, the field of spectral graph theory has developed rapidly, and has gradually formed into a relatively complete theoretical system. Since then several monographs have been published [13, 25, 27, 28, 47, 68, 118].

Spectral graph theory is not only closely related to linear algebra, combinatorial matrix theory, discrete mathematics, number theory, group theory and other branches of mathematics, but also has a wide range of applications in chemistry, physics, biology, computer science, information science, network science and many other fields. For example, networks consisting of nodes and links can be represented by a graph (where the nodes and links are represented by vertices and edges in the graph, respectively). Networks with the largest possible eigenvalues (to be defined later) have some remarkable properties. They deliver messages very quickly, so it is easy to route messages from one vertex to another. They have no bottlenecks, so they are not disabled by the failure of a few nodes or links. Also, the size of the spectral radius (to be defined later) can directly reflect the ability of the network to resist virus transmission: the smaller the adjacency spectral radius, the stronger the ability of the network to resist virus transmission. The study of spectral graph theory has attracted the attention of experts and scholars at home and abroad, and has become a very active research field in graph theory. The study of spectral graph theory can not only enrich and perfect its theoretical system, but also play a role in promoting the development of algebraic graph theory, combinatorial matrix theory and related fields.

Spectral graph theory mainly studies the properties of graphs related to the characteristic polynomials, eigenvalues and eigenvectors of matrices associated with the graph. The most commonly studied graph matrices are its adjacency matrix, its Laplacian matrix, and its signless Laplacian matrix. The most commonly studied spectral properties are the spectral radius (the maximum of the absolute values of the eigenvalues), the k-th spectral moment (the sum of the k-th powers of the eigenvalues), the spread (the maximum of the absolute values of the differences between any two eigenvalues), and the sum of the k largest eigenvalues. In this thesis, we mainly focus on the spectral moment (in Chapters 2 and 3) and the spectral radius (in Chapters 4 and 5) of digraphs.

In general, what we call a graph is an undirected graph. An undirected graph is used to describe a particular relationship between objects, and it requires that the particular relationship is symmetric. In real life, however, many relationships are not symmetric, such as the relationship between winners and losers in a race, the relationship between routes in a traffic network, or the relationship between processes in engineering. Digraphs form the natural extension of graphs to reflect the asymmetric relationships among pairs of objects. This demonstrates the need and practical importance of studying digraphs.

The matrices of undirected graphs are nonnegative real symmetric matrices, and their eigenvalues are all real numbers. But the matrices of digraphs are not necessarily symmetric, and their eigenvalues are generally complex numbers. As a result, the research methods and techniques that are used for undirected graphs are often difficult to apply to digraphs. As examples we name the concept of Rayleigh entropy and the Cauchy interlacing theorem, without going into details. This fact is increasing the difficulty of studying the spectral properties of digraphs. Therefore, researchers often study the spectral properties of matrices of digraphs with some given parameters, including their dichromatic number (the smallest integer r such that the digraph has a partition of its vertex set into r sets, each inducing an acyclic subdigraph), their clique number (the maximum number of mutually adjacent vertices), their girth (the length of a shortest directed cycle), their vertex connectivity (the minimum number of vertices whose deletion yields the resulting digraph non-strongly connected), and their arc connectivity (the minimum number of arcs whose deletion yields the resulting digraph non-strongly connected).

In this thesis, the main parameter involved in our study of the spectral properties of digraphs is their dichromatic number. This digraph parameter was introduced 40 years ago by Neumann-Lara [98]. Since then, several groups of scholars studied the dichromatic number of digraphs and structural properties related to the dichromatic number of digraphs, see [3, 7, 23, 24, 50, 60, 61, 116, 117]. Bokal et al. [7] introduced the circular chromatic number of a digraph and showed that the coloring theory for digraphs is similar to the coloring theory for undirected graphs when independent sets of vertices are replaced by acyclic sets. Steiner [117] proved that every oriented graph in which the out-neighborhood of every vertex induces a transitive tournament can be partitioned into two acyclic induced subdigraphs. Other groups of researchers have focused on algebraic properties related to the dichromatic number of digraphs, see [32, 43, 62, 74, 78, 89, 96, 132]. The first connection between the dichromatic number and algebraic properties related to eigenvalues of digraphs was made by Mohar in [96]. He extended Wilf's classical eigenvalue upper bound on the chromatic number of undirected graphs to the analogue for digraphs in terms of the dichromatic number and the spectral radius of the adjacency matrix. Lin and Shu [78] characterized the digraphs with given dichromatic number which have the maximal spectral radius. Kim et al. [62] provided a new proof of the results by Lin and Shu [78]. Many of the results in this thesis deal with the algebraic and structural properties related to the dichromatic number of digraphs.

More in particular, we study the spectral properties (spectral moment or spectral radius) of digraphs with a fixed dichromatic number, focusing on different matrices. To be more precise, we focus on the Laplacian matrix in Chapter 2, the A_α-matrix in Chapters 3 and 4, and the eccentricity matrix in Chapter 5.

After providing some basic terminology and notation in Section 1.1, we will introduce the concepts for different digraph matrices in detail in Section 1.2, and the research progress with respect to the spectral moment and spectral radius in Section 1.3. In the later sections of this chapter, we will recall some known lemmas used for our results, and provide an overview of our main contributions to the field.

1.1 Terminology and notation

In this section, we introduce some basic terminology and notation. All digraphs considered in this thesis are connected digraphs without loops or multiple arcs, unless otherwise indicated. For terminology and notation not defined here, we refer the reader to [8].

For a digraph G, we use $\mathscr{V}(G)$ and $\mathscr{A}(G)$ to denote the vertex set and arc set of G, respectively, and we use $n = |\mathscr{V}(G)|$ and $e = |\mathscr{A}(G)|$ to denote the *order* and *size* of G, respectively. We denote an arc from a vertex u to a vertex v by (u, v), and we call u the *tail* and v the *head* of the arc (u, v).

For two disjoint subdigraphs $G_1, G_2 \subseteq G$, we write $G_1 \to G_2$ if $(u, v) \in \mathscr{A}(G)$ for every $u \in \mathscr{V}(G_1)$ and $v \in \mathscr{V}(G_2)$, and $G_1 \nrightarrow G_2$ if $(u, v) \notin \mathscr{A}(G)$ for every $u \in \mathscr{V}(G_1)$ and $v \in \mathscr{V}(G_2)$. We also use $G_1 \mapsto G_2$ to denote $G_1 \to G_2$ and $G_2 \nrightarrow G_1$.

For a vertex $v \in \mathscr{V}(G)$, the *outdegree* $d^+_G(v)$ is the number of arcs in $\mathscr{A}(G)$ whose tail is v, while the *indegree* $d^-_G(v)$ is the number of arcs in $\mathscr{A}(G)$ whose head is v. We denote by $\Delta^+(G)$ the *maximum outdegree* of G, $\Delta^-(G)$ the *maximum indegree* of G, $\delta^+(G)$ the *minimum outdegree* of G and $\delta^-(G)$ the *minimum indegree* of G, respectively.

A *directed walk* π of length ℓ from vertex u to vertex v in G is a sequence of vertices π: $u = v_0, v_1, \ldots, v_\ell = v$, where (v_{k-1}, v_k) is an arc of G for any $1 \le k \le \ell$. If $u = v$, then π is called a *directed closed walk*. If all vertices of the directed walk π of length ℓ are distinct, then we call it a *directed path*, and denote it by $P_{\ell+1}$; a directed closed walk of length ℓ in which all except the end vertices are distinct is called a *directed cycle*, and denoted by C_ℓ. We let $c_\ell(v)$ denote the number of directed closed walks of length ℓ starting at vertex v, and $c_\ell = \sum_{v \in \mathscr{V}(G)} c_\ell(v)$ to denote the total number of directed closed walks of length ℓ (clearly involving a lot of double counting).

The *distance* $d(u, v)$ between the vertices $u, v \in \mathscr{V}(G)$ is defined as the length (i.e. the number of arcs) of a shortest directed path from u to v. The *out-eccentricity* $e^+(u)$ of the vertex u of G is defined as $e^+(u) = \max\{d(u, v) | v \in \mathscr{V}(G)\}$, while the *in-eccentricity* $e^-(u)$ of the vertex u of G is defined as $e^-(u) = \max\{d(v, u) | v \in \mathscr{V}(G)\}$. The *diameter* $diam(G)$ of G is defined as: $diam(G) = \max\{e^+(u) | u \in \mathscr{V}(G)\} = \max\{e^-(u) | u \in \mathscr{V}(G)\}$.

A digraph G is *acyclic* if it has no directed cycles. A vertex set $F \subseteq \mathscr{V}(G)$ is acyclic if its induced subdigraph $G[F]$ in G is acyclic. A partition of $\mathscr{V}(G)$ into r acyclic sets is called an *r-coloring* of G. Adopting the definition of [98], the minimum integer r for which there exists an r-coloring of G is the *dichromatic* *number* $\chi(G)$ of G.

We next introduce some special classes of digraphs. For a digraph G, the *underlying graph* is a graph obtained from G by ignoring the direction on the arcs of G, i.e., by replacing each arc (u, v) of G with an edge joining u and v (possibly yielding multiple edges).

A digraph is *connected* if its underlying graph is connected. A digraph G is *strongly connected* if for each $u, v \in \mathscr{V}(G)$, there is a directed path from u to v and one from v to u. A *strong component* of a digraph G is a maximal strongly connected subdigraph of G.

A *directed tree* is a digraph obtained from an undirected tree by assigning a direction to each edge, i.e., a digraph with n vertices and $n-1$ arcs whose underlying graph does not contain any cycles. If $n = 1$, then the directed tree is an isolated vertex.

As illustrated in Figure 1.1, an *in-tree* is a directed tree for which the outdegree of each vertex is at most one. Hence, an in-tree has exactly one vertex with outdegree 0, and such a vertex is called the *root* of the in-tree.

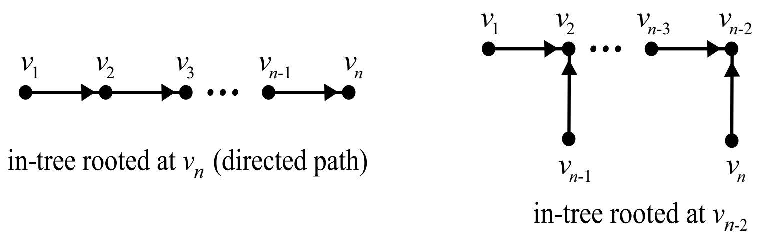


Figure 1.1: Two different in-trees.

As illustrated in Figure 1.2, an *out-star* $\overrightarrow{K}_{1,n-1}$ of order n is a directed tree which has one vertex with outdegree $n-1$ and all other vertices with outdegree 0, while an *in-star* $\overleftarrow{K}_{1,n-1}$ of order n is a directed tree which has one vertex with indegree $n-1$ and all other vertices with indegree 0.

Let B_n be a *book* digraph of order n which $\mathscr{V}(B_n) = \{v_1, v_2, \ldots, v_n\}$ and $\mathscr{A}(B_n) = \{(v_1, v_n), (v_1, v_i), (v_i, v_n) | i = 2, 3, \ldots, n-1\}$, see Figure 1.3.

A *tournament* is a digraph obtained from an undirected complete graph by assigning a direction to each edge. A *transitive tournament* is a tournament G

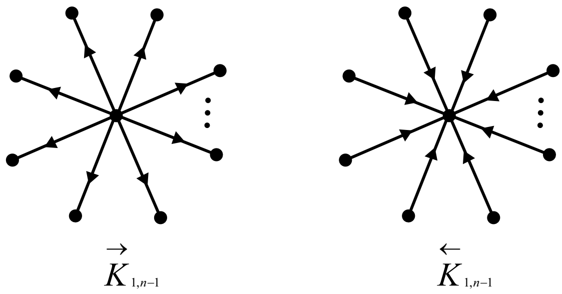


Figure 1.2: The out-star $\overrightarrow{K}_{1,n-1}$ and the in-star $\overleftarrow{K}_{1,n-1}$.

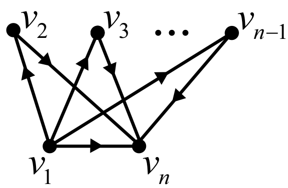


Figure 1.3: The book digraph B_n.

satisfying the following condition: if $(u,v) \in \mathscr{A}(G)$ and $(v,w) \in \mathscr{A}(G)$, then $(u,w) \in \mathscr{A}(G)$.

Every undirected graph H determines a *bidirected graph* $\overleftrightarrow{H}$ that is obtained from H by replacing each edge with two oppositely arcs joining the same pair of vertices. We use $\overleftrightarrow{K}_n$ to denote the *bidirected complete graph* of order n, $G = \overleftrightarrow{K}_{n_1,n_2,\ldots,n_r}$ to denote the *bidirected complete r-partite graph*, and $\overleftrightarrow{C}_n$ to denote the *bidirected cycle* of order n.

The *join* of two vertex-disjoint digraphs G_1 and G_2, denoted by $G_1 \vee G_2$, is the digraph having vertex set $\mathscr{V}(G_1) \cup \mathscr{V}(G_2)$ and arc set $\mathscr{A}(G_1) \cup \mathscr{A}(G_2) \cup \{(u,v),(v,u) | u \in \mathscr{V}(G_1), v \in \mathscr{V}(G_2)\}$. We use $G_1 \vee G_2 \vee \cdots \vee G_r$ as shorthand for the join $G_1 \vee (G_2 \vee (\cdots \vee G_r))$ of $r \geq 3$ vertex-disjoint digraphs $G_1, G_2, \ldots, G_r$.

We use $\mathscr{G}_{n,r}$ to denote the set of digraphs of order n with dichromatic number r. We say that a digraph with dichromatic number r is a *join digraph* if it is the join of r acyclic digraphs. In particular, we let $\bigvee_{i=1}^{r} V^i$ denote the join digraph in $\mathscr{G}_{n,r}$ which is isomorphic to $V^1 \vee V^2 \vee \cdots \vee V^r$, in which each V^i is an acyclic digraph with n_i vertices, and we assume that $\sum_{i=1}^{r} n_i = n$.

1.2 Digraphs matrices

As we noted before, several different matrices have been introduced and studied in the context of spectral properties of digraphs. We will define them in this section and treat them in more detail in the following subsections. At the end of this section the reader will find a small example to illustrate these matrices. Among the mostly studied matrices, we focus on the adjacency matrix $A(G)$ [11, 14, 59, 106, 112, 119], the Laplacian matrix $L(G)$ [2, 5, 107, 110, 136], the signless Laplacian matrix $Q(G)$ [10,55,65,72,131], the distance matrix $D(G)$ [30,44,79,82,129], and the A_α-matrix $A_\alpha(G)$ [4,40,89,130,133]. We refer the interested reader to the following sources for details on other digraph matrices [53, 71, 74, 128, 132].

Let I_n be a unit matrix of order n and let $J_{n\times m}$ be an all 1-matrix of order $n \times m$. We use J_n to denote the all 1-matrix of order $n \times n$.

Let $M(G)$ be a square $n \times n$-matrix associated with a digraph G. Then the *characteristic polynomial* $\phi_{M(G)}(x)$ of G (of order n) is $\phi_{M(G)}(x) = |xI_n - M(G)|$, where $|\cdot|$ denotes the *determinant*. The roots of $\phi_{M(G)}(x)$ are the $M(G)$-*eigenvalues* of G. The $M(G)$-*spectrum* of G is a multiset consisting of the $M(G)$-eigenvalues, denoted by $Spec_M(G)$. The eigenvalue of $M(G)$ with the largest modulus is called the $M(G)$-*spectral radius* of G, denoted by $\rho_M(G) = \rho(M(G))$. We next introduce the different digraphs matrices in detail.

We assume that $\mathscr{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and use d_i^+ as shorthand for $d_G^+(v_i)$.

The *adjacency matrix* $A(G) = (a_{ij})_{n\times n}$ of G is a $(0, 1)$-square matrix whose (i, j)-entry equals 1 if (v_i, v_j) is an arc of G, and equals 0 otherwise.

The *Laplacian matrix* $L(G)$ and the *signless Laplacian matrix* $Q(G)$ of G are $L(G) = D^+(G) - A(G)$ and $Q(G) = D^+(G) + A(G)$, respectively, where $D^+(G) = diag(d_1^+, d_2^+, \ldots, d_n^+)$ is the *diagonal outdegree matrix* of G.

The A_α-*matrix* of G is

$$A_\alpha(G) = \alpha D^+(G) + (1 - \alpha)A(G),$$

where $\alpha \in [0, 1]$. It is clear that the A_α-matrix is a natural common extension of the adjacency matrix $A(G) = A_0(G)$ and the signless Laplacian matrix $Q(G) = 2A_{\frac{1}{2}}(G)$. Since $D^+(G)$ is not very interesting to study, we only consider $\alpha \in [0, 1)$.

Because the concept of distance only makes sense on strongly connected digraphs, the concepts of distance matrix and eccentricity matrix also only make sense on strongly connected digraphs. So, whenever we consider these matrices we implicitly assume that the associated digraphs are strongly connected, i.e., all distances between pairs of vertices are finite.

The *distance matrix* $D(G) = (d_{ij})_{n\times n}$ of G is a matrix whose (i, j)-entry equals $d(v_i, v_j)$, where $i, j = 1, 2, \ldots, n$.

The *eccentricity matrix* $\varepsilon(G)$ of G is obtained from the distance matrix of G by keeping the largest distances in each row and each column, and leaving 0 in the remaining ones, as follows:

$$\varepsilon(G)_{ij} = \begin{cases} d(v_i, v_j), & \text{if } d(v_i, v_j) = \min\{e^+(v_i), e^-(v_j)\}, \\ 0, & \text{otherwise.} \end{cases}$$

All of the above matrices are nonnegative matrices except for the Laplacian matrix. As we have seen, the A_α-matrix can be regarded as an extension of the adjacency matrix and the signless Laplacian matrix. The adjacency matrix and the eccentricity matrix can be regarded as the two extremes of the distance matrix, only keeping the smallest and largest distances as entries, respectively, although they are not extremal in a mathematical sense. The adjacency matrix is by far the mostly studied digraph matrix. In this thesis we mainly focus on the spectral properties of the Laplacian matrix, the A_α-matrix and the eccentricity matrix of digraphs. The reported research has mainly theoretical value and significance. Next, in each of the following subsections we will give a short overview of the research progress with respect to the Laplacian matrix, the A_α-matrix and the eccentricity matrix of digraphs, respectively.

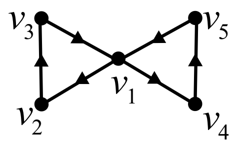


Figure 1.4: The bicyclic digraph $\infty[3,3]$.

We give a simple digraph to illustrate the above matrices. Let $\infty[3,3]$ be the bicyclic digraph shown in Figure 1.4. Then

$$A(\infty[3,3]) = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$L(\infty[3,3]) = \begin{pmatrix} 2 & -1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$A_\alpha(\infty[3,3]) = \begin{pmatrix} 2\alpha & 1-\alpha & 0 & 1-\alpha & 0 \\ 0 & \alpha & 1-\alpha & 0 & 0 \\ 1-\alpha & 0 & \alpha & 0 & 0 \\ 0 & 0 & 0 & \alpha & 1-\alpha \\ 1-\alpha & 0 & 0 & 0 & \alpha \end{pmatrix},$$

$$D(\infty[3,3]) = \begin{pmatrix} 0 & 1 & 2 & 1 & 2 \\ 2 & 0 & 1 & 3 & 4 \\ 1 & 2 & 0 & 2 & 3 \\ 2 & 3 & 4 & 0 & 1 \\ 1 & 2 & 3 & 2 & 0 \end{pmatrix}, \ \varepsilon(\infty[3,3]) = \begin{pmatrix} 0 & 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 3 & 4 \\ 0 & 0 & 0 & 0 & 3 \\ 2 & 3 & 4 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \end{pmatrix}.$$

1.2.1 Laplacian matrix

Within spectral graph theory the Laplacian matrix is well-studied, and it is known to have nice properties. As an example, the number of occurrences of 0 in its eigenvalues is the number of connected regions of the graph. Moreover, its smallest non-zero eigenvalue is the algebraic connectivity of the graph.

One of the classic results on the Laplacian matrix is in fact a conjecture due to Brouwer [13]. In Brouwer's conjecture it is conjectured that the sum of the k largest Laplacian eigenvalues of an undirected graph H is

$$S_k(H) \leq e(H) + \binom{k+1}{2},$$

for all $k = 1, 2, \ldots, n$, where $e(H)$ is the number of edges of H. The general conjecture is still open, but it has been verified for many special cases. Over time, Brouwer's conjecture has resulted in many interesting results [15, 33, 38, 52, 108]. Some scholars have focused on the study of the Laplacian spectral radius [1, 87, 142], and some on the study of the Laplacian spread [5, 16, 18], among other spectral properties. In this thesis we mainly focus on the Laplacian energy. We will introduce it by a short historical overview.

Graph energy is one of the main concepts in chemical graph theory, and as such is the central concept in one of the few chemically motivated branches in discrete mathematics. Graph energy goes back to the late 1970s, when it was introduced by Gutman [45] as the sum of the absolute values of the eigenvalues of the adjacency matrix of a graph. More recently, in 2006, Gutman and Zhou [48] and Lazić [66] independently defined different versions of the Laplacian energy of a graph, where the version of Lazić is defined as the sum of the squares of the eigenvalues of the Laplacian matrix of the graph. The latter definition was extended to digraphs in 2010 by Perera and Mizoguchi [107]. In a paper of 2015 [110], Qi et al. obtained lower and upper bounds on the Laplacian energy of digraphs and also characterized the extremal digraphs. Very recently, in a paper of 2020 [136], Yang and Wang determined the directed trees, unicyclic digraphs and bicyclic digraphs which attain the maximal and minimal Laplacian energy among all digraphs with n vertices, respectively.

In this thesis, our main results in Chapter 2 are closely related to and motivated by the aforementioned results obtained in [110] and [136]. We consider classes of digraphs with a fixed dichromatic number and obtain the digraphs which attain the minimal and maximal Laplacian energy among these classes of digraphs.

1.2.2 A_α-matrix

Research on the A_α-matrix began in 2017, when Nikiforov [99] proposed the A_α-matrix of an undirected graph H of order n as

$$A_\alpha(H) = \alpha D(H) + (1-\alpha)A(H),$$

where $A(H)$ is the adjacency matrix and $D(H)$ is the diagonal degree matrix of H, and $\alpha \in [0,1)$.

Subsequently, several different groups of researchers have studied the properties of the A_α-matrix of undirected graphs. In 2017, Nikiforov et al. [100] obtained several results about the A_α-matrices of trees, and established upper and lower bounds on the spectral radius of the A_α-matrices of arbitrary graphs. In 2019, Lin et al. [77] proved that some graphs are determined by their A_α-spectra. In 2020, Liu et al. [85] presented several upper and lower bounds on the k-th largest eigenvalue of the A_α-matrix and characterized the extremal graphs corresponding to some of these obtained bounds. In 2022, Li and Sun [70] showed that in the set of connected graphs with fixed order and size, the graphs with the maximum A_α-index are the nested split graphs (i.e. threshold graphs). More results about the A_α-matrix of graphs can be found in [12, 69, 75, 76, 81, 83, 86, 101].

In 2019, the concept of the A_α-matrix of a graph has been extended to digraphs by Liu et al. [89]. They also characterized the digraph which has the maximal A_α spectral radius in $\mathscr{G}_{n,r}$. In Chapter 4, in one of our main results we give an alternative approach for characterizing the digraph with the maximal A_α spectral radius in $\mathscr{G}_{n,r}$.

In 2020, Xi and Wang [133] established lower bounds on $\Delta^+(G) - \rho_\alpha(G)$ for strongly connected irregular digraphs with given maximum outdegree $\Delta^+(G)$, involving some other parameters. Here $\rho_\alpha(G)$ denotes the spectral radius of $A_\alpha(G)$. In 2022, Xi et al. [130] determined the digraphs which attain the maximum (or minimum) A_α spectral radius among all strongly connected digraphs with given parameters such as the girth, the clique number, the vertex connectivity or the arc connectivity. Ganie and Baghipur [40] obtained lower bounds for the spectral radius of $A_\alpha(G)$ in terms of the number of vertices, arcs and directed closed walks of G. More results regarding the A_α-matrix of digraphs can be found in [4, 37, 39, 134, 139].

It can be observed that the literature about the A_α-matrix of digraphs is not as rich as it is for the adjacency and Laplacian matrix. This has motivated the work we will present in Chapters 3 and 4. There we consider the A_α spectral moment and the A_α spectral radius of digraphs with a fixed dichromatic number, respectively.

1.2.3 Eccentricity matrix

The eccentricity matrix of a graph was introduced by Randić [113] in 2013 under the name D_{MAX}-matrix, and was renamed the eccentricity matrix by Wang et al. [120] in 2018.

As we have seen before, the eccentricity matrix of a graph is obtained from the distance matrix by keeping the largest distances in each row and each column, and leaving 0 in the remaining ones. This matrix can be interpreted as the opposite of the adjacency matrix, which is instead constructed from the distance matrix of a graph by keeping for each row and each column only the distances are equal to 1. Hence, the adjacency matrix can be viewed as a D_{MIN}-matrix and the eccentricity matrix can be viewed as a D_{MAX}-matrix.

Since 2018, there have appeared quite a few results about the eccentricity matrix of undirected graphs. Wang et al. [120] showed that the eccentricity matrices of trees are irreducible. In 2019, Wang et al. [123] investigated the relationship between the ε-energy (the sum of the absolute values of the eigenvalues of the eccentricity matrix) and the A-energy (the sum of the absolute values of the eigenvalues of the adjacency matrix). They also provided upper and lower bounds for the ε-energy, and showed that the extremal graphs are a kind of self-centered graphs. In 2020, Wei et al. [124]

characterized the extremal trees of given diameter having the minimum ε-spectral radius. In 2021, Patel et al. [104] studied the irreducibility and the spectrum of the eccentricity matrix for particular classes of graphs, namely windmill graphs, the coalescence of complete graphs, and the coalescence of two cycles. In 2022, Wang et al. [121] showed that when the order n tends to infinity, the fractions of non-isomorphic cospectral graphs with respect to the adjacency and the eccentricity matrix behave like those only concerning the self-centered graphs with diameter two. More results regarding the eccentricity matrix of undirected graphs can be found in [51, 67, 92–94, 111, 114, 122, 125]. However, there is still little reported research on the eccentricity matrix of digraphs.

In 2022, Yang and Wang [137] first extended the concept of eccentricity matrix from graphs to digraphs. They considered the irreducibility of the eccentricity matrix of a digraph with diameter 2, and obtained a lower bound on the spectral radius of the eccentricity matrix of a digraph with diameter 2.

With the above as our motivation, we continued our research on the eccentricity matrix of digraphs. In Chapter 5, we obtain lower bounds for the eccentricity spectral radius among all join digraphs with a fixed dichromatic number.

1.3 Spectral moment and spectral radius

Spectral graph theory is an important research subject within algebraic graph theory, studying the structural properties of a graph by relating the structure to the eigenvalues and eigenvectors of matrices associated with the graph. There are many defined and studied concepts related to the eigenvalues of a matrix, such as its spectral radius, spectral moment, spread, energy, etc. In this thesis, we mainly focus on the spectral moment (Chapters 2 and 3) and the spectral radius (Chapters 4 and 5) of matrices associated with digraphs. Next, we will give a short overview of the most relevant concepts and results regarding the spectral moment and the spectral radius of matrices of (di)graphs, respectively.

1.3.1 Spectral moment

For a fixed nonnegative integer k, the k-th adjacency spectral moment of a digraph G is defined as

$$SM_k(G) = \sum_{i=1}^{n} z_i^k,$$

where z_i are the eigenvalues of $A(G)$. It is known and straightforward to show that the latter sum equals c_k, the total number of directed closed walks of length k in G. Similarly, for the Laplacian matrix and A_α-matrix, the k-th spectral moments of G are

$$LSM_k(G) = \sum_{i=1}^{n} \lambda_i^k \text{ and } SM_\alpha^k(G) = \sum_{i=1}^{n} \lambda_{\alpha i}^k,$$

where λ_i and $\lambda_{\alpha i}$ are the eigenvalues of $L(G)$ and $A_\alpha(G)$, respectively.

For an undirected graph H, let

$$SM_k(H) = \sum_{i=1}^{n} \nu_i^k$$

be the k-th spectral moment of H, where ν_i are the eigenvalues of $A(H)$. Let

$$SM(H) = \left(SM_0(H), SM_1(H), \ldots, SM_{n-1}(H)\right)$$

be the sequence of spectral moments of H. Several groups of researchers have focused on the study of this sequence of spectral moments of graphs. Some recent and very recent results involving the sequence of spectral moments of graphs can be found in [21, 29, 34, 35, 103]. In another direction, scholars have related the spectral moments of an undirected graph H to the energy $E(H) = \sum_{i=1}^{n} |\nu_i|$. In fact, in [105], de la Peña et al. proved

$$E(H) \geq \left(SM_r(H)\right)^2 \left(SM_s(H) SM_t(H)\right)^{-1/2},$$

when H is a bipartite graph with at least one edge and r, s, t are even positive integers such that $4r = s + t + 2$. And in [146], Zhou et al. defined the moment-like quantities $SM_k^*(G) = \sum_{i=1}^n |\nu_i|^k$ and proved

$$E(H) \geq \left(SM_r^*(H)\right)^2 \left(SM_s^*(H)SM_t^*(H)\right)^{-1/2},$$

when H is a graph with at least one edge and r, s, t are nonnegative real numbers such that $4r = s + t + 2$. Obviously, the result in [105] is a special case of [146].

Most studies on spectral moments, however, have focused on the adjacency matrix of graphs. For results on the spectral moments of other graph matrices associated with undirected graphs the reader is referred to [88, 97, 126]. For digraphs, results about the spectral moments of matrices are generally lacking. This motivated us to study the spectral moments of the Laplacian matrix and the A_α-matrix of digraphs.

1.3.2 Spectral radius

The spectral radius of a matrix is the maximum of the absolute values of the eigenvalues of that matrix. Apart from the theoretical relevance, the spectral radius has been studied in the context of applications. As we mentioned before, as an example the adjacency spectral radius can reflect the ability of networks to withstand virus transmission. Here we are mainly interested in the theoretical implications. Within algebraic graph theory, the research regarding the spectral radius of various different matrices has attracted considerable attention. Researchers have in particular paid attention to the adjacency spectral radius [22, 54, 63, 84, 140], the Laplacian spectral radius [1, 87, 142, 144, 145], the signless Laplacian spectral radius [19, 20, 58, 73, 147], the distance spectral radius [9, 95, 102, 141, 143], and the A_α spectral radius [17, 57, 76, 90, 135].

However, all of the above references deal with undirected graphs. Although a great deal of research has been done on spectral radii in conjunction with various structural parameters and invariants of graphs, compared to the above lists, results on digraphs are relatively scarce. Early results on the spectral radius of digraphs can be found in the survey [14]. Recently, some new results about the spectral radius of digraphs have appeared. In 2012, Lin et al. [80] established sharp upper and lower bounds for digraphs with some given graph parameters, such as the clique number, girth, and vertex connectivity, and characterized the corresponding extremal graphs. In 2016, Drury and Lin [32] determined the digraphs that have the minimum and second minimum spectral radius among all strongly connected digraphs with given order and dichromatic number. In 2021, Xi et al. [129] completely determined the strongly connected digraphs minimizing the spectral radius among all strongly connected digraphs with order n and diameter d, for $d = 1,2,3,4,5,6,7,n-1$. In 2022, Shan et al. [115] characterized the extremal digraphs with the maximal or minimal α-spectral radius among some digraph classes, such as rose digraphs, generalized theta digraphs, and tri-ring digraphs with given size m. In 2023, Ganie and Carmona [41] established an increasing sequence of lower bounds for the spectral radius of digraphs. For more results on digraphs see [4,10,39,40,42,55,59,64,65,71,82,89,128,130–132]. In this thesis, we mainly study the spectral radii of the A_α-matrix and the eccentricity matrix of digraphs.

1.4 Some known results

In this section, we will list some known results for later reference. First, since we will focus on digraphs with a fixed dichromatic number, we recall some useful lemmas involving r-critical digraphs that appeared in a paper due to Mohar [96]. Let G be a digraph and recall that $\chi(G)$ denotes the dichromatic number of G, i.e., the smallest integer r such that G has a partition of $\mathcal{V}(G)$ into r sets, each inducing an acyclic subdigraph. Suppose that $v \in \mathcal{V}(G)$ is a vertex such that $\chi(G-v) < \chi(G)$. Then we say that v is a critical vertex. If every vertex of G is critical and $\chi(G) = r$, then we say that G is an r-critical digraph. Note that every digraph with dichromatic number at least r contains an induced subdigraph that is r-critical. The following results relate the degrees of critical vertices to the dichromatic number, and determine some structure of the extremal cases. These results turn out to be very useful for our purposes.

Lemma 1.1 (Mohar [96]). *If v is a critical vertex in a digraph G with dichromatic number r, then $d_G^+(v) \geq r-1$ and $d_G^-(v) \geq r-1$.*

Lemma 1.2 (Mohar [96]). *Let G be an r-critical digraph of order n in which every vertex v satisfies $d_G^+(v) = d_G^-(v) = r-1$. Then one of the following cases occurs:*
(i) $r=2$ and G is a directed cycle of length $n \geq 2$.
(ii) $r=3$ and G is a bidirected cycle of odd length $n \geq 3$.
(iii) G is a bidirected complete graph of order $r \geq 4$.

Because a lot of properties of spectral radii involve irreducibility of matrices, we recall the concept of an irreducible matrix. Note that we assume throughout the sequel that all matrices are square matrices. A matrix M is said to be *reducible* if there exists a permutation matrix P such that

$$M = P \begin{pmatrix} M_{11} & 0 \\ M_{21} & M_{22} \end{pmatrix} P^T,$$

where M_{11} and M_{22} are square blocks. If no such permutation matrix P exists, then M is said to be *irreducible*.

We next introduce some notation we adopted from [6] to define what we mean by $A \leq B$, $A < B$, and $A \ll B$ for two $n \times n$ matrices A and B.

Definition 1.1 (Berman and Plemmons [6]). Let $A = (a_{ij})$, $B = (b_{ij})$ be two $n \times n$ matrices. If $a_{ij} \leq b_{ij}$ for all i and j, then $A \leq B$. If $A \leq B$ and $A \neq B$, then $A < B$. If $a_{ij} < b_{ij}$ for all i and j, then $A \ll B$.

We list a number of known results on matrices and their spectral radii.

Lemma 1.3 (Berman and Plemmons [6]). *Let $A = (a_{ij})$, $B = (b_{ij})$ be two $n \times n$ matrices with spectral radii $\rho(A)$ and $\rho(B)$, respectively. If $0 \leq A \leq B$, then $\rho(A) \leq \rho(B)$. Furthermore, If $0 \leq A < B$ and B is irreducible, then $\rho(A) < \rho(B)$.*

Here we use 0 to denote the all-zero $n \times n$ matrix.

Lemma 1.4 (Horn and Johnson [56]). *Let $M = (m_{ij})_{n\times n}$ be a nonnegative matrix with spectral radius $\rho(M)$. Then*

$$\min_{1\le i\le n}\sum_{j=1}^{n} m_{ij} \le \rho(M) \le \max_{1\le i\le n}\sum_{j=1}^{n} m_{ij}.$$

If M is irreducible, one of the equality holds if and only if the row sums of M are all equal. And

$$\min_{1\le j\le n}\sum_{i=1}^{n} m_{ij} \le \rho(M) \le \max_{1\le j\le n}\sum_{i=1}^{n} m_{ij}.$$

If M is irreducible, one of the equality holds if and only if the column sums of M are all equal.

Lemma 1.5 (Horn and Johnson [56]). *Let M be an irreducible and nonnegative matrix of order n. Then*
(a) $\rho(M) > 0$.
(b) $\rho(M)$ is an algebraically simple eigenvalue of M.
(c) there is a unique real vector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ such that $M\mathbf{x} = \rho(M)\mathbf{x}$ and $x_1 + x_2 + \cdots + x_n = 1$; this vector is positive.
(d) there is a unique real vector $\mathbf{y} = (y_1, y_2, \ldots, y_n)^T$ such that $\mathbf{y}^T M = \rho(M)\mathbf{y}^T$ and $x_1y_1 + \cdots + x_ny_n = 1$; this vector is positive.

Lemma 1.6 (Horn and Johnson [56]). *If M is a nonnegative matrix and $\mathbf{x} \ge 0$ is a nonnegative vector such that $M\mathbf{x} \ge \beta\mathbf{x}$ for some $\beta \in \mathbb{R}$, then $\rho(M) \ge \beta$. Furthermore, if M is irreducible and $M\mathbf{x} > \beta\mathbf{x}$, then $\rho(M) > \beta$.*

We also need the following definition and result regarding an equitable quotient matrix.

Definition 1.2 (Brouwer and Haemers [13]). Let M be a complex matrix of order n described in the following block form

$$M = \begin{bmatrix} M_{11} & \cdots & M_{1t} \\ \vdots & \ddots & \vdots \\ M_{t1} & \cdots & M_{tt} \end{bmatrix},$$

where the blocks M_{ij} are $n_i \times n_j$ matrices for any $1 \le i, j \le t$ and $n = n_1 + n_2 + \cdots + n_t$. For $1 \le i, j \le t$, let b_{ij} be the average row sum of M_{ij}, i.e. b_{ij} is the sum of all entries in M_{ij} divided by the number of rows. Then $B(M) = (b_{ij})$ (or simply B) is called the quotient matrix of M. If for each pair i, j, the row sum of the matrix M_{ij} is the same for each row, then B is called an equitable quotient matrix of M.

Lemma 1.7 (You, Yang, So and Xi [138]). *Let M be a nonnegative matrix, and let B be the equitable quotient matrix of M as defined in Definition 1.2. If B is irreducible, then $\rho(B) = \rho(M)$.*

The following lemma is adopted from [8] and describes what is known as a topological ordering of an acyclic digraph.

Lemma 1.8 (Bondy and Murty [8]). *Let G be a digraph with no directed cycle. Then $\delta^-(G) = 0$ and there is an ordering $v_1, v_2, \ldots, v_n$ of $\mathcal{V}(G)$ such that, for $1 \le i \le n$, every arc of G with head v_i has its tail in $\{v_1, v_2, \ldots, v_{i-1}\}$.*

We also recall Karamata's inequality for later use. Let I be an interval on the real line and let f denote a real-valued, convex function defined on I. If $x_1 \ge x_2 \ge \cdots \ge x_n$ and $y_1 \ge y_2 \ge \cdots \ge y_n$ are numbers in I such that $(x_1, x_2, \ldots, x_n)$ majorizes $(y_1, y_2, \ldots, y_n)$, then

$$f(x_1) + f(x_2) + \cdots + f(x_n) \ge f(y_1) + f(y_2) + \cdots + f(y_n).$$

Moreover, if f is a strictly convex function, then the inequality holds with equality if and only if $x_i = y_i$ for all $i = 1, 2, \ldots, n$. Here majorization means that $(x_1, x_2, \ldots, x_n)$ and $(y_1, y_2, \ldots, y_n)$ satisfy

$$x_1 + x_2 + \cdots + x_i \ge y_1 + y_2 + \cdots + y_i,$$

for all $i = 1, 2, \ldots, n-1$, and

$$x_1 + x_2 + \cdots + x_n = y_1 + y_2 + \cdots + y_n.$$

We complete this introductory chapter by giving a brief outline of our main contributions to the field.

1.5 Outline of the main results of this thesis

This thesis consists of five main chapters. Apart from this introductory chapter, the other four chapters are based on previously submitted papers. These four chapters mainly consider the spectral moments or the spectral radius of digraphs with a fixed dichromatic number, involving the Laplacian matrix, the A_α matrix, and the eccentricity matrix. The remainder of this thesis is organized as follows.

In Chapter 2, we obtain the digraphs which attain the minimal and maximal Laplacian energy (also known as the second Laplacian spectral moment) among all (join) digraphs in $\mathscr{G}_{n,r}$. The minimal Laplacian energy is attained by bidirected complete graphs and in-trees. The maximal Laplacian energy is attained by the join digraphs $G = \bigvee_{i=1}^{r} V^i$, in which each V^i is a transitive tournament and $|\mathscr{V}(V^i) - \mathscr{V}(V^j)| \leq 1$. These extremal digraphs are the same as the ones with the maximal adjacency spectral radius in [78] (and also with the maximal A_α spectral radius in [89]). In addition, we determine sharp upper and lower bounds for the third Laplacian spectral moment among all join digraphs in $\mathscr{G}_{n,r}$.

In Chapter 3, we obtain the digraphs which attain the minimal and maximal A_α energy (also known as the second A_α spectral moment) among all (join) digraphs in $\mathscr{G}_{n,r}$. We also determine sharp bounds for the third A_α spectral moment among all join digraphs in $\mathscr{G}_{n,r}$. These results generalize the results about the second and third Laplacian spectral moments of digraphs in Chapter 2.

In Chapter 4, by using the equitable quotient matrix, we obtain the digraph which has the maximal A_α spectral radius among all digraphs in $\mathscr{G}_{n,r}$. This provides a new proof for the results of Liu et al. [89]. Also, among all digraphs in $\mathscr{G}_{n,r}$, this extremal digraph for the A_α spectral radius is the same as the extremal digraph for the adjacency spectral radius, the Laplacian energy, and the A_α energy. Moreover, we obtain the digraph which has the minimal A_α spectral radius among the join of in-trees in $\mathscr{G}_{n,r}$.

In Chapter 5, we consider bounds for the spectral radius of join digraphs in $\mathscr{G}_{n,r}$ involving the eccentricity matrix. We obtain lower bounds for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$, and derive upper bounds for the eccentricity spectral radius of some special join digraphs in $\mathscr{G}_{n,r}$. These extremal digraphs for the eccentricity spectral radius are very different from those in the other chapters.

Chapter 2

Bounds for the Laplacian spectral moments of digraphs

In this chapter, we characterize the digraphs which attain the minimal and maximal Laplacian energy within classes of digraphs with a fixed dichromatic number. We determine sharp bounds for the third Laplacian spectral moment within the special subclass which we define as join digraphs. In addition, we leave some open problems.

2.1 Introduction

Recall that the Laplacian matrix $L(G)$ of G is defined by $L(G) = D^+(G) - A(G)$, where $A(G)$ is an adjacency matrix and $D^+(G) = diag(d_1^+, d_2^+, \ldots, d_n^+)$ is a diagonal outdegree matrix of G. Hence, $L(G) = (\ell_{ij})$ is an $n \times n$ matrix, where

$$\ell_{ij} = \begin{cases} d_i^+, & \text{if } i = j, \\ -1, & \text{if } (v_i, v_j) \in \mathscr{A}(G), \\ 0, & \text{otherwise.} \end{cases}$$

As we mentioned in Subsection 1.3.1, the results about the spectral moments of the adjacency matrix or the Laplacian matrix of digraphs are generally lacking. In this chapter, we are mainly concerned with the second and third Laplacian spectral moments of digraphs. Obviously,

$$LSM_0(G) = \sum_{i=1}^{n} \lambda_i^0 = n$$

and

$$LSM_1(G) = \sum_{i=1}^{n} \lambda_i^1 = \sum_{i=1}^{n} d_i^+ = e(G).$$

For $k = 2$, the second Laplacian spectral moment was first studied by Perera and Mizoguchi in [107], where they defined the Laplacian energy of a digraph G as

$$LE(G) = \sum_{i=1}^{n} \lambda_i^2.$$

This is a direct analogue of the definition $LE(H) = \sum_{i=1}^{n} \lambda_i^2$ that Lazić introduced in [66] for the Laplacian energy of an undirected graph H with vertex set $\{v_1, v_2, \ldots, v_n\}$. In [66], he also proved that $LE(H) = \sum_{i=1}^{n} d_i(d_i + 1)$, where d_i is the degree of v_i in H.

As we mentioned in Subsection 1.2.1, there exist many alternative definitions for graph energies of graphs and digraphs, as witnessed by the sources [46, 47, 68]. This shows the popularity of this topic within chemical graph theory. Nevertheless, there are just a few published papers on the Laplacian energy of digraphs. They mainly deal with obtaining the lower and upper bounds for $LE(G)$ and characterizing the extremal digraphs, as it was done in [110] for general digraphs, and for the special graph classes of directed trees, unicyclic digraphs and bicyclic digraphs in [136]. We extend these results to digraphs with a fixed dichromatic number.

Throughout this chapter, we consider only connected digraphs without loops or multiple arcs. Recall that $\mathscr{G}_{n,r}$ is denoted the set of digraphs of order n with dichromatic number r. And for the join digraph $\bigvee_{i=1}^{r} V^i$, we mainly consider each V^i is a connected acyclic digraph with n_i vertices with $\sum_{i=1}^{r} n_i = n$ and $n_1 \geq n_2 \geq \cdots \geq n_r$.

The rest of the chapter is organized as follows. In Section 2.2, we obtain the digraphs which attain the minimal and maximal Laplacian energy $LE(G)$

among all (join) digraphs in $\mathcal{G}_{n,r}$. In Section 2.3, we determine sharp upper and lower bounds for the third Laplacian spectral moment $LSM_3(G)$ among all join digraphs in $\mathcal{G}_{n,r}$. We finish the chapter with some concluding remarks and open problems in Section 2.4.

2.2 Extremal digraphs for the Laplacian energy

In this section, we will characterize the digraphs which attain the minimal and maximal Laplacian energy $LE(G)$ among all join digraphs (Subsection 2.2.1) and all digraphs (Subsection 2.2.2) in $\mathcal{G}_{n,r}$. First, we list some known results and lemmas that we use in our proofs. Recall that for any digraph G of order n we assume that $\mathcal{V}(G) = \{v_1, v_2, \ldots, v_n\}$, that d_i^+ denotes the outdegree of v_i, and that we use c_2 to indicate the total number of directed closed walks of length 2 in G.

Lemma 2.1 (Qi et al. [110])**.** *Let G be a digraph of order n. Then*

$$LE(G) = \sum_{i=1}^{n} (d_i^+)^2 + c_2.$$

Lemma 2.2 (Perera and Mizoguchi [107], Qi et al. [110])**.** *Let G be a digraph of order n. Then*

$$n-1 \leq LE(G) \leq n^2(n-1).$$

Moreover, the first inequality is an equality if and only if G is an in-tree, and the second inequality is an equality if and only if G is a bidirected complete graph.

We use the above two lemmas to prove the following counterpart of Lemma 2.2 for acyclic digraphs. We also need to use the Karamata's inequality introduced in Section 1.4.

Lemma 2.3. *Let G be an acyclic digraph of order n. Then*

$$n-1 \leq LE(G) \leq \frac{n(n-1)(2n-1)}{6}.$$

Moreover, the first inequality is an equality if and only if G is an in-tree, and the second inequality is an equality if and only if G is a transitive tournament.

Proof. The statements about the lower bound follow directly from Lemma 2.2. Lemma 2.1 implies that $LE(G) = \sum_{i=1}^{n}(d_i^+)^2$ for an acyclic digraph G. So we need to find the maximum possible value of $\sum_{i=1}^{n}(d_i^+)^2$ among all acyclic digraphs.

By Lemma 1.8, any acyclic digraph admits a topological ordering, i.e., an ordering of its vertices $\{v_1, v_2, \ldots, v_n\}$ such that for every arc (v_i, v_j), we have $i < j$. Using Karamata's inequality, for the acyclic digraph with order n and size e, $\sum_{i=1}^{n}(d_i^+)^2$ is maximized when the outdegree sequence is $(n-1, n-2, \ldots, n-x, y, 0, \ldots, 0)$, where $1 \leq x \leq n$, $0 \leq y \leq n-x-2$ and $\frac{(n-1+n-x)x}{2} + y = e$. Clearly,

$$\sum_{i=1}^{n}(n-i)^2 \geq \sum_{i=1}^{x}(n-i)^2 + y^2.$$

That is, $\sum_{i=1}^{n}(d_i^+)^2$ is maximized when arcs (v_i, v_j) exist for all $i < j$ and $j \leq n$, so when $d_i^+ = n-i$ for $i = 1, \ldots, n$. Hence, using a well-known expression for the sum of squares, we obtain

$$LE(G) = \sum_{i=1}^{n}(d_i^+)^2 \leq \sum_{i=1}^{n}(n-i)^2 = \frac{n(n-1)(2n-1)}{6}.$$

The above inequality is an equality if and only if $d_i^+ = n-i$ for $i = 1, \ldots, n$. It is an easy exercise and a folklore result that this is only possible if G is a transitive tournament. $\square$

2.2.1 Extremal digraphs for the Laplacian energy among all join digraphs

In our first main results, we will determine the digraphs which attain the minimal and maximal Laplacian energy $LE(G)$ among all join digraphs in $\mathcal{G}_{n,r}$. We need the following inequality in our proofs of the main results in this subsection.

Lemma 2.4. *Let $f(x) = x^2(a-bx)$ for an integer variable x and two fixed real numbers a and b. Suppose x_i and x_j are chosen such that $x_i - x_j \geq 2$ and*

$x_j < \frac{a}{3b} - 1$. *Then*

$$f(x_i - 1) + f(x_j + 1) < f(x_i) + f(x_j).$$

Proof. Since

$$\begin{aligned}
&f(x_i - 1) + f(x_j + 1) \\
&= (x_i - 1)^2[a - b(x_i - 1)] + (x_j + 1)^2[a - b(x_j + 1)] \\
&= x_i^2(a - bx_i) + bx_i^2 + (1 - 2x_i)(a - bx_i + b) \\
&+ x_j^2(a - bx_j) - bx_j^2 + (1 + 2x_j)(a - bx_j - b),
\end{aligned}$$

we have

$$\begin{aligned}
&[f(x_i - 1) + f(x_j + 1)] - [f(x_i) + f(x_j)] \\
&= bx_i^2 + (1 - 2x_i)(a - bx_i + b) - bx_j^2 + (1 + 2x_j)(a - bx_j - b) \\
&= (x_j - x_i)(-3bx_i - 3bx_j + 2a - 3b) - 6bx_i + 2a \\
&\leq -2(-3bx_i - 3bx_j + 2a - 3b) - 6bx_i + 2a \\
&= 6bx_j - 2a + 6b < 6b\left(\frac{a}{3b} - 1\right) - 2a + 6b = 0.
\end{aligned}$$

□

The next result characterizes the digraphs which attain the minimal Laplacian energy $LE(G)$ among all join digraphs $\bigvee_{i=1}^{r} V^i$ in $\mathscr{G}_{n,r}$.

Theorem 2.5. *Let* $G = \bigvee_{i=1}^{r} V^i$. *Then*

$$LE(G) \geq (r - 1)n^2 + r^2 n - r^3,$$

with equality holding if and only if each V^i *is an in-tree,* $n_1 = n - r + 1$*, and* $n_2 = \cdots = n_r = 1$.

Proof. Let $\{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ be the vertex set of V^i, where $i = 1, 2, \ldots, r$. Let $d_G^+(v_j^i)$ be the outdegree of v_j^i in G and $d_{V^i}^+(v_j^i)$ be the outdegree of v_j^i in V^i, where $j = 1, 2, \ldots, n_i$. Obviously, we have $d_G^+(v_j^i) = n - n_i + d_{V^i}^+(v_j^i)$, where $j = 1, 2, \ldots, n_i$ and $i = 1, 2, \ldots, r$. Since V^i is acyclic and connected, we know that $\sum_{j=1}^{n_i} d^+_{V^i}(v^i_j) = e(V^i) \geq n_i - 1$, with equality if and only if V^i is a directed tree. Using Lemma 2.3, we also have $\sum_{j=1}^{n_i} \left(d^+_{V^i}(v^i_j)\right)^2 \geq n_i - 1$, with equality if and only if V^i is an in-tree.

Hence, starting with the expression from Lemma 2.1, we have

$$\begin{aligned}
LE(G) &= \sum_{i=1}^{n} (d^+_i)^2 + c_2 \\
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i} \left(d^+_G(v^i_j)\right)^2 + 2\sum_{i<j} n_i n_j \\
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i} \left(n - n_i + d^+_{V^i}(v^i_j)\right)^2 + \left[\left(\sum_{i=1}^{r} n_i\right)^2 - \sum_{i=1}^{r} n_i^2\right] \\
&= \sum_{i=1}^{r}\left[\sum_{j=1}^{n_i}(n-n_i)^2 + 2(n-n_i)\sum_{j=1}^{n_i} d^+_{V^i}(v^i_j) + \sum_{j=1}^{n_i}\left(d^+_{V^i}(v^i_j)\right)^2\right] \\
&+ \left(n^2 - \sum_{i=1}^{r} n_i^2\right) \geq \left(n^3 + \sum_{i=1}^{r} n_i^3 - 2n\sum_{i=1}^{r} n_i^2\right) \\
&+ \sum_{i=1}^{r}\left[2(n-n_i)(n_i-1) + (n_i-1)\right] + \left(n^2 - \sum_{i=1}^{r} n_i^2\right) \\
&= \left(n^3 + 3n^2 - (2r-3)n - r\right) + \sum_{i=1}^{r} n_i^2(n_i - 2n - 3).
\end{aligned}$$

Next, we are going to use Lemma 2.4 to determine the minimum value of the above sum $\sum_{i=1}^{r} n_i^2(n_i - 2n - 3)$. Since $n_i - 2n - 3 < 0$, this is equivalent to determining the maximum value of $\sum_{i=1}^{r} n_i^2(2n + 3 - n_i)$.

Let $f(x) = x^2(2n+3-x)$ and $F(x_1, x_2, \ldots, x_r) = \sum_{i=1}^{r} f(x_i)$, where $\sum_{i=1}^{r} x_i = n$ and $1 \leq x_i \leq n - r + 1$. Suppose that $x_i - x_j \geq 2$ for some x_i and x_j. Then, since $x_i + x_j \leq n - (r-2)$, we have $x_j \leq \frac{n-r}{2}$. Now, let $a = 2n+3$ and $b = 1$. Since $x_j \leq \frac{n-r}{2} < \frac{a}{3b} - 1$, using Lemma 2.4, we get $f(x_i - 1) + f(x_j + 1) < f(x_i) + f(x_j)$. Then we have $F(x_1, \ldots, x_i - 1, \ldots, x_j + 1, \ldots, x_r) < F(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_r)$. This implies that $\sum_{i=1}^{r} x_i^2(2n+3-x_i)$ is maximal when $x_1 = n - r + 1$ and $x_2 = \cdots = x_r = 1$. If there are no x_i, x_j

such that $x_i - x_j \geq 2$, then $|x_i - x_j| \leq 1$ for each $1 \leq i, j \leq r$. For any $x_i \geq x_j$, let $x_i' = x_i + 1$ and $x_j' = x_j - 1$. Then $x_i' - x_j' = x_i + 1 - x_j + 1 \geq 2$ and

$$f(x_i) + f(x_j) = f(x_i' - 1) + f(x_j' + 1) < f(x_i') + f(x_j').$$

Concluding, we obtain

$$\begin{aligned}
LE(G) &\geq \left(n^3 + 3n^2 - (2r-3)n - r\right) + \sum_{i=1}^{r} n_i^2(n_i - 2n - 3) \\
&\geq \left(n^3 + 3n^2 - (2r-3)n - r\right) \\
&\quad + (n-r+1)^2(n-r+1-2n-3) + (r-1)(1-2n-3) \\
&= (r-1)n^2 + r^2 n - r^3,
\end{aligned}$$

with equality holding here and above if and only if each V^i is an in-tree, $n_1 = n - r + 1$, and $n_2 = \cdots = n_r = 1$. $\square$

The next result characterizes the digraphs which attain the maximal Laplacian energy $LE(G)$ among all join digraphs $\bigvee_{i=1}^{r} V^i$ in $\mathscr{G}_{n,r}$. We will distinguish the cases that r is a divisor of n, denoted by $r \mid n$, and that r does not divide n, denoted by $r \nmid n$.

Theorem 2.6. *Let $G = \bigvee_{i=1}^{r} V^i$. Then the following inequalities hold:*
(i) If $r \mid n$, we have

$$LE(G) \leq \left(1 + \frac{1}{3r^2} - \frac{1}{r}\right) n^3 - \frac{1}{2r} n^2 + \frac{1}{6} n,$$

with equality holding if and only if each V^i is a transitive tournament with $n_i = \frac{n}{r}$.
(ii) If $r \nmid n$, we have

$$LE(G) \leq n^3 + \frac{1}{6} n + p - q,$$

where $p = \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right)\left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right)$ and $q = \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)\left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right)$. The inequality is an equality if and only if each V^i is a transitive tournament, with $n_s = \left\lceil \frac{n}{r} \right\rceil$ for $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ and $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ for $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$.

Proof. Similarly as in the proof of Theorem 2.5, using Lemma 2.3, we have $\sum_{j=1}^{n_i} d_{V^i}^+(v_j^i) = e(V^i) \leq \frac{n_i(n_i-1)}{2}$ and $\sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^2 \leq \frac{n_i(n_i-1)(2n_i-1)}{6}$, with equality in the latter inequality if and only if V^i is a transitive tournament.

Hence, using Lemma 2.1, we have

$$
\begin{aligned}
LE(G) &= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^2 + 2\sum_{i<j} n_i n_j \\
&= \sum_{i=1}^{r}\left[\sum_{j=1}^{n_i}(n-n_i)^2 + 2(n-n_i)\sum_{j=1}^{n_i} d_{V^i}^+(v_j^i) + \sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^2\right] \\
&+ \left(n^2 - \sum_{i=1}^{r} n_i^2\right) \leq \left(n^3 + \sum_{i=1}^{r} n_i^3 - 2n\sum_{i=1}^{r} n_i^2\right) \\
&+ \sum_{i=1}^{r}\left[2(n-n_i)\frac{n_i(n_i-1)}{2} + \frac{n_i(n_i-1)(2n_i-1)}{6}\right] + \left(n^2 - \sum_{i=1}^{r} n_i^2\right) \\
&= \left(n^3 + \frac{1}{6}n\right) + \sum_{i=1}^{r} n_i^2\left(\frac{1}{3}n_i - n - \frac{1}{2}\right).
\end{aligned}
$$

Next, we are going to use Lemma 2.4 to determine the maximum value of the above sum $\sum_{i=1}^{r} n_i^2\left(\frac{1}{3}n_i - n - \frac{1}{2}\right)$. Since $\frac{1}{3}n_i - n - \frac{1}{2} < 0$, this is equivalent to determining the minimum value of $\sum_{i=1}^{r} n_i^2\left(n + \frac{1}{2} - \frac{1}{3}n_i\right)$.

Let $f(x) = x^2\left(n + \frac{1}{2} - \frac{1}{3}x\right)$ and $F(x_1, x_2, \ldots, x_r) = \sum_{i=1}^{r} f(x_i)$, where $\sum_{i=1}^{r} x_i = n$ and $1 \leq x_i \leq n - r + 1$. Let $a = n + \frac{1}{2}$ and $b = \frac{1}{3}$. Since $x_j < \frac{a}{3b} - 1$, using Lemma 2.4, we get $f(x_i - 1) + f(x_j + 1) < f(x_i) + f(x_j)$ for any x_i, x_j with $x_i - x_j \geq 2$. Then we have $F(x_1, \ldots, x_i - 1, \ldots, x_j + 1, \ldots, x_r) < F(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_r)$. That is, when $|x_i - x_j| \leq 1$, $\sum_{i=1}^{r} x_i^2\left(n + \frac{1}{2} - \frac{1}{3}x_i\right)$ is minimal.

(i) If $r \mid n$, then $|n_i - n_j| \leq 1$ implies $n_i = \frac{n}{r}$ for all $i = 1, 2, \ldots, r$. Therefore, we obtain

$$
\begin{aligned}
LE(G) &\leq \left(n^3 + \frac{1}{6}n\right) + \sum_{i=1}^{r} n_i^2\left(\frac{1}{3}n_i - n - \frac{1}{2}\right) \\
&\leq \left(n^3 + \frac{1}{6}n\right) + r\left(\frac{n}{r}\right)^2\left(\frac{n}{3r} - n - \frac{1}{2}\right)
\end{aligned}
$$

$$= \left(1 + \frac{1}{3r^2} - \frac{1}{r}\right) n^3 - \frac{1}{2r} n^2 + \frac{1}{6} n,$$

with equality if and only if each V^i is a transitive tournament of order $n_i = \frac{n}{r}$.
(ii) If $r \nmid n$, then $|n_i - n_j| \le 1$ implies $n_s = \left\lceil \frac{n}{r} \right\rceil$ for $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ and $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ for $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$. Therefore, we obtain

$$\begin{aligned}
LE(G) &\le \left(n^3 + \frac{1}{6}n\right) + \sum_{i=1}^{r} n_i^2 \left(\frac{1}{3} n_i - n - \frac{1}{2}\right) \\
&\le \left(n^3 + \frac{1}{6}n\right) + \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right) \left\lceil \frac{n}{r} \right\rceil^2 \left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right) \\
&+ \left(r - n + r\left\lfloor \frac{n}{r} \right\rfloor\right) \left\lfloor \frac{n}{r} \right\rfloor^2 \left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right) \\
&= \left(n^3 + \frac{1}{6}n\right) + \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right) \left\lceil \frac{n}{r} \right\rceil^2 \left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right) \\
&- \left(n - r\left\lceil \frac{n}{r} \right\rceil\right) \left\lfloor \frac{n}{r} \right\rfloor^2 \left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right) \\
&= n^3 + \frac{1}{6}n + p - q,
\end{aligned}$$

where $p = \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right)\left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right)$ and $q = \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)$ $\left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right)$. Obviously, the inequality is an equality if and only if each V^i is a transitive tournament, with $n_s = \left\lceil \frac{n}{r} \right\rceil$ for $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ and $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ for $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$.

This completes the proof of Theorem 2.6. □

Let $G[n_1, n_2, \ldots, n_r]$ denote the join $\bigvee_{i=1}^{r} V^i$ in which each V^i is either an in-tree or a transitive tournament, respectively. Then by Lemma 2.4 and from the proof of Theorem 2.5 (or Theorem 2.6, respectively), we can find a size relationship with respect to the Laplacian energies of the digraphs $G[n_1, n_2, \ldots, n_r] \in \mathscr{G}_{n,r}$ for different choices of the n_i. We give the following example with $n = 10$ and $r = 4$ to illustrate this, as shown in Figure 2.1. Every arrow points to a digraph with a higher Laplacian energy.

$$\begin{tikzcd}
 & & G[7,1,1,1] \arrow[d] & & \\
 & & G[6,2,1,1] \arrow[dl] \arrow[dr] & & \\
 & G[5,3,1,1] \arrow[rr] \arrow[dl] \arrow[dr] & & G[5,2,2,1] \arrow[dl] \arrow[dr] & \\
G[4,4,1,1] \arrow[rr] & & G[4,3,2,1] \arrow[rr] \arrow[dl] \arrow[dr] & & G[4,2,2,2] \arrow[dl] \\
 & G[3,3,3,1] \arrow[rr] & & G[3,3,2,2] &
\end{tikzcd}$$

Figure 2.1: The size relationship of the Laplacian energies of $G[n_1, n_2, n_3, n_4] \in \mathscr{G}_{10,4}$.

2.2.2 Extremal digraphs for the Laplacian energy among all digraphs

In our second main results, we will determine the digraphs which attain the minimal and maximal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$.

Recall that G is an r-critical digraph if every vertex $v \in \mathscr{V}(G)$ satisfies $\chi(G-v) < \chi(G) = r$. In order to characterize the digraphs which attain the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$, we need Lemmas 1.1 and 1.2 involving r-critical digraphs in Mohar [96]. Note that every digraph with dichromatic number at least r contains an induced subdigraph that is r-critical. In addition, we also need the following lemma.

Lemma 2.7. *Let G be a digraph in $\mathscr{G}_{n,r}$, and let G' be an r-critical subdigraph of G. If G attains the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$, then $d_G^+(v) = 1$ for any $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$ and $d_G^+(u) = d_{G'}^+(u)$ for any $u \in \mathscr{V}(G')$.*

Proof. Suppose that G attains the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$. First, we prove $d_G^+(v) = 1$ for any $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$. We start with the following claim.

Claim 2.1. $d_G^+(v) \neq 0$ for any $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$.

Suppose there exists a vertex $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$ such that $d_G^+(v) = 0$. Then $d_G^-(v) \geq 1$, since G is connected. Let $(w, v) \in \mathscr{A}(G)$ for $w \in \mathscr{V}(G)$. Let G^1 be obtained from G by reversing the direction on the arc (w, v), denoted as

$$G^1 = G - (w, v) + (v, w).$$

Then

$$LE(G^1) = LE(G) - \left(d_G^+(w)\right)^2 + \left(d_G^+(w) - 1\right)^2 + 1 = LE(G) - 2(d_G^+(w) - 1).$$

We discuss the possible choices for w, and derive contradictions in all of the three cases.

Case 1. $w \in \mathscr{V}(G')$. Since G' is r-critical, $d_{G'}^+(w) \geq 1$. So we have $d_G^+(w) > 1$. Then $LE(G^1) < LE(G)$, a contradiction to $LE(G)$ being minimal.

Case 2. $w \in \mathscr{V}(G) \setminus \mathscr{V}(G')$ and $d_G^+(w) > 1$. Obviously $LE(G^1) < LE(G)$, a contradiction.

Case 3. $w \in \mathscr{V}(G) \setminus \mathscr{V}(G')$ and $d_G^+(w) = 1$. Then $LE(G^1) = LE(G)$ and we know $d_{G^1}^+(w) = 0$. So, for G^1 there also exists a vertex $v \in \mathscr{V}(G^1) \setminus \mathscr{V}(G')$ such that $d_{G^1}^+(v) = 0$. We use the following procedure:

$H^0 := G$;
$i := 0$;
while $\exists\, v \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ s.t. $d_{H^i}^+(v) = 0$ **do begin**
  select a vertex $w \in \mathscr{V}(H^i)$ with $(w, v) \in \mathscr{A}(H^i)$;
  $H^{i+1} := H^i - (w, v) + (v, w)$;
  $i := i + 1$;
end.

The resulting digraph H we obtain at the termination of this procedure has no vertex $v \in \mathscr{V}(H) \setminus \mathscr{V}(G')$ such that $d_H^+(v) = 0$. By the procedure, for the vertex $w \in \mathscr{V}(H^i)$ with $(w, v) \in \mathscr{A}(H^i)$, we consider three cases:

(a) $w \in \mathscr{V}(G')$;
(b) $w \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ with $d_{H^i}^+(w) > 1$;
(c) $w \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ with $d_{H^i}^+(w) = 1$.

There is at least one H^i such that $w \in \mathscr{V}(G')$, or $w \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ with $d^+_{H^i}(w) > 1$. Otherwise, for every H^i, $w \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ with $d^+_{H^i}(w) = 1$. But this is impossible since $H^{i+1} = H^i - (w,v) + (v,w)$ and G is connected. Now, as in Case 1 and Case 2 above, if there exists H^i such that $w \in \mathscr{V}(G')$, or $w \in \mathscr{V}(H^i) \setminus \mathscr{V}(G')$ with $d^+_{H^i}(w) > 1$, then $LE(H^{i+1}) < LE(H^i) \leq LE(G)$. Hence, as above we conclude that $LE(H) < LE(G)$, a contradiction. This completes the proof of Claim 2.1.

We also need the following claim.

Claim 2.2. Every component of $G - \mathscr{V}(G')$ is an in-tree, the root of which is an inneighbor of exactly one vertex of G'.

Let T be a component of $G - \mathscr{V}(G')$. Then Lemma 2.2 implies that T is an in-tree. Let $v_0 \in \mathscr{V}(T)$ be the root of T. From Claim 2.1, we have $d^+_G(v_0) \neq 0$. Since G is connected, by the minimality of $LE(G)$, $d^+_G(v_0) = 1$. That is, the root of the in-tree T is the inneighbor of exactly one vertex of G'. This completes the proof of Claim 2.2.

From Claims 2.1 and 2.2, we get that $d^+_G(v) = 1$ for any $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$. Next we will prove that $d^+_G(u) = d^+_{G'}(u)$ for any $u \in \mathscr{V}(G')$.

Suppose there exists a vertex $u \in \mathscr{V}(G')$ such that $d^+_G(u) > d^+_{G'}(u)$. Then there exists an arc $(u,v) \in \mathscr{A}(G)$ for $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$. Let

$$G^2 = G - (u,v).$$

Claim 2.2 implies that G^2 is connected. Clearly, $LE(G^2) < LE(G)$, a contradiction. Hence, we conclude that $d^+_G(u) = d^+_{G'}(u)$ for any $u \in \mathscr{V}(G')$. $\square$

Now, we are ready to present and prove the main result of this section. It characterizes the digraphs which attain the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$.

Theorem 2.8. *Let G be a digraph in $\mathscr{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r = 2$, we have

$$LE(G) \geq \begin{cases} 4, & \text{if } n = 2, \\ n, & \text{if } n \geq 3. \end{cases}$$

If $n = 2$, the inequality is an equality if and only if G is a directed cycle C_2. If $n \geq 3$, the inequality is an equality if and only if G contains a directed cycle $C_{n'}$ ($n' \geq 3$) and every component (if any) of $G - \mathcal{V}(C_{n'})$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $C_{n'}$.
(ii) If $r \geq 3$, we have

$$LE(G) \geq n + r^3 - r^2 - r,$$

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component (if any) of $G - \mathcal{V}(\overleftrightarrow{K}_r)$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $\overleftrightarrow{K}_r$.

Proof. Let G be a digraph in $\mathcal{G}_{n,r}$. Then G must contain an induced subdigraph G' of order n' that is r-critical. From Lemma 2.7, we obtain that if G attains the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathcal{G}_{n,r}$, then $d_G^+(v) = 1$ for any $v \in \mathcal{V}(G) \setminus \mathcal{V}(G')$ and $d_G^+(u) = d_{G'}^+(u)$ for any $u \in \mathcal{V}(G')$. That is, G contains an r-critical digraph G' and every component of $G - \mathcal{V}(G')$ is an in-tree, the root of which is an inneighbor of exactly one vertex of G'. So, we have

$$LE(G) \geq LE(G') + n - n' = \sum_{u \in \mathcal{V}(G')} \left(d_{G'}^+(u)\right)^2 + c_2(G') + n - n'.$$

We next characterize the r-critical digraphs which attain the minimal Laplacian energy.

By definition, every vertex of G' is critical. Hence, using Lemma 1.1, we know that each vertex $u \in \mathcal{V}(G')$ satisfies $d_{G'}^+(u) \geq r - 1$ and $d_{G'}^-(u) \geq r - 1$. Applying the characterizations of Lemma 1.2, the following cases need to be considered.

Case 1. $r = 2$.

If $r = 2$ and $n = 2$, then $G = G' = C_2$. So, $LE(G) = 4$.

If $r = 2$ and $n \geq 3$, then

$$\begin{aligned} LE(G) &\geq \sum_{u \in \mathcal{V}(G')} \left(d_{G'}^+(u)\right)^2 + c_2(G') + n - n' \\ &\geq n'(r-1) + 0 + n - n' = n, \end{aligned}$$

with equality holding if and only if $G' = C_{n'}$ ($n' \geq 3$) and every component (if any) of $G - \mathscr{V}(C_{n'})$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $C_{n'}$.

So, (i) follows.

Case 2. $r \geq 3$. We distinguish three subcases.

Case 2.1. If $n' = r$, then $d^+_{G'}(u) = r - 1$ for any $u \in \mathscr{V}(G')$. That is, $G' = \overleftrightarrow{K}_r$. In that case,

$$\begin{aligned} LE(G) &\geq LE(\overleftrightarrow{K}_r) + n - n' \\ &= r(r-1)^2 + r(r-1) + n - r \\ &= n + r^3 - r^2 - r, \end{aligned}$$

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component of $G - \mathscr{V}(\overleftrightarrow{K}_r)$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $\overleftrightarrow{K}_r$.

Case 2.2. If $n' = r + 1$, since $d^+_{G'}(u) \geq r - 1$ for any $u \in \mathscr{V}(G')$, we have

$$e(G') \geq (r+1)(r-1) \text{ and } \frac{c_2(G')}{2} \geq e(G') - \frac{(r+1)r}{2}.$$

So,

$$\begin{aligned} LE(G) &\geq \sum_{u \in \mathscr{V}(G')} \left(d^+_{G'}(u)\right)^2 + c_2(G') + n - n' \\ &\geq (r+1)(r-1)^2 + 2(r+1)(r-1) - (r+1)r + n - (r+1) \\ &= n + r^3 - 3r - 2. \end{aligned}$$

Case 2.3. If $n' \geq r + 2$ and $r \geq 4$, then

$$\begin{aligned} LE(G) &\geq \sum_{u \in \mathscr{V}(G')} \left(d^+_{G'}(u)\right)^2 + c_2(G') + n - n' \\ &\geq n'(r-1)^2 + 0 + n - n' \\ &\geq n + r^3 - 4r. \end{aligned}$$

If $n' \geq r+2$ and $r=3$, by Lemma 1.2, then

$$\begin{aligned} LE(G) &\geq \sum_{u\in\mathscr{V}(G')} \left(d^+_{G'}(u)\right)^2 + c_2(G') + n - n' \\ &\geq 4n' + 2n' + n - n' \\ &\geq n + 25. \end{aligned}$$

Since

$$(n+r^3-3r-2)-(n+r^3-r^2-r) = r^2-2r-2 > 0 \ (r \geq 3),$$

$$(n+r^3-4r)-(n+r^3-r^2-r) = r^2-3r > 0 \ (r \geq 4)$$

and

$$n+25 > n+15,$$

we obtain

$$LE(G) \geq n + r^3 - r^2 - r,$$

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component of $G - \mathscr{V}(\overleftrightarrow{K}_r)$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $\overleftrightarrow{K}_r$. So, (ii) follows.

This completes the proof of Theorem 2.8. □

As an illustration of the above theorem, Figure 2.2 shows all digraphs in $\mathscr{G}_{6,3}$ attaining the minimal Laplacian energy.

The next result characterizes the digraphs which attain the maximal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$. It is an easy consequence of Theorem 2.6, which we state without proof.

Theorem 2.9. *Let G be a digraph in $\mathscr{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r \mid n$, we have

$$LE(G) \leq \left(1 + \frac{1}{3r^2} - \frac{1}{r}\right) n^3 - \frac{1}{2r} n^2 + \frac{1}{6} n,$$

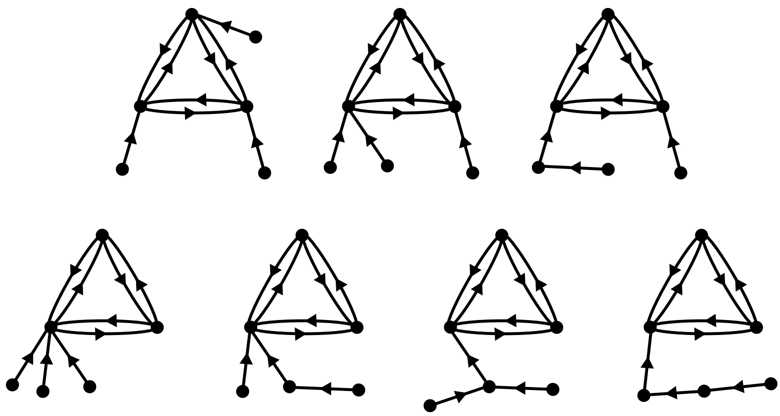


Figure 2.2: The digraphs in $\mathcal{G}_{6,3}$ with the minimal Laplacian energy.

with equality holding if and only if $G = \bigvee_{i=1}^{r} V^i$ *and each* V^i *is a transitive tournament with* $n_i = \frac{n}{r}$.
(ii) If $r \nmid n$, *we have*

$$LE(G) \leq n^3 + \frac{1}{6}n + p - q,$$

where $p = \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right)\left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right)$ *and* $q = \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)$ $\left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right)$. *The inequality is an equality if and only if* $G = \bigvee_{i=1}^{r} V^i$ *and each* V^i *is a transitive tournament, with* $n_s = \left\lceil \frac{n}{r} \right\rceil$ *for* $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ *and* $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ *for* $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$.

2.3 Bounds for the third Laplacian spectral moment

In this section, we will determine sharp bounds for the third Laplacian spectral moment $LSM_3(G)$ of join digraphs in $\mathcal{G}_{n,r}$. First, we present a general formula for $LSM_3(G)$ of a digraph G. Recall that we assume G has vertex set $\{v_1, v_2, \ldots, v_n\}$, with outdegrees $d_1^+, d_2^+, \ldots, d_n^+$, and that $\left(c_2^{(1)}, c_2^{(2)}, \ldots, c_2^{(n)}\right)$ denotes the directed closed walk sequence of length 2. We let c_3 denote the total number of directed closed walks of length 3 in G.

Lemma 2.10. *Let G be a digraph of order n. Then*

$$LSM_3(G) = \sum_{i=1}^{n}(d_i^+)^3 + 3\sum_{i=1}^{n} d_i^+ c_2^{(i)} - c_3.$$

Proof. Since the Laplacian matrix is an $n \times n$ matrix $L(G) = (\ell_{ij})$, where

$$\ell_{ij} = \begin{cases} d_i^+, & \text{if } i = j, \\ -1, & \text{if } (v_i, v_j) \in \mathscr{A}(G), \\ 0, & \text{otherwise,} \end{cases}$$

we have

$$LSM_3(G) = \sum_{i=1}^{n} \lambda_i^3 = tr\left((L(G))^3\right) = \sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \ell_{j_1 j_2}\ell_{j_2 j_3}\ell_{j_3 j_1}.$$

For the different (possible) choices of j_1, j_2, j_3, we presented the respective values in Table 2.1.

So, we get $LSM_3(G) = \sum_{i=1}^{n}(d_i^+)^3 + 3\sum_{i=1}^{n} d_i^+ c_2^{(i)} - c_3$. □

Table 2.1: The values of $\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \ell_{j_1 j_2}\ell_{j_2 j_3}\ell_{j_3 j_1}$ for different choices of j_1, j_2, j_3.

j_1, j_2, j_3			$\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \ell_{j_1 j_2}\ell_{j_2 j_3}\ell_{j_3 j_1}$
$j_1 = j_2$	$j_2 = j_3$	$j_3 = j_1$	$\sum_{i=1}^{n}(d_i^+)^3$
		$j_3 \neq j_1$	non-existent
	$j_2 \neq j_3$	$j_3 = j_1$	non-existent
		$j_3 \neq j_1$	$\sum_{i=1}^{n} d_i^+ c_2^{(i)}$
$j_1 \neq j_2$	$j_2 = j_3$	$j_3 = j_1$	non-existent
		$j_3 \neq j_1$	$\sum_{i=1}^{n} d_i^+ c_2^{(i)}$
	$j_2 \neq j_3$	$j_3 = j_1$	$\sum_{i=1}^{n} d_i^+ c_2^{(i)}$
		$j_3 \neq j_1$	$-c_3$

We will use the above lemma to obtain an expression for $LSM_3(G)$ in case $G = \bigvee_{i=1}^{r} V^i$. We adopt the notation of the previous section.

Lemma 2.11. *Let $G = \bigvee_{i=1}^{r} V^i$. Then*

$$LSM_3(G) = \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 + 3\sum_{i=1}^{r} n_i(n-n_i)^2 - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i).$$

Proof. From Lemma 2.10, we obtain

$$LSM_3(G) = \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 + 3\sum_{i=1}^{r}\sum_{j=1}^{n_i} d_G^+(v_j^i)c_2(v_j^i) - c_3.$$

We also recall that $d_G^+(v_j^i) = n - n_i + d_{V^i}^+(v_j^i)$ and $c_2(v_j^i) = n - n_i$, for $j = 1, 2, \dots, n_i$ and $i = 1, 2, \dots, r$. So, we next consider c_3.

Let $c_3(v_j^i)$ be the number of directed closed walks of length 3 associated with v_j^i. Then $c_3 = \sum_{i=1}^{r}\sum_{j=1}^{n_i} c_3(v_j^i)$ is the total number of directed closed walks of length 3 in G. Actually, any directed closed walk of length 3 associated with v_j^i is a triangle that starts and ends in v_j^i. For any $v_j^i \in \mathscr{V}(V^i)$, we denote the associated triangles by $v_j^i \to u \to w \to v_j^i$ and discuss the possible choices for u and w, and their contribution to the total number of triangles.

Case 1. $u \in \mathscr{V}(V^i)$. The total contribution is clearly $d_{V^i}^+(v_j^i)(n-n_i)$.

Case 2. $u \notin \mathscr{V}(V^i)$. Let $u \in \mathscr{V}(V^s)$ for $s \neq i$. Next, we consider w.

Case 2.1. $w \in \mathscr{V}(V^s)$. Then the total contribution is $\sum_{t=1}^{n_s} d_{V^s}^+(v_t^s)$.

Case 2.2. $w \notin \mathscr{V}(V^s)$. Then the total contribution is $n_s\left[(n-n_s-n_i)+d_{V^i}^-(v_j^i)\right]$.

Hence, in Case 2, we get a total contribution of

$$\sum_{s\neq i}\left[\sum_{t=1}^{n_s} d_{V^s}^+(v_t^s) + n_s\left[(n-n_s-n_i)+d_{V^i}^-(v_j^i)\right]\right].$$

Summing up, we get

$$c_3 = \sum_{i=1}^{r}\sum_{j=1}^{n_i} c_3(v_j^i)$$

$$= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[d^+_{V^i}(v^i_j)(n-n_i) + \sum_{s\neq i}\left[\sum_{t=1}^{n_s} d^+_{V^s}(v^s_t) + n_s\left[(n-n_s-n_i)+d^-_{V^i}(v^i_j)\right]\right]\right].$$

Thus, $LSM_3(G)$

$$\begin{aligned}
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d^+_G(v^i_j)\right)^3 + 3\sum_{i=1}^{r}\sum_{j=1}^{n_i} d^+_G(v^i_j)c_2(v^i_j) - c_3\\
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d^+_G(v^i_j)\right)^3 + 3\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(n-n_i+d^+_{V^i}(v^i_j)\right)(n-n_i)\\
&- \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[d^+_{V^i}(v^i_j)(n-n_i) + \sum_{s\neq i}\left[\sum_{t=1}^{n_s} d^+_{V^s}(v^s_t) + n_s\left[(n-n_s-n_i)+d^-_{V^i}(v^i_j)\right]\right]\right]\\
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d^+_G(v^i_j)\right)^3 + 3\sum_{i=1}^{r}\left[n_i(n-n_i)^2 + (n-n_i)e(V^i)\right] - \sum_{i=1}^{r}(n-n_i)e(V^i)\\
&- \sum_{i=1}^{r}\left[n_i\sum_{s\neq i}e(V^s) + n_i\sum_{s\neq i}n_s(n-n_s-n_i) + e(V^i)\sum_{s\neq i}n_s\right]\\
&= \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d^+_G(v^i_j)\right)^3 + 3\sum_{i=1}^{r}n_i(n-n_i)^2 - \sum_{i=1}^{r}n_i\sum_{s\neq i}n_s(n-n_s-n_i)\\
&+ \sum_{i=1}^{r}e(V^i)\left[2(n-n_i) - \sum_{s\neq i}n_s\right] - \sum_{i=1}^{r}n_i\sum_{s\neq i}e(V^s).
\end{aligned}$$

Since

$$\begin{aligned}
&\sum_{i=1}^{r}e(V^i)\left[2(n-n_i) - \sum_{s\neq i}n_s\right] - \sum_{i=1}^{r}n_i\sum_{s\neq i}e(V^s)\\
&= \sum_{i=1}^{r}e(V^i)(n-n_i) - \sum_{i=1}^{r}n_i\sum_{s\neq i}e(V^s)\\
&= n\sum_{i=1}^{r}e(V^i) - \sum_{i=1}^{r}n_i\left[e(V^i) + \sum_{s\neq i}e(V^s)\right]\\
&= n\sum_{i=1}^{r}e(V^i) - \sum_{i=1}^{r}n_i\left(\sum_{i=1}^{r}e(V^i)\right)\\
&= 0,
\end{aligned}$$

we obtain

$$LSM_3(G) = \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 + 3\sum_{i=1}^{r} n_i(n-n_i)^2 - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i).$$

This completes the proof of the lemma. □

Next, using the above expression we will determine sharp bounds for $LSM_3(G)$ of join digraphs in $\mathcal{G}_{n,r}$.

Theorem 2.12. *Let $G = \bigvee_{i=1}^{r} V^i$. Then*

(i)

$$\begin{aligned} LSM_3(G) \geq & \sum_{i=1}^{r}\left[-n_i^4 + (3n+6)n_i^3 - (3n^2+12n+6)n_i^2\right] \\ & + n(n^3+6n^2+9n+4) - r(3n^2+3n+1) \\ & - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i), \end{aligned}$$

with equality holding if and only if each V^i is an in-tree.

(ii)

$$\begin{aligned} LSM_3(G) \leq & \sum_{i=1}^{r}\left[-\frac{1}{4}n_i^4 + \left(n+\frac{5}{2}\right)n_i^3 - \left(\frac{3n^2}{2}+\frac{9n}{2}+\frac{1}{4}\right)n_i^2\right] \\ & + n^2\left(n^2+\frac{3n}{2}+\frac{1}{2}\right) - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i), \end{aligned}$$

with equality holding if and only if each V^i is a transitive tournament.

Proof. We start with the expression from Lemma 2.11.

$$LSM_3(G) = \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 + 3\sum_{i=1}^{r} n_i(n-n_i)^2 - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i).$$

Since $d_G^+(v_j^i) = n - n_i + d_{V^i}^+(v_j^i)$, for the first summation on the right-hand side, we obtain the following equality.

$$\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 = \sum_{i=1}^{r} n_i(n-n_i)^3$$
$$+\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[\left(d_{V^i}^+(v_j^i)\right)^3 + 3(n-n_i)\left(d_{V^i}^+(v_j^i)\right)^2 + 3(n-n_i)^2 d_{V^i}^+(v_j^i)\right].$$

Using Lemma 2.3, its proof, and similar calculations, we obtain the following lower and upper bounds which we will use to simplify some of the terms on the right-hand side of the above expression.

$$n_i - 1 \leq \sum_{j=1}^{n_i} d_{V^i}^+(v_j^i) \leq \frac{n_i(n_i-1)}{2},$$

$$n_i - 1 \leq \sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^2 \leq \frac{n_i(n_i-1)(2n_i-1)}{6},$$

$$n_i - 1 \leq \sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^3 \leq \frac{n_i^2(n_i-1)^2}{4}.$$

In all of the above three inequalities, the lower bounds are only attained if V^i is an in-tree, and the upper bounds are only attained if V^i is a transitive tournament.

Combining the above terms, for the lower bound on $LSM_3(G)$ we obtain

$$LSM_3(G) = \sum_{i=1}^{r} n_i(n-n_i)^3$$
$$+\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[\left(d_{V^i}^+(v_j^i)\right)^3 + 3(n-n_i)\left(d_{V^i}^+(v_j^i)\right)^2 + 3(n-n_i)^2 d_{V^i}^+(v_j^i)\right]$$
$$+3\sum_{i=1}^{r} n_i(n-n_i)^2 - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i)$$
$$\geq \sum_{i=1}^{r}\left[n_i(n-n_i)^3 + (n_i-1) + 3(n-n_i)(n_i-1) + 3(n-n_i)^2(n_i-1)\right]$$

$$+3\sum_{i=1}^{r} n_i(n-n_i)^2 - \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i)$$
$$=\sum_{i=1}^{r}\left[-n_i^4+(3n+6)n_i^3-(3n^2+12n+6)n_i^2+(n^3+6n^2+9n+4)n_i\right]$$
$$-r(3n^2+3n+1)-\sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i),$$

with equality holding if and only if each V^i is an in-tree with n_i vertices.

For the upper bound we obtain

$$LSM_3(G)=\sum_{i=1}^{r} n_i(n-n_i)^3$$
$$+\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[\left(d_{V^i}^+(v_j^i)\right)^3+3(n-n_i)\left(d_{V^i}^+(v_j^i)\right)^2+3(n-n_i)^2 d_{V^i}^+(v_j^i)\right]$$
$$+3\sum_{i=1}^{r} n_i(n-n_i)^2-\sum_{i=1}^{r} n_i\sum_{s\neq i} n_s(n-n_s-n_i)$$
$$\leq \sum_{i=1}^{r}\left[n_i(n-n_i)^3+\frac{n_i^2(n_i-1)^2}{4}+3(n-n_i)\frac{n_i(n_i-1)(2n_i-1)}{6}\right.$$
$$\left.+3(n-n_i)^2\frac{n_i(n_i-1)}{2}\right]+3\sum_{i=1}^{r} n_i(n-n_i)^2-\sum_{i=1}^{r} n_i\sum_{s\neq i} n_s(n-n_s-n_i)$$
$$=\sum_{i=1}^{r}\left[-\frac{1}{4}n_i^4+\left(n+\frac{5}{2}\right)n_i^3-\left(\frac{3n^2}{2}+\frac{9n}{2}+\frac{1}{4}\right)n_i^2+\left(n^3+\frac{3n^2}{2}+\frac{n}{2}\right)n_i\right]$$
$$-\sum_{i=1}^{r} n_i\sum_{s\neq i} n_s(n-n_s-n_i),$$

with equality holding if and only if each V^i is a transitive tournament with n_i vertices. □

Unfortunately, we are not able to characterize the extremal digraphs for $LSM_3(G)$ precisely, as counterparts of Theorem 2.5 and Theorem 2.6, except for the case when $r=2$. Based on the expressions in Theorem 2.12, we next determine the digraphs which attain the minimal and maximal value of $LSM_3(G)$ among the join digraphs in $\mathscr{G}_{n,2}$.

Corollary 2.13. *Let $G = V^1 \vee V^2$. Then*

(i) $LSM_3(G) \geq n^3 + 8n - 16$,
with equality holding if and only if V^1 and V^2 are in-trees with $n_1 = n-1$ and $n_2 = 1$.

(ii) $LSM_3(G) \leq \begin{cases} \frac{1}{32}(15n^4 - 4n^3 + 12n^2), & \text{if } n \text{ is even,} \\ \frac{1}{32}(15n^4 - 4n^3 + 6n^2 - 12n - 5), & \text{if } n \text{ is odd,} \end{cases}$

with equality holding if and only if V^1 and V^2 are transitive tournaments with $n_1 = \left\lceil \frac{n}{2} \right\rceil$ and $n_2 = \left\lfloor \frac{n}{2} \right\rfloor$.

Proof.
(i) Since $n_1 \geq n_2$, we have $\left\lceil \frac{n}{2} \right\rceil \leq n_1 \leq n-1$ and $1 \leq n_2 \leq \left\lfloor \frac{n}{2} \right\rfloor$. Let $n_2 = x$ and $n_1 = n - x$. Using Theorem 2.12, we have

$$\begin{aligned} LSM_3(G) \geq & -\left(n_1^4 + n_2^4\right) + (3n+6)\left(n_1^3 + n_2^3\right) - (3n^2 + 12n + 6)\left(n_1^2 + n_2^2\right) \\ & + n(n^3 + 6n^2 + 9n + 4) - 2(3n^2 + 3n + 1) \\ & = -\left((n-x)^4 + x^4\right) + (3n+6)\left((n-x)^3 + x^3\right) \\ & - (3n^2 + 12n + 6)\left((n-x)^2 + x^2\right) \\ & + n(n^3 + 6n^2 + 9n + 4) - 2(3n^2 + 3n + 1) \\ & = -2x^4 + 4nx^3 - (3n^2 + 6n + 12)x^2 + (n^3 + 6n^2 + 12n)x \\ & - (3n^2 + 2n + 2). \end{aligned}$$

Let $f(x) = -2x^4 + 4nx^3 - (3n^2 + 6n + 12)x^2 + (n^3 + 6n^2 + 12n)x - (3n^2 + 2n + 2)$. Next, we prove that $f(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$.

Since $f'(x) = -8x^3 + 12nx^2 - (6n^2 + 12n + 24)x + (n^3 + 6n^2 + 12n)$ and $f''(x) = -24x^2 + 24nx - (6n^2 + 12n + 24)$, we get $f''(x) < 0$ when $1 \leq x \leq \frac{n}{2}$. So, $f'(x)$ is a decreasing function and $f'(x) \geq f'(x)_{min} = f'(\frac{n}{2}) = 0$. Hence, $f(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$, and consequently $f(x) \geq f(1) = n^3 + 8n - 16$.

Concluding, we obtain $LSM_3(G) \geq n^3 + 8n - 16$, with equality holding if and only if V^1 and V^2 are in-trees with $n_1 = n-1$ and $n_2 = 1$.

(ii) Similarly as in the proof of (i), using Theorem 2.12, we have

$$\begin{aligned}
LSM_3(G) \leq & -\frac{1}{4}\left(n_1^4 + n_2^4\right) + \left(n + \frac{5}{2}\right)\left(n_1^3 + n_2^3\right) \\
& - \left(\frac{3n^2}{2} + \frac{9n}{2} + \frac{1}{4}\right)\left(n_1^2 + n_2^2\right) + n^2\left(n^2 + \frac{3n}{2} + \frac{1}{2}\right) \\
& = -\frac{1}{4}\left((n-x)^4 + x^4\right) + \left(n + \frac{5}{2}\right)\left((n-x)^3 + x^3\right) \\
& - \left(\frac{3n^2}{2} + \frac{9n}{2} + \frac{1}{4}\right)\left((n-x)^2 + x^2\right) + n^2\left(n^2 + \frac{3n}{2} + \frac{1}{2}\right) \\
& = -\frac{1}{2}x^4 + nx^3 - \frac{1}{2}(3n^2 + 3n + 1)x^2 + \frac{1}{2}(2n^3 + 3n^2 + n)x \\
& + \frac{1}{4}(n^4 - 2n^3 + n^2).
\end{aligned}$$

Let $g(x) = -\frac{1}{2}x^4 + nx^3 - \frac{1}{2}(3n^2 + 3n + 1)x^2 + \frac{1}{2}(2n^3 + 3n^2 + n)x + \frac{1}{4}(n^4 - 2n^3 + n^2)$. Next, we prove that $g(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$.

Since $g'(x) = -2x^3 + 3nx^2 - (3n^2 + 3n + 1)x + \frac{1}{2}(2n^3 + 3n^2 + n)$ and $g''(x) = -6x^2 + 6nx - (3n^2 + 3n + 1)$, we get $g''(x) < 0$ when $1 \leq x \leq \frac{n}{2}$. So, $g'(x)$ is a decreasing function and $g'(x) \geq g'(x)_{min} = g'(\frac{n}{2}) = 0$. Hence, $g(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$, and consequently $g(x) \leq g(\frac{n}{2})$.

Substituting $x = \frac{n}{2}$ if n is even, and $x = \left\lfloor \frac{n}{2} \right\rfloor = \frac{n-1}{2}$ if n is odd, we obtain $LSM_3(G) \leq \frac{1}{32}(15n^4 - 4n^3 + 12n^2)$ for even n, and $LSM_3(G) \leq \frac{1}{32}(15n^4 - 4n^3 + 6n^2 - 12n - 5)$ for odd n, with equality holding if and only if V^1 and V^2 are transitive tournaments with $n_1 = \left\lceil \frac{n}{2} \right\rceil$ and $n_2 = \left\lfloor \frac{n}{2} \right\rfloor$. □

2.4 Concluding remarks

In Subsection 2.2.1 of this chapter, we fully characterized the extremal digraphs with a fixed dichromatic number that attain the minimal and maximal second Laplacian spectral moment among all join digraphs in $\mathscr{G}_{n,r}$. From Theorem 2.5 and Theorem 2.6, we know that the extremal digraphs are isomorphic to $\bigvee_{i=1}^{r} V^i$, where each V^i is an in-tree with $n_1 = n - r + 1$ and $n_2 = \cdots = n_r = 1$, and each V^i is a transitive tournament with $n_i = \left\lceil \frac{n}{r} \right\rceil$ or $n_i = \left\lfloor \frac{n}{r} \right\rfloor$, respectively.

In addition, in Subsection 2.2.2 of this chapter, we characterized the extremal digraphs that attain the minimal and maximal second Laplacian spectral moment among all digraphs in $\mathscr{G}_{n,r}$. In particular, the extremal digraphs in Theorem 2.8 for the minimal second Laplacian spectral moment differ considerably from those in Theorem 2.5, and required a different proof approach.

We were unable to provide such a full characterization of the extremal digraphs for the third Laplacian spectral moment. However, restricting ourselves to join digraphs we demonstrated that in-trees and transitive tournaments play a key role there, too. From Theorem 2.12, we know that also for the third Laplacian spectral moment the extremal join digraphs are isomorphic to $\bigvee_{i=1}^{r} V^i$, where each V^i is either an in-tree (for attaining the minimum), or a transitive tournament (for the maximum), but we could not determine the optimum values of n_i, except for the case when $r = 2$. For $r = 2$, we obtained a full characterization in Corollary 2.13, showing exactly the same extremal join digraphs as for the second Laplacian spectral moment. We complete this section with some examples of the extremal join digraphs in $\mathscr{G}_{n,3}$ for the third Laplacian spectral moment, as shown in Table 2.2. Here we used $G[n_1, n_2, n_3]$ to denote the digraph $V^1 \vee V^2 \vee V^3$, and we used Lemma 2.11 and Theorem 2.12 to determine the extremal join digraphs.

From Table 2.2, we conclude that the extremal join digraphs in $\mathscr{G}_{n,3}$ for the third Laplacian spectral moment are the same as for the second Laplacian spectral moment for $n = 5, 6, 7, 8, 9, 10, 15, 20$. This might suggest that the extremal join digraphs in $\mathscr{G}_{n,3}$ for the second and third Laplacian spectral moment are the same for all values of n, but we were unable to confirm this. We leave the full characterization of the extremal join digraphs in $\mathscr{G}_{n,r}$ for the third Laplacian spectral moment as an open problem.

Problem 2.1. Characterize the extremal digraphs for the third Laplacian spectral moment among all join digraphs with a fixed dichromatic number.

We have partially solved the above problem by narrowing the extremal

Table 2.2: The extremal join digraphs in $\mathscr{G}_{n,3}$ for the third Laplacian spectral moment.

$\mathscr{G}_{n,3}$	The minimal join digraphs for the third Laplacian spectral moment when each V^i is an in-tree	The maximal join digraphs for the third Laplacian spectral moment when each V^i is a transitive tournament
$\mathscr{G}_{5,3}$	$G[3,1,1]$	$G[2,2,1]$
$\mathscr{G}_{6,3}$	$G[4,1,1]$	$G[2,2,2]$
$\mathscr{G}_{7,3}$	$G[5,1,1]$	$G[3,2,2]$
$\mathscr{G}_{8,3}$	$G[6,1,1]$	$G[3,3,2]$
$\mathscr{G}_{9,3}$	$G[7,1,1]$	$G[3,3,3]$
$\mathscr{G}_{10,3}$	$G[8,1,1]$	$G[4,3,3]$
$\mathscr{G}_{15,3}$	$G[13,1,1]$	$G[5,5,5]$
$\mathscr{G}_{20,3}$	$G[18,1,1]$	$G[7,7,6]$

digraphs down to join digraphs $\bigvee_{i=1}^{r} V^i$, where either each V^i is an in-tree or each V^i is a transitive tournament. In this chapter, we did not consider the k-th Laplacian spectral moment for higher values of $k \geq 4$. We leave this as another challenging open problem.

Problem 2.2. Characterize the extremal digraphs for the k-th Laplacian spectral moment among all join digraphs with a fixed dichromatic number, for a fixed integer $k \geq 4$.

We also leave the characterization for general digraphs with a fixed dichromatic number as an open problem. In the light of Theorem 2.8, we think this could be particularly challenging for the minimal spectral moments.

Problem 2.3. Characterize the extremal digraphs for the k-th Laplacian spectral moment among all digraphs with a fixed dichromatic number, for a fixed integer $k \geq 3$.

Chapter 3

Bounds for the A_α spectral moments of digraphs

In this chapter, we obtain the digraphs which attain the minimal and maximal A_α energy (also known as the second A_α spectral moment) within classes of digraphs with a fixed dichromatic number. We also determine sharp bounds for the third A_α spectral moment within the special subclass which we define as join digraphs. These results generalize the results about the second and third Laplacian spectral moments of digraphs in Chapter 2.

3.1 Introduction

As mentioned in Chapter 2, our research is motivated by different variants of the concept of graph energy. This concept was originally introduced by Gutman [45], based on the eigenvalues of the adjacency matrix. Graph energies are mainly studied within the area which is usually referred to as chemical graph theory. Later variants of graph energy are based on the eigenvalues of other matrices associated with the graph, like the (signless) Laplacian matrix. These concepts have also been extended to digraphs.

In order to study the differences and similarities of the adjacency matrix and the signless Laplacian matrix, Nikiforov [99] proposed to study what he named the A_α-matrix of a graph, which is a convex linear combination of α times its diagonal degree matrix plus $1-\alpha$ times its adjacency matrix. This is a natural way to get a grip on the influence of the summands in the expression of the signless Laplacian matrix on the behavior of the matrix. In [89], Liu et al. extended the concept of A_α-matrix of a graph to a digraph. The A_α-matrix of a digraph G is defined by

$$A_\alpha(G) = \alpha D^+(G) + (1-\alpha)A(G),$$

where $\alpha \in [0,1)$. Following up on this idea, several groups of researchers have studied the properties of this A_α-matrix and its counterpart for digraphs (See, e.g., [4, 12, 37, 39, 40, 69, 70, 75–77, 81, 83, 85, 86, 90, 100, 101, 130, 133, 134, 139]).

For a fixed nonnegative integer k, the k-th A_α spectral moment of a digraph G is defined as

$$SM_\alpha^k(G) = \sum_{i=1}^{n} \lambda_{\alpha i}^k,$$

where $\lambda_{\alpha i}$ are the eigenvalues of $A_\alpha(G)$. In Chapter 2, we define the k-th Laplacian spectral moment of G as

$$LSM_k(G) = \sum_{i=1}^{n} \lambda_i^k,$$

where λ_i are the eigenvalues of $L(G)$. We characterized the digraphs which attain the minimal and maximal Laplacian energy within classes of digraphs with a fixed dichromatic number. And we determined sharp bounds for the third Laplacian spectral moment within the special subclass which we define as join digraphs. Note that, we mainly consider the join digraph $\bigvee_{i=1}^{r} V^i$ which each V^i is a connected acyclic digraph with n_i vertices with $\sum_{i=1}^{r} n_i = n$ and $n_1 \geq n_2 \geq \cdots \geq n_r$. In this chapter, we continue this line of research and our results are closely related to the results we obtained in Chapter 2 about the second and third Laplacian spectral moments of digraphs with a fixed dichromatic number.

We start with two results on the energy in terms of the second spectral moments of the Laplacian matrix and the A_α-matrix. The first result is due to Perera and Mizoguchi. In [107], they studied the Laplacian energy $LE(G)$ of a digraph by using the second spectral moment. See Lemma 2.1,

$$LE(G) = \sum_{i=1}^{n}(d_i^+)^2 + c_2.$$

This is followed by a result due to Xi. In [127], she defined and studied the A_α energy $E_\alpha(G)$ of a digraph by using the second spectral moment.

Lemma 3.1 (Xi [127]). *Let G be a digraph of order n. Then*

$$E_\alpha(G) = \alpha^2 \sum_{i=1}^{n}(d_i^+)^2 + (1-\alpha)^2 c_2.$$

In Chapter 2, we studied the third Laplacian spectral moment $LSM_3(G)$ of a digraph. See Lemma 2.10,

$$LSM_3(G) = \sum_{i=1}^{n}(d_i^+)^3 + 3\sum_{i=1}^{n} d_i^+ c_2^{(i)} - c_3.$$

In our first new contribution, we extend the concept to the A_α-matrix of a digraph and derive the following expression for the third spectral moment.

Lemma 3.2. *Let G be a digraph of order n. Then*

$$SM_\alpha^3(G) = \alpha^3 \sum_{i=1}^{n}(d_i^+)^3 + 3\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)} + (1-\alpha)^3 c_3.$$

Proof. The A_α-matrix of G is defined by

$$A_\alpha(G) = \alpha D^+(G) + (1-\alpha)A(G).$$

Then for $A_\alpha(G) = (\alpha_{ij})_{n\times n}$,

$$\alpha_{ij} = \begin{cases} \alpha d_i^+, & \text{if } i = j, \\ 1-\alpha, & \text{if } (v_i, v_j) \in \mathscr{A}(G), \\ 0, & \text{otherwise,} \end{cases}$$

and we have

$$SM_\alpha^3(G) = \sum_{i=1}^{n} \lambda_{\alpha i}^3 = tr\left((A_\alpha(G))^3\right) = \sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \alpha_{j_1j_2}\alpha_{j_2j_3}\alpha_{j_3j_1}.$$

For the different (possible) choices of j_1, j_2, j_3, we presented the respective values in Table 3.1.

Table 3.1: The values of $\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \alpha_{j_1j_2}\alpha_{j_2j_3}\alpha_{j_3j_1}$ for different choices of j_1, j_2, j_3.

j_1, j_2, j_3			$\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \alpha_{j_1j_2}\alpha_{j_2j_3}\alpha_{j_3j_1}$
$j_1 = j_2$	$j_2 = j_3$	$j_3 = j_1$	$\alpha^3 \sum_{i=1}^{n}(d_i^+)^3$
		$j_3 \neq j_1$	non-existent
	$j_2 \neq j_3$	$j_3 = j_1$	non-existent
		$j_3 \neq j_1$	$\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)}$
$j_1 \neq j_2$	$j_2 = j_3$	$j_3 = j_1$	non-existent
		$j_3 \neq j_1$	$\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)}$
	$j_2 \neq j_3$	$j_3 = j_1$	$\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)}$
		$j_3 \neq j_1$	$(1-\alpha)^3 c_3$

So, by summing up all the values from the table, we get

$$SM_\alpha^3(G) = \alpha^3 \sum_{i=1}^{n}(d_i^+)^3 + 3\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)} + (1-\alpha)^3 c_3.$$

□

Comparing the expressions for $L(G)$ and $A_\alpha(G)$ in Lemmas 2.1, 2.10, 3.1 and 3.2, we can easily deduce that the coefficients of α^2 and α^3 for the second and third spectral moments of $A_\alpha(G)$ are equal to the second and third spectral moments of $L(G)$, respectively.

$$\begin{aligned}
E_\alpha(G) &= \alpha^2 \sum_{i=1}^{n} (d_i^+)^2 + (1-\alpha)^2 c_2 \\
&= \alpha^2 \left(\sum_{i=1}^{n} (d_i^+)^2 + c_2 \right) - 2\alpha c_2 + c_2 \\
&= \alpha^2 LE(G) + (-2\alpha + 1) c_2,
\end{aligned}$$

and

$$\begin{aligned}
SM_\alpha^3(G) &= \alpha^3 \sum_{i=1}^{n} (d_i^+)^3 + 3\alpha(1-\alpha)^2 \sum_{i=1}^{n} d_i^+ c_2^{(i)} + (1-\alpha)^3 c_3 \\
&= \alpha^3 \left(\sum_{i=1}^{n} (d_i^+)^3 + 3 \sum_{i=1}^{n} d_i^+ c_2^{(i)} - c_3 \right) \\
&\quad + 3\alpha^2 \left(-2 \sum_{i=1}^{n} d_i^+ c_2^{(i)} + c_3 \right) + 3\alpha \left(\sum_{i=1}^{n} d_i^+ c_2^{(i)} - c_3 \right) + c_3 \\
&= \alpha^3 LSM_3(G) + 3\alpha(-2\alpha + 1) \sum_{i=1}^{n} d_i^+ c_2^{(i)} + (3\alpha^2 - 3\alpha + 1) c_3.
\end{aligned}$$

In this sense, this results extend the results in Chapter 2. In the next sections, we use the above expression for $E_\alpha(G)$ to characterize the digraphs attaining the minimal and maximal A_α energy among all join digraphs and all digraphs in $\mathcal{G}_{n,r}$, and we determine sharp bounds for the third A_α spectral moment among all join digraphs in $\mathcal{G}_{n,r}$.

3.2 Extremal digraphs for the A_α energy

In this section, we will characterize the digraphs which attain the minimal and maximal A_α energy $E_\alpha(G)$ among all join digraphs and all digraphs in

$\mathscr{G}_{n,r}$. First, we determine the extremal digraphs for the A_α energy among all join digraphs $\bigvee_{i=1}^{r} V^i$ in $\mathscr{G}_{n,r}$.

From Lemma 2.3, we get

$$n-1 \leq LE(G) \leq \frac{n(n-1)(2n-1)}{6},$$

the first equality holds if and only if G is an in-tree, and the second equality holds if and only if G is a transitive tournament.

We make use of the above result and its consequence for $E_\alpha(G)$. Since $E_\alpha(G) = \alpha^2 LE(G) + (-2\alpha+1)c_2$, the following corollary is immediate.

Corollary 3.3. *Let G be an acyclic digraph of order n. Then*

$$\alpha^2(n-1) \leq E_\alpha(G) \leq \frac{\alpha^2 n(n-1)(2n-1)}{6}.$$

Moreover, the first inequality is an equality if and only if G is an in-tree, and the second inequality is an equality if and only if G is a transitive tournament.

Using Lemma 2.4, we have the following results.

Theorem 3.4. *Let $G = \bigvee_{i=1}^{r} V^i$. Then the following inequalities hold:*
(i)

$$E_\alpha(G) \geq \alpha^2\left((r-1)n^2 + r^2 n - r^3\right) + (-2\alpha+1)\left(2(r-1)n - r^2 + r\right),$$

with equality holding if and only if each V^i is an in-tree with $n_1 = n-r+1$ and $n_2 = \cdots = n_r = 1$.
(ii) If $r \mid n$,

$$E_\alpha(G) \leq \alpha^2\left(\left(1+\frac{1}{3r^2}-\frac{1}{r}\right)n^3 - \frac{n^2}{2r} + \frac{n}{6}\right) + (-2\alpha+1)\left(1-\frac{1}{r}\right)n^2,$$

with equality holding if and only if each V^i is a transitive tournament with $n_i = \frac{n}{r}$.
(iii) If $r \nmid n$,

$$E_\alpha(G) \leq \alpha^2\left(n^3 + \frac{n}{6} + p - q\right) + (-2\alpha+1)\left(n^2 - \left\lceil\frac{n}{r}\right\rceil^2\left(n - r\left\lfloor\frac{n}{r}\right\rfloor\right)\right)$$

$$+\left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)\Bigg),$$

where $p = \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right)\left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right)$ *and* $q = \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)$ $\left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right)$. *The inequality is an equality if and only if each V^i is a transitive tournament, with $n_s = \left\lceil \frac{n}{r} \right\rceil$ for $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ and $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ for $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$.*

Proof. Let $\{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ be the vertex set of V^i, where $i = 1, 2, \ldots, r$. Let $d_G^+(v_j^i)$ be the outdegree of v_j^i in G and $d_{V^i}^+(v_j^i)$ be the outdegree of v_j^i in V^i, where $j = 1, 2, \ldots, n_i$. Using Lemma 3.1, we have

$$\begin{aligned}
E_\alpha(G) &= \alpha^2 \sum_{i=1}^{n} (d_i^+)^2 + (1-\alpha)^2 c_2 \\
&= \alpha^2 \sum_{i=1}^{r} \sum_{j=1}^{n_i} \left(d_G^+(v_j^i)\right)^2 + (1-\alpha)^2 2 \sum_{i<j} n_i n_j \\
&= \alpha^2 \sum_{i=1}^{r} \sum_{j=1}^{n_i} \left(n - n_i + d_{V^i}^+(v_j^i)\right)^2 + (1-\alpha)^2 \left[\left(\sum_{i=1}^{r} n_i\right)^2 - \sum_{i=1}^{r} n_i^2\right] \\
&= \alpha^2 \sum_{i=1}^{r} \left[\sum_{j=1}^{n_i} (n-n_i)^2 + 2(n-n_i) \sum_{j=1}^{n_i} d_{V^i}^+(v_j^i) + \sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^2\right] \\
&\quad + (1-\alpha)^2 \left(n^2 - \sum_{i=1}^{r} n_i^2\right).
\end{aligned}$$

Since V^i is acyclic and connected, using Karamata's inequality, we have

$$n_i - 1 \le \sum_{j=1}^{n_i} d_{V^i}^+(v_j^i) \le \frac{n_i(n_i-1)}{2},$$

$$n_i - 1 \le \sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^2 \le \frac{n_i(n_i-1)(2n_i-1)}{6}.$$

In all of the above inequalities, the lower bounds are only attained if V^i is an in-tree, and the upper bounds are only attained if V^i is a transitive tournament.

Hence, we obtain

$$\begin{aligned}
&\left(\alpha^2\left(n^3+3n^2-(2r-3)n-r\right)-2\alpha n^2+n^2\right)+\alpha^2\sum_{i=1}^{r}n_i^3\\
&-\left(\alpha^2(2n+3)-2\alpha+1\right)\sum_{i=1}^{r}n_i^2\le E_\alpha(G)\\
&\le\left(\alpha^2\left(n^3+\frac{n}{6}\right)-2\alpha n^2+n^2\right)+\frac{\alpha^2}{3}\sum_{i=1}^{r}n_i^3-\left(\alpha^2\left(n+\frac{1}{2}\right)-2\alpha+1\right)\sum_{i=1}^{r}n_i^2.
\end{aligned}$$

Let $f(x)=x^2(a-bx)$ and $F(x_1,x_2,\dots,x_r)=\sum_{i=1}^{r}f(x_i)$, where $\sum_{i=1}^{r}x_i=n$ and $1\le x_i\le n-r+1$. From Lemma 2.4, if $x_i-x_j\ge 2$ and $x_j<\frac{a}{3b}-1$ for some x_i and x_j, we have $f(x_i-1)+f(x_j+1)<f(x_i)+f(x_j)$. Then we have $F(x_1,\dots,x_i-1,\dots,x_j+1,\dots,x_r)<F(x_1,\dots,x_i,\dots,x_j,\dots,x_r)$.

For

$$\begin{aligned}
&\alpha^2\sum_{i=1}^{r}n_i^3-\left(\alpha^2(2n+3)-2\alpha+1\right)\sum_{i=1}^{r}n_i^2\\
&=\sum_{i=1}^{r}n_i^2\left(\alpha^2 n_i-\left(\alpha^2(2n+3)-2\alpha+1\right)\right)\\
&=-\sum_{i=1}^{r}n_i^2\left(\alpha^2(2n+3)-2\alpha+1-\alpha^2 n_i\right),
\end{aligned}$$

let $f_1(n_i)=n_i^2\left(\alpha^2(2n+3)-2\alpha+1-\alpha^2 n_i\right)$. Since $\frac{\alpha^2(2n+3)-2\alpha+1}{3\alpha^2}-1=\frac{2\alpha^2 n-2\alpha+1}{3\alpha^2}>\frac{n-r}{2}\ge n_j$ if $n_i-n_j\ge 2$, $F_1(n_1,n_2,\dots,n_r)=\sum_{i=1}^{r}f_1(n_i)$ is maximal when $n_1=n-r+1$ and $n_2=\cdots=n_r=1$. That is, $E_\alpha(G)$ is minimal when $n_1=n-r+1$ and $n_2=\cdots=n_r=1$.

Similarly, for

$$\frac{\alpha^2}{3}\sum_{i=1}^{r}n_i^3-\left(\alpha^2\left(n+\frac{1}{2}\right)-2\alpha+1\right)\sum_{i=1}^{r}n_i^2$$

$$= \sum_{i=1}^{r} n_i^2 \left(\frac{\alpha^2}{3} n_i - \left(\alpha^2 \left(n + \frac{1}{2} \right) - 2\alpha + 1 \right) \right)$$
$$= -\sum_{i=1}^{r} n_i^2 \left(\alpha^2 \left(n + \frac{1}{2} \right) - 2\alpha + 1 - \frac{\alpha^2}{3} n_i \right),$$

let $f_2(n_i) = n_i^2 \left(\alpha^2 \left(n + \frac{1}{2} \right) - 2\alpha + 1 - \frac{\alpha^2}{3} n_i \right)$. Since $\frac{\alpha^2 \left(n+\frac{1}{2}\right) - 2\alpha + 1}{\alpha^2} - 1 = \frac{\alpha^2 \left(n-\frac{1}{2}\right) - 2\alpha + 1}{\alpha^2} > \frac{n-r}{2} \geq n_j$ if $n_i - n_j \geq 2$, $F_2(n_1, n_2, \ldots, n_r) = \sum_{i=1}^{r} f_2(n_i)$ is minimal when $|n_i - n_j| \leq 1$. That is, $E_\alpha(G)$ is maximal when $n_i = \left\lceil \frac{n}{r} \right\rceil$ or $n_i = \left\lfloor \frac{n}{r} \right\rfloor$.

Concluding,

(i) $E_\alpha(G)$

$$\begin{aligned}
&\geq \left(\alpha^2 \left(n^3 + 3n^2 - (2r-3)n - r \right) - 2\alpha n^2 + n^2 \right) \\
&+ \alpha^2 \sum_{i=1}^{r} n_i^3 - \left(\alpha^2 (2n+3) - 2\alpha + 1 \right) \sum_{i=1}^{r} n_i^2 \\
&\geq \left(\alpha^2 \left(n^3 + 3n^2 - (2r-3)n - r \right) - 2\alpha n^2 + n^2 \right) + \alpha^2 \left((n-r+1)^3 + (r-1) \right) \\
&- \left(\alpha^2 (2n+3) - 2\alpha + 1 \right) \left((n-r+1)^2 + (r-1) \right) \\
&= \alpha^2 \left((r-1)n^2 + r^2 n - r^3 \right) - 2\alpha \left(2(r-1)n - r^2 + r \right) + \left(2(r-1)n - r^2 + r \right) \\
&= \alpha^2 \left((r-1)n^2 + r^2 n - r^3 \right) + (-2\alpha + 1) \left(2(r-1)n - r^2 + r \right),
\end{aligned}$$

with equality holding if and only if each V^i is an in-tree with $n_1 = n - r + 1$ and $n_2 = \cdots = n_r = 1$.

(ii) If $r \mid n$, $E_\alpha(G)$

$$\begin{aligned}
&\leq \left(\alpha^2 \left(n^3 + \frac{n}{6} \right) - 2\alpha n^2 + n^2 \right) + \frac{\alpha^2}{3} \sum_{i=1}^{r} n_i^3 - \left(\alpha^2 \left(n + \frac{1}{2} \right) - 2\alpha + 1 \right) \sum_{i=1}^{r} n_i^2 \\
&\leq \left(\alpha^2 \left(n^3 + \frac{n}{6} \right) - 2\alpha n^2 + n^2 \right) + \frac{\alpha^2}{3} r \left(\frac{n}{r} \right)^3 - \left(\alpha^2 \left(n + \frac{1}{2} \right) - 2\alpha + 1 \right) r \left(\frac{n}{r} \right)^2 \\
&= \alpha^2 \left(\left(1 + \frac{1}{3r^2} - \frac{1}{r} \right) n^3 - \frac{n^2}{2r} + \frac{n}{6} \right) - 2\alpha \left(1 - \frac{1}{r} \right) n^2 + \left(1 - \frac{1}{r} \right) n^2 \\
&= \alpha^2 \left(\left(1 + \frac{1}{3r^2} - \frac{1}{r} \right) n^3 - \frac{n^2}{2r} + \frac{n}{6} \right) + (-2\alpha + 1) \left(1 - \frac{1}{r} \right) n^2,
\end{aligned}$$

with equality holding if and only if each V^i is a transitive tournament with $n_i = \frac{n}{r}$.

(iii) If $r \nmid n$, $E_\alpha(G)$

$$
\begin{aligned}
&\le \left(\alpha^2\left(n^3+\frac{n}{6}\right)-2\alpha n^2+n^2\right)+\sum_{i=1}^{r} n_i^2\left(\alpha^2\left(\frac{1}{3}n_i-n-\frac{1}{2}\right)+2\alpha-1\right)\\
&\le \left(\alpha^2\left(n^3+\frac{n}{6}\right)-2\alpha n^2+n^2\right)+\left\lceil\frac{n}{r}\right\rceil^2\left(n-r\left\lfloor\frac{n}{r}\right\rfloor\right)\left(\alpha^2\left(\frac{1}{3}\left\lceil\frac{n}{r}\right\rceil-n-\frac{1}{2}\right)\right.\\
&\left.+2\alpha-1\right)-\left\lfloor\frac{n}{r}\right\rfloor^2\left(n-r\left\lceil\frac{n}{r}\right\rceil\right)\left(\alpha^2\left(\frac{1}{3}\left\lfloor\frac{n}{r}\right\rfloor-n-\frac{1}{2}\right)+2\alpha-1\right)\\
&=\alpha^2\left(n^3+\frac{n}{6}+p-q\right)+(-2\alpha+1)\Bigg(n^2-\left\lceil\frac{n}{r}\right\rceil^2\left(n-r\left\lfloor\frac{n}{r}\right\rfloor\right)\\
&+\left\lfloor\frac{n}{r}\right\rfloor^2\left(n-r\left\lceil\frac{n}{r}\right\rceil\right)\Bigg),
\end{aligned}
$$

where $p=\left\lceil\frac{n}{r}\right\rceil^2\left(n-r\left\lfloor\frac{n}{r}\right\rfloor\right)\left(\frac{1}{3}\left\lceil\frac{n}{r}\right\rceil-n-\frac{1}{2}\right)$ and $q=\left\lfloor\frac{n}{r}\right\rfloor^2\left(n-r\left\lceil\frac{n}{r}\right\rceil\right)$ $\left(\frac{1}{3}\left\lfloor\frac{n}{r}\right\rfloor-n-\frac{1}{2}\right)$. The inequality is an equality if and only if each V^i is a transitive tournament, with $n_s=\left\lceil\frac{n}{r}\right\rceil$ for $s=1,2,\ldots,n-r\left\lfloor\frac{n}{r}\right\rfloor$ and $n_t=\left\lfloor\frac{n}{r}\right\rfloor$ for $t=n-r\left\lfloor\frac{n}{r}\right\rfloor+1, n-r\left\lfloor\frac{n}{r}\right\rfloor+2,\ldots,r$.

This completes the proof. □

For the join digraphs $G=\bigvee_{i=1}^{r}V^i$ in $\mathscr{G}_{n,r}$, $E_\alpha(G)$ and $LE(G)$ have the same extremal digraphs by Theorem 3.4 above and Theorems 2.5, 2.6 in Chapter 2. Actually, we know $c_2=n^2-\sum_{i=1}^{r}n_i^2$. Using Karamata's inequality, $\sum_{i=1}^{r}n_i^2$ is maximal when $n_1=n-r+1$ and $n_2=\cdots=n_r=1$ and minimal when $|n_i-n_j|\le 1$. Since

$$
E_\alpha(G)=\alpha^2LE(G)+(-2\alpha+1)c_2=\alpha^2LE(G)+(-2\alpha+1)\left(n^2-\sum_{i=1}^{r}n_i^2\right),
$$

in case $0\le\alpha\le\frac{1}{2}$, we can deduce that $E_\alpha(G)$ and $LE(G)$ have the same extremal digraphs directly. But when $\frac{1}{2}<\alpha<1$, we can not directly get the bounds of $E_\alpha(G)$ based on the bounds of $LE(G)$. In particular, when $\alpha=\frac{1}{2}$, Yang and Wang [136] have shown that results on the Laplacian energy of a digraph are also applicable to its signless Laplacian energy. We omit the details.

Next, we will determine the digraphs which attain the minimal and maximal A_α energy $E_\alpha(G)$ among all digraphs in $\mathscr{G}_{n,r}$. Using Lemmas 1.1, 1.2

and 2.7, in Chapter 2, we were able to characterize the digraphs which attain the minimal Laplacian energy $LE(G)$ among all digraphs in $\mathscr{G}_{n,r}$, see Theorem 2.8.

From Theorem 2.8, it is rather natural to expect that the same digraphs attain the minimal A_α energy among all digraphs in $\mathscr{G}_{n,r}$. However, the following two digraphs illustrated in Figure 3.1 show that the minimal digraphs for the A_α energy and the Laplacian energy can be different (when α is in some range).

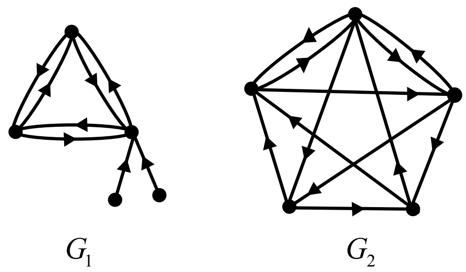


Figure 3.1: Different minimal digraphs for $LE(G)$ and $E_\alpha(G)$.

It is easy to check that both digraphs illustrated in Figure 3.1 belong to $\mathscr{G}_{5,3}$. From Theorem 2.8, we know that G_1 is an example of a digraph attaining the minimal Laplacian energy, whereas G_2 is not. But for the A_α energy, we obtain $E_\alpha(G_1) = 14\alpha^2 + 6(1-\alpha)^2$ and $E_\alpha(G_2) = 30\alpha^2 + 4(1-\alpha)^2$. Hence, $E_\alpha(G_1) \geq E_\alpha(G_2)$ when $\alpha \in [0, \frac{2\sqrt{2}-1}{7}]$, and $E_{\frac{1}{4}}(G_1) > E_{\frac{1}{4}}(G_2)$. Hence, the minimal digraphs for the A_α energy and the Laplacian energy can be different when α is in some range. It is natural to ask what happens for other values of α outside this range. In fact, our next result shows that the A_α energy and Laplacian energy among all digraphs in $\mathscr{G}_{n,r}$ have the same minimal digraphs when $\alpha \in [\frac{1}{2}, 1)$. We need the Lemma 2.7 and its straightforward consequence.

Using Lemma 2.7, it is easy to prove the following corollary of the above lemma.

Corollary 3.5. *Let G be a digraph in $\mathscr{G}_{n,r}$, and let G' be an r-critical subdigraph of G. If G attains the minimal A_α energy $E_\alpha(G)$ among all digraphs in $\mathscr{G}_{n,r}$, then $d_G^+(v)=1$ for any $v\in\mathscr{V}(G)\setminus\mathscr{V}(G')$ and $d_G^+(u)=d_{G'}^+(u)$ for any $u\in\mathscr{V}(G')$.*

Proof. Let G' of order n' be an r-critical subdigraph of G. Then using Lemma 2.7, we know

$$\begin{aligned} LE(G) &\geq \sum_{v\in\mathscr{V}(G)\setminus\mathscr{V}(G')} \left(d_G^+(v)\right)^2 + \sum_{u\in\mathscr{V}(G')} \left(d_G^+(u)\right)^2 + c_2(G') \\ &\geq \sum_{v\in\mathscr{V}(G)\setminus\mathscr{V}(G')} 1 + \sum_{u\in\mathscr{V}(G')} \left(d_{G'}^+(u)\right)^2 + c_2(G') \\ &= LE(G') + n - n'. \end{aligned}$$

So,

$$\begin{aligned} E_\alpha(G) &\geq \alpha^2 \left(\sum_{v\in\mathscr{V}(G)\setminus\mathscr{V}(G')} \left(d_G^+(v)\right)^2 + \sum_{u\in\mathscr{V}(G')} \left(d_G^+(u)\right)^2 \right) + (1-\alpha)^2 c_2(G') \\ &\geq \alpha^2 \left(\sum_{v\in\mathscr{V}(G)\setminus\mathscr{V}(G')} 1 + \sum_{u\in\mathscr{V}(G')} \left(d_{G'}^+(u)\right)^2 \right) + (1-\alpha)^2 c_2(G') \\ &= E_\alpha(G') + \alpha^2(n-n'). \end{aligned}$$

Hence, if G attains the minimal A_α energy $E_\alpha(G)$ among all digraphs in $\mathscr{G}_{n,r}$, then $d_G^+(v)=1$ for any $v\in\mathscr{V}(G)\setminus\mathscr{V}(G')$ and $d_G^+(u)=d_{G'}^+(u)$ for any $u\in\mathscr{V}(G')$. □

We use the above corollary to prove our next result.

Theorem 3.6. *Let G be a digraph in $\mathscr{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r=2$, we have

$$E_\alpha(G) \geq \begin{cases} 4\alpha^2 - 4\alpha + 2, & \text{if } n=2, \\ \alpha^2 n, & \text{if } n\geq 3. \end{cases}$$

If $n = 2$, the inequality is an equality if and only if G is a directed cycle C_2. If $n \geq 3$, the inequality is an equality if and only if G contains a directed cycle $C_{n'}$ ($n' \geq 3$) and every component (if any) of $G - \mathscr{V}(C_{n'})$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $C_{n'}$.
(ii) When $\alpha \in [\frac{1}{2}, 1)$ and $r \geq 3$, we have

$$E_\alpha(G) \geq \alpha^2(n + r^3 - r^2 - r) + (-2\alpha + 1)r(r-1),$$

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component (if any) of $G - \mathscr{V}(\overleftrightarrow{K}_r)$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $\overleftrightarrow{K}_r$.

Proof. Let G be a digraph in $\mathscr{G}_{n,r}$. Then G must contain an induced subdigraph G' of order n' that is r-critical. From Corollary 3.5, we obtain that if G attains the minimal A_α energy $E_\alpha(G)$ among all digraphs in $\mathscr{G}_{n,r}$, then $d_G^+(v) = 1$ for any $v \in \mathscr{V}(G) \setminus \mathscr{V}(G')$ and $d_G^+(u) = d_{G'}^+(u)$ for any $u \in \mathscr{V}(G')$. That is, G contains an r-critical digraph G' and every component of $G - \mathscr{V}(G')$ is an in-tree, the root of which is an inneighbor of exactly one vertex of G'. From the proof of Corollary 3.5, we also get

$$E_\alpha(G) \geq E_\alpha(G') + \alpha^2(n - n') = \alpha^2 \sum_{u \in \mathscr{V}(G')} \left(d_{G'}^+(u)\right)^2 + (1-\alpha)^2 c_2(G') + \alpha^2(n - n').$$

Next, we distinguish the cases $r = 2$ and $r \geq 3$.

Case 1. $r = 2$.
We consider the two subcases $n = 2$ and $n \geq 3$.

Case 1.1. Suppose $n = 2$. Then $G = G' = C_2$, and $E_\alpha(C_2) = 4\alpha^2 - 4\alpha + 2$.

Case 1.2. Suppose $n \geq 3$. Using Lemma 1.1, we get that $d_{G'}^+(u) \geq r - 1 = 1$ for any $u \in \mathscr{V}(G')$. If $d_{G'}^+(u) = 1$ for any $u \in \mathscr{V}(G')$, using Lemma 1.2, we can get $c_2(G') = 0$ if G' is a directed cycle of length $n' \geq 3$. So, we conclude that

$$E_\alpha(G) \geq \alpha^2 \sum_{u \in \mathscr{V}(G')} \left(d_{G'}^+(u)\right)^2 + (1-\alpha)^2 c_2(G') + \alpha^2(n - n') \geq \alpha^2 n,$$

with equality if and only if G contains a directed cycle $C_{n'}$ ($n' \geq 3$) and every component (if any) of $G - \mathscr{V}(C_{n'})$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $C_{n'}$.

Case 2. $r \geq 3$.

Then $d^+_{G'}(u) \geq r-1$ for any $u \in \mathscr{V}(G')$ by Lemma 1.1.

If $n' = r$, then $d^+_{G'}(u) = r-1$ for any $u \in \mathscr{V}(G')$. From Lemma 1.2, we have $r = 3$ and G' is a bidirected cycle of odd length $n' = 3$, or G' is a bidirected complete graph of order $r \geq 4$. That is, if $n' = r$, then $d^+_{G'}(u) = r-1$ for any $u \in \mathscr{V}(G')$, $G' = \overleftrightarrow{K}_r$ of order $r \geq 3$, and

$$\begin{aligned}
&\alpha^2 \sum_{u \in \mathscr{V}(\overleftrightarrow{K}_r)} \left(d^+_{\overleftrightarrow{K}_r}(u) \right)^2 + (1-\alpha)^2 c_2(\overleftrightarrow{K}_r) + \alpha^2(n-r) \\
&= \alpha^2 r(r-1)^2 + (1-\alpha)^2 r(r-1) + \alpha^2(n-r).
\end{aligned}$$

If $n' = r+1$, since $d^+_{G'}(u) \geq r-1$ for any $u \in \mathscr{V}(G')$, we get $e(G') \geq (r+1)(r-1)$ and $\frac{c_2(G')}{2} \geq e(G') - \frac{(r+1)r}{2}$. So

$$\begin{aligned}
E_\alpha(G) &\geq \alpha^2 \sum_{u \in \mathscr{V}(G')} \left(d^+_{G'}(u) \right)^2 + (1-\alpha)^2 c_2(G') + \alpha^2(n-n') \\
&\geq \alpha^2(r+1)(r-1)^2 + (1-\alpha)^2(r(r-1)-2) + \alpha^2(n-r-1).
\end{aligned}$$

If $n' \geq r+2$, then

$$\begin{aligned}
E_\alpha(G) &\geq \alpha^2 \sum_{u \in \mathscr{V}(G')} \left(d^+_{G'}(u) \right)^2 + (1-\alpha)^2 c_2(G') + \alpha^2(n-n') \\
&\geq \alpha^2 n'(r-1)^2 + 0 + \alpha^2(n-n').
\end{aligned}$$

When $n' = r+1$ and $\alpha \in [\frac{1}{2}, 1)$, we have

$$\begin{aligned}
&\left(\alpha^2(r+1)(r-1)^2 + (1-\alpha)^2(r(r-1)-2) + \alpha^2(n-r-1) \right) \\
&- \left(\alpha^2 r(r-1)^2 + (1-\alpha)^2 r(r-1) + \alpha^2(n-r) \right) \\
&= \alpha^2(r^2-2r-2) + 4\alpha - 2 \\
&> 0.
\end{aligned}$$

When $n' \geq r+2$ and $\alpha \in (\frac{1}{2}, 1)$, we have

$$\begin{aligned}
&\left(\alpha^2 n'(r-1)^2 + 0 + \alpha^2(n-n')\right) \\
&- \left(\alpha^2 r(r-1)^2 + (1-\alpha)^2 r(r-1) + \alpha^2(n-r)\right) \\
&= \alpha^2 r\left(n'(r-2) - r^2 + r + 1\right) + (2\alpha-1)r(r-1) \\
&\geq \alpha^2 r\left((r+2)(r-2) - r^2 + r + 1\right) + (2\alpha-1)r(r-1) \\
&= \alpha^2 r(r-3) + (2\alpha-1)r(r-1) \\
&> 0.
\end{aligned}$$

And when $\alpha = \frac{1}{2}$, we know $E_{\frac{1}{2}}(G) = \frac{1}{4}LE(G)$.

Hence, when $\alpha \in [\frac{1}{2}, 1)$, if $r \geq 3$,

$$\begin{aligned}
E_\alpha(G) &\geq \alpha^2 r(r-1)^2 + (1-\alpha)^2 r(r-1) + \alpha^2(n-r) \\
&= \alpha^2(n + r^3 - r^2 - r) + (-2\alpha+1)r(r-1),
\end{aligned}$$

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component (if any) of $G - \mathscr{V}(\overleftrightarrow{K}_r)$ is an in-tree, the root of which is an inneighbor of exactly one vertex of $\overleftrightarrow{K}_r$.

□

The next result characterizes the digraphs which attain the maximal A_α energy $E_\alpha(G)$ among all digraphs in $\mathscr{G}_{n,r}$. It is an easy consequence of Theorem 3.4, so we omit the proof.

Theorem 3.7. *Let G be a digraph in $\mathscr{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r \mid n$,

$$E_\alpha(G) \leq \alpha^2\left(\left(1 + \frac{1}{3r^2} - \frac{1}{r}\right)n^3 - \frac{n^2}{2r} + \frac{n}{6}\right) + (-2\alpha+1)\left(1 - \frac{1}{r}\right)n^2,$$

with equality holding if and only if $G = \bigvee_{i=1}^{r} V^i$ and each V^i is a transitive tournament with $n_i = \frac{n}{r}$.

(ii) If $r \nmid n$,

$$E_\alpha(G) \leq \alpha^2 \left(n^3 + \frac{n}{6} + p - q\right) + (-2\alpha+1)\Bigg(n^2 - \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right) + \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)\Bigg),$$

where $p = \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r\left\lfloor \frac{n}{r} \right\rfloor\right)\left(\frac{1}{3}\left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right)$ *and* $q = \left\lfloor \frac{n}{r} \right\rfloor^2 \left(n - r\left\lceil \frac{n}{r} \right\rceil\right)\left(\frac{1}{3}\left\lfloor \frac{n}{r} \right\rfloor - n - \frac{1}{2}\right)$. *The inequality is an equality if and only if* $G = \bigvee_{i=1}^r V^i$ *and each* V^i *is a transitive tournament, with* $n_s = \left\lceil \frac{n}{r} \right\rceil$ *for* $s = 1, 2, \ldots, n - r\left\lfloor \frac{n}{r} \right\rfloor$ *and* $n_t = \left\lfloor \frac{n}{r} \right\rfloor$ *for* $t = n - r\left\lfloor \frac{n}{r} \right\rfloor + 1, n - r\left\lfloor \frac{n}{r} \right\rfloor + 2, \ldots, r$.

3.3 Bounds for the third A_α spectral moment

In this section, we will determine sharp bounds for the third A_α spectral moment $SM_\alpha^3(G)$ of join digraphs $G = \bigvee_{i=1}^r V^i$ in $\mathscr{G}_{n,r}$.

Using the expressions for $LSM_3(G)$ and $SM_\alpha^3(G)$ in Lemmas 2.10 and 3.2, we can derive that

$$SM_\alpha^3(G) = \alpha^3 LSM_3(G) + 3\alpha(-2\alpha+1)\sum_{i=1}^n d_i^+ c_2^{(i)} + (3\alpha^2 - 3\alpha + 1)c_3.$$

However, this does not imply that we can obtain sharp bounds for $SM_\alpha^3(G)$ directly from the sharp bounds that were obtained for $LSM_3(G)$ earlier. We will first derive an alternative expression for $SM_\alpha^3(G)$, making use of the following earlier result in the proof of Lemma 2.11.

Lemma 3.8. *Let $G = \bigvee_{i=1}^r V^i$. Then*

$$c_3 = \sum_{i=1}^r \sum_{j=1}^{n_i} \left[d_{V^i}^+(v_j^i)(n - n_i) + \sum_{s \neq i} \left[\sum_{t=1}^{n_s} d_{V^s}^+(v_t^s) + n_s \left[(n - n_s - n_i) + d_{V^i}^-(v_j^i) \right] \right] \right].$$

Lemma 3.9. *Let* $G = \bigvee_{i=1}^{r} V^i$. *Then*

$$SM_\alpha^3(G) = \alpha^3 \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(n - n_i + d_{V^i}^+(v_j^i)\right)^3 + 3\alpha(1-\alpha)^2\sum_{i=1}^{r} n_i(n-n_i)^2$$
$$+ 3(1-\alpha)^2\sum_{i=1}^{r}\sum_{j=1}^{n_i} d_{V^i}^+(v_j^i)(n-n_i) + (1-\alpha)^3\sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i).$$

Proof. From Lemma 3.2, we obtain

$$SM_\alpha^3(G) = \alpha^3 \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(d_G^+(v_j^i)\right)^3 + 3\alpha(1-\alpha)^2\sum_{i=1}^{r}\sum_{j=1}^{n_i} d_G^+(v_j^i)c_2(v_j^i)$$
$$+ (1-\alpha)^3 c_3.$$

Recall that $d_G^+(v_j^i) = n - n_i + d_{V^i}^+(v_j^i)$ and $c_2(v_j^i) = n - n_i$, for $j = 1, 2, \ldots, n_i$ and $i = 1, 2, \ldots, r$. Then

$$\sum_{i=1}^{r}\sum_{j=1}^{n_i} d_G^+(v_j^i)c_2(v_j^i) = \sum_{i=1}^{r} n_i(n-n_i)^2 + \sum_{i=1}^{r} e(V^i)(n-n_i).$$

By Lemma 3.8,

$$c_3 = \sum_{i=1}^{r}\sum_{j=1}^{n_i}\left[d_{V^i}^+(v_j^i)(n-n_i) + \sum_{s\neq i}\left[\sum_{t=1}^{n_s} d_{V^s}^+(v_t^s) + n_s\left[(n-n_s-n_i) + d_{V^i}^-(v_j^i)\right]\right]\right]$$
$$= \sum_{i=1}^{r} e(V^i)(n-n_i) + \sum_{i=1}^{r}\left[n_i\sum_{s\neq i} e(V^s) + n_i\sum_{s\neq i} n_s(n-n_s-n_i) + e(V^i)\sum_{s\neq i} n_s\right].$$

We also get

$$3\alpha(1-\alpha)^2\sum_{i=1}^{r} e(V^i)(n-n_i) + (1-\alpha)^3\sum_{i=1}^{r} e(V^i)(n-n_i)$$
$$+ (1-\alpha)^3\sum_{i=1}^{r} e(V^i)\sum_{s\neq i} n_s = (1-\alpha)^2(\alpha+2)\sum_{i=1}^{r} e(V^i)(n-n_i),$$

and

$$\begin{aligned}
&(1-\alpha)^2(\alpha+2)\sum_{i=1}^{r} e(V^i)(n-n_i)+(1-\alpha)^3\sum_{i=1}^{r} n_i \sum_{s\neq i} e(V^s)\\
&=(1-\alpha)^2(\alpha+2)n\sum_{i=1}^{r} e(V^i)+(1-\alpha)^2(1-\alpha-3)\sum_{i=1}^{r} e(V^i)n_i\\
&+(1-\alpha)^3\sum_{i=1}^{r} n_i \sum_{s\neq i} e(V^s)\\
&=(1-\alpha)^2(\alpha+2)n\sum_{i=1}^{r} e(V^i)-3(1-\alpha)^2\sum_{i=1}^{r} e(V^i)n_i\\
&+(1-\alpha)^3\sum_{i=1}^{r} n_i \left[e(V^i)+\sum_{s\neq i} e(V^s)\right]\\
&=(1-\alpha)^2\sum_{i=1}^{r} e(V^i)\left[(\alpha+2)n-3n_i\right]+(1-\alpha)^3\sum_{i=1}^{r} n_i \sum_{s=1}^{r} e(V^s)\\
&=(1-\alpha)^2\sum_{i=1}^{r} e(V^i)\left[(\alpha+2)n-3n_i\right]+(1-\alpha)^3 n\sum_{s=1}^{r} e(V^s)\\
&=(1-\alpha)^2\sum_{i=1}^{r} e(V^i)\left[(\alpha+2)n-3n_i+(1-\alpha)n\right]\\
&=3(1-\alpha)^2\sum_{i=1}^{r} e(V^i)(n-n_i).
\end{aligned}$$

Combining the above equations, we obtain

$$\begin{aligned}
SM_\alpha^3(G)=\alpha^3\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(n-n_i+d_{V^i}^+(v_j^i)\right)^3+3\alpha(1-\alpha)^2\sum_{i=1}^{r} n_i(n-n_i)^2\\
+3(1-\alpha)^2\sum_{i=1}^{r}\sum_{j=1}^{n_i} d_{V^i}^+(v_j^i)(n-n_i)+(1-\alpha)^3\sum_{i=1}^{r} n_i\sum_{s\neq i} n_s(n-n_s-n_i).
\end{aligned}$$

□

Next, using the above expression we will determine sharp bounds for $SM_\alpha^3(G)$ of join digraphs in $\mathcal{G}_{n,r}$.

Theorem 3.10. *Let $G = \bigvee_{i=1}^{r} V^i$. Then*

(i)

$$
\begin{aligned}
SM_\alpha^3(G) \geq & -\alpha^3 \sum_{i=1}^{r} n_i^4 + 3\left(\alpha^3(n+1) + \alpha(1-\alpha)^2\right) \sum_{i=1}^{r} n_i^3 \\
& - 3\left(\alpha^3(n^2+2n+2) + 2\alpha(1-\alpha)^2 n + (1-\alpha)^2\right) \sum_{i=1}^{r} n_i^2 \\
& + \alpha^3\left(n(n^3+3n^2+9n+4) - r(3n^2+3n+1)\right) + 3\alpha(1-\alpha)^2 n^3 \\
& + 3(1-\alpha)^2(n^2+n-rn) + (1-\alpha)^3 \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i),
\end{aligned}
$$

with equality holding if and only if each V^i is an in-tree.

(ii)

$$
\begin{aligned}
SM_\alpha^3(G) \leq & -\frac{\alpha^3}{4} \sum_{i=1}^{r} n_i^4 + \left(\alpha^3\left(n-\frac{1}{2}\right) + 3\alpha(1-\alpha)^2 - \frac{3}{2}(1-\alpha)^2\right) \sum_{i=1}^{r} n_i^3 \\
& - \left(\alpha^3\left(\frac{3n^2}{2} - \frac{3n}{2} + \frac{1}{4}\right) + 6\alpha(1-\alpha)^2 n - \frac{3}{2}(1-\alpha)^2(n+1)\right) \sum_{i=1}^{r} n_i^2 \\
& + \alpha^3\left(n^4 - \frac{3n^3}{2} + \frac{n^2}{2}\right) + 3\alpha(1-\alpha)^2 n^3 - (1-\alpha)^2 \frac{3n^2}{2} \\
& + (1-\alpha)^3 \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i),
\end{aligned}
$$

with equality holding if and only if each V^i is a transitive tournament.

Proof. From Lemma 3.9, since

$$
\begin{aligned}
SM_\alpha^3(G) = & \alpha^3 \sum_{i=1}^{r} \sum_{j=1}^{n_i} \left(n - n_i + d_{V^i}^+(v_j^i)\right)^3 + 3\alpha(1-\alpha)^2 \sum_{i=1}^{r} n_i(n-n_i)^2 \\
& + 3(1-\alpha)^2 \sum_{i=1}^{r} \sum_{j=1}^{n_i} d_{V^i}^+(v_j^i)(n-n_i) + (1-\alpha)^3 \sum_{i=1}^{r} n_i \sum_{s\neq i} n_s(n-n_s-n_i),
\end{aligned}
$$

and

$$
\sum_{i=1}^{r} \sum_{j=1}^{n_i} \left(n - n_i + d_{V^i}^+(v_j^i)\right)^3 = \sum_{i=1}^{r} \left[n_i(n-n_i)^3 + \sum_{j=1}^{n_i} \left(d_{V^i}^+(v_j^i)\right)^3 \right.
$$

$$+3(n-n_i)\sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^2+3(n-n_i)^2\sum_{j=1}^{n_i}d_{V^i}^+(v_j^i)\Bigg],$$

we only need to consider the bounds of $\sum_{j=1}^{n_i} d_{V^i}^+(v_j^i)$, $\sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^2$ and $\sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^3$. Using Karamata's inequality, we have

$$n_i-1\le\sum_{j=1}^{n_i}d_{V^i}^+(v_j^i)\le\frac{n_i(n_i-1)}{2},$$

$$n_i-1\le\sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^2\le\frac{n_i(n_i-1)(2n_i-1)}{6},$$

$$n_i-1\le\sum_{j=1}^{n_i}\left(d_{V^i}^+(v_j^i)\right)^3\le\frac{n_i^2(n_i-1)^2}{4}.$$

In all of the above three inequalities, the lower bounds are only attained if V^i is an in-tree, and the upper bounds are only attained if V^i is a transitive tournament. Combining the above terms, for the lower bound we obtain

$$\begin{aligned}
&SM_\alpha^3(G)\\
&\ge\alpha^3\sum_{i=1}^{r}\left[n_i(n-n_i)^3+(n_i-1)+3(n-n_i)(n_i-1)+3(n-n_i)^2(n_i-1)\right]\\
&+3\alpha(1-\alpha)^2\sum_{i=1}^{r}n_i(n-n_i)^2+3(1-\alpha)^2\sum_{i=1}^{r}(n-n_i)(n_i-1)\\
&+(1-\alpha)^3\sum_{i=1}^{r}n_i\sum_{s\ne i}n_s(n-n_s-n_i)\\
&=-\alpha^3\sum_{i=1}^{r}n_i^4+3\left(\alpha^3(n+1)+\alpha(1-\alpha)^2\right)\sum_{i=1}^{r}n_i^3\\
&-3\left(\alpha^3(n^2+2n+2)+2\alpha(1-\alpha)^2n+(1-\alpha)^2\right)\sum_{i=1}^{r}n_i^2\\
&+\alpha^3\left(n(n^3+3n^2+9n+4)-r(3n^2+3n+1)\right)+3\alpha(1-\alpha)^2n^3
\end{aligned}$$

$$+3(1-\alpha)^2(n^2+n-rn)+(1-\alpha)^3\sum_{i=1}^{r}n_i\sum_{s\neq i}n_s(n-n_s-n_i),$$

with equality holding if and only if each V^i is an in-tree with n_i vertices.

For the upper bound we obtain

$$\begin{aligned}
&SM_\alpha^3(G)\\
&\leq \alpha^3\sum_{i=1}^{r}\left[n_i(n-n_i)^3+\frac{n_i^2(n_i-1)^2}{4}+3(n-n_i)\frac{n_i(n_i-1)(2n_i-1)}{6}\right.\\
&\left.+3(n-n_i)^2\frac{n_i(n_i-1)}{2}\right]+3\alpha(1-\alpha)^2\sum_{i=1}^{r}n_i(n-n_i)^2\\
&+3(1-\alpha)^2\sum_{i=1}^{r}(n-n_i)\frac{n_i(n_i-1)}{2}+(1-\alpha)^3\sum_{i=1}^{r}n_i\sum_{s\neq i}n_s(n-n_s-n_i)\\
&=-\frac{\alpha^3}{4}\sum_{i=1}^{r}n_i^4+\left(\alpha^3\left(n-\frac{1}{2}\right)+3\alpha(1-\alpha)^2-\frac{3}{2}(1-\alpha)^2\right)\sum_{i=1}^{r}n_i^3\\
&-\left(\alpha^3\left(\frac{3n^2}{2}-\frac{3n}{2}+\frac{1}{4}\right)+6\alpha(1-\alpha)^2n-\frac{3}{2}(1-\alpha)^2(n+1)\right)\sum_{i=1}^{r}n_i^2\\
&+\alpha^3\left(n^4-\frac{3n^3}{2}+\frac{n^2}{2}\right)+3\alpha(1-\alpha)^2n^3-(1-\alpha)^2\frac{3n^2}{2}\\
&+(1-\alpha)^3\sum_{i=1}^{r}n_i\sum_{s\neq i}n_s(n-n_s-n_i),
\end{aligned}$$

with equality holding if and only if each V^i is a transitive tournament with n_i vertices. □

Unfortunately, the above expressions for the lower and upper bounds still contain n_i, and we see no way to get rid of these terms. Hence, we did not derive tight bounds for $SM_\alpha^3(G)$ similar to the bounds in Theorem 3.4. However, we can obtain such tight bounds for $SM_\alpha^3(G)$ among the join digraphs in $\mathcal{G}_{n,2}$.

Corollary 3.11. *Let $G=V^1\vee V^2$. Then*

(i) $SM_\alpha^3(G)\geq\alpha^3\left(n^3+8n-16\right)+3\alpha^2(-2n^2+3n-2)+3\alpha(n^2-3n+4)+3(n-2)$,

with equality holding if and only if V^1 and V^2 are in-trees with $n_1 = n-1$ and $n_2 = 1$.

$$\text{(ii) } SM_\alpha^3(G) \leq \begin{cases} \frac{1}{32}\big[\alpha^3(15n^4-4n^3+12n^2)-12\alpha^2(3n^3+2n^2) \\ +48\alpha n^2+12(n^3-2n^2)\big], & \text{if } n \text{ is even,} \\ \frac{1}{32}\big[\alpha^3(15n^4-4n^3+6n^2-12n-5) \\ -12\alpha^2(3n^3+2n^2-3n-2) \\ +48\alpha(n^2-1)+12(n^3-2n^2-n+2)\big], & \text{if } n \text{ is odd,} \end{cases}$$

with equality holding if and only if V^1 and V^2 are transitive tournaments with $n_1 = \left\lceil \frac{n}{2} \right\rceil$ and $n_2 = \left\lfloor \frac{n}{2} \right\rfloor$.

Proof.

(i) If $r=2$, $n = n_1+n_2$. Let $n_2 = x$ and $n_1 = n-x$, where $1 \leq n_2 \leq \left\lfloor \frac{n}{2} \right\rfloor$. Using Theorem 3.10, we only need to consider

$$\begin{aligned} &-\alpha^3\left(x^4+(n-x)^4\right)+3\left(\alpha^3(n+1)+\alpha(1-\alpha)^2\right)\left(x^3+(n-x)^3\right) \\ &-3\left(\alpha^3(n^2+2n+2)+2\alpha(1-\alpha)^2n+(1-\alpha)^2\right)\left(x^2+(n-x)^2\right). \end{aligned}$$

Let $f(x) = a\left(x^4+(n-x)^4\right)+b\left(x^3+(n-x)^3\right)+c\left(x^2+(n-x)^2\right)$, where $a=-\alpha^3$, $b=3\big(\alpha^3(n+1)+\alpha(1-\alpha)^2\big)$ and $c=-3\big(\alpha^3(n^2+2n+2)+2\alpha(1-\alpha)^2n+(1-\alpha)^2\big)$. Then

$$\begin{aligned} f(x) = {} & 2ax^4-4anx^3+(6an^2+3bn+2c)x^2-(4an^3+3bn^2+2cn)x \\ & +(an^4+bn^3+cn^2). \end{aligned}$$

Next, we prove that $f(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$.

When $1 \leq x \leq \frac{n}{2}$, since

$$f'(x) = 8ax^3-12anx^2+2(6an^2+3bn+2c)x-(4an^3+3bn^2+2cn),$$

$$f''(x) = 24ax^2-24anx+2(6an^2+3bn+2c)$$

and

$$f'''(x) = 48ax-24an \geq 0,$$

$f''(x)$ is an increasing function and

$$\begin{aligned} f''(x)_{max} &= f''(\frac{n}{2}) = 6an^2 + 6bn + 4c \\ &= -6\alpha(2\alpha^2 - 2\alpha + 1)n - 12(2\alpha^3 + \alpha^2 - 2\alpha + 1). \end{aligned}$$

Since $2\alpha^2 - 2\alpha + 1 > 0$ and $2\alpha^3 + \alpha^2 - 2\alpha + 1 > 0$ when $\alpha \in [0, 1)$, $f''(x) \leq 0$. So $f'(x)$ is a decreasing function and

$$f'(x)_{min} = f'(\frac{n}{2}) = 0.$$

Hence, $f'(x) \geq 0$ and $f(x)$ is an increasing function when $1 \leq x \leq \frac{n}{2}$, and consequently

$$\begin{aligned} f(x) \geq f(1) = &-\alpha^3 \left(n^4 + 5n^3 + 3n^2 - 10n + 14\right) + 3\alpha^2(2n^3 - 3n^2 + 4n - 2) \\ &- 3\alpha(n^3 - 3n^2 + 5n - 4) - 3(n^2 - 2n + 2). \end{aligned}$$

Concluding, $SM^3_\alpha(G)$ is minimal when $n_1 = n - 1$ and $n_2 = 1$. Thus,

$$SM^3_\alpha(G) \geq \alpha^3 \left(n^3 + 8n - 16\right) + 3\alpha^2(-2n^2 + 3n - 2) + 3\alpha(n^2 - 3n + 4) + 3(n - 2),$$

with equality holding if and only if V^1 and V^2 are in-trees with $n_1 = n - 1$ and $n_2 = 1$.

(ii) Similarly as in the proof of (i), if $r = 2$, $n = n_1 + n_2$. Let $n_2 = x$ and $n_1 = n - x$, where $1 \leq n_2 \leq \left\lfloor \frac{n}{2} \right\rfloor$. Using Theorem 3.10, we only need to consider

$$\begin{aligned} &-\frac{\alpha^3}{4}\left(x^4 + (n-x)^4\right) + \left(\alpha^3\left(n - \frac{1}{2}\right) + 3\alpha(1-\alpha)^2 - \frac{3}{2}(1-\alpha)^2\right)\left(x^3 + (n-x)^3\right) \\ &-\left(\alpha^3\left(\frac{3n^2}{2} - \frac{3n}{2} + \frac{1}{4}\right) + 6\alpha(1-\alpha)^2 n - \frac{3}{2}(1-\alpha)^2(n+1)\right)\left(x^2 + (n-x)^2\right). \end{aligned}$$

Let $g(x) = a'\left(x^4 + (n-x)^4\right) + b'\left(x^3 + (n-x)^3\right) + c'\left(x^2 + (n-x)^2\right)$, where $a' = -\frac{\alpha^3}{4}$, $b' = \alpha^3\left(n - \frac{1}{2}\right) + 3\alpha(1-\alpha)^2 - \frac{3}{2}(1-\alpha)^2$ and $c = -\big(\alpha^3\big(\frac{3n^2}{2} -$

$\frac{3n}{2}+\frac{1}{4})+6\alpha(1-\alpha)^2 n-\frac{3}{2}(1-\alpha)^2(n+1)\big)$. Then

$$g(x)=2a'x^4-4a'nx^3+(6a'n^2+3b'n+2c')x^2 \\ -(4a'n^3+3b'n^2+2c'n)x+(a'n^4+b'n^3+c'n^2).$$

Next, we prove that $g(x)$ is an increasing function when $1\le x\le \frac{n}{2}$.

When $1\le x\le \frac{n}{2}$, since

$$g'(x)=8a'x^3-12a'nx^2+2(6a'n^2+3b'n+2c')x-(4a'n^3+3b'n^2+2c'n),$$

$$g''(x)=24a'x^2-24a'nx+2(6a'n^2+3b'n+2c')$$

and

$$g'''(x)=48a'x-24a'n\ge 0,$$

$g''(x)$ is an increasing function and

$$\begin{aligned} g''(x)_{max} &= g''(\frac{n}{2})=6a'n^2+6b'n+4c' \\ &= -\left(3\alpha^3\left(\frac{n}{2}+1\right)-9\alpha^2+1\right)n-\alpha(\alpha^2-6\alpha+12)-(2n-6). \end{aligned}$$

If $n=3$, $g''(\frac{n}{2})=-\frac{47}{2}\alpha^3+33\alpha^2-12\alpha-3<0$ when $\alpha\in[0,1)$. If $n=4$, $g''(\frac{n}{2})=-37\alpha^3+42\alpha^2-12\alpha-6<0$ when $\alpha\in[0,1)$. Next, we show that also in case $n\ge 5$, $g''(\frac{n}{2})<0$ when $\alpha\in[0,1)$.

For this, we use the help function $h(x)=3\left(\frac{n}{2}+1\right)x^3-9x^2+1$. Then $h'(x)=9\left(\frac{n}{2}+1\right)x^2-18x=\frac{9}{2}x((n+2)x-4)$. If $h'(x)=0$, then $x=0$ or $x=\frac{4}{n+2}$. $h(x)$ is decreasing on $[0,\frac{4}{n+2}]$ and increasing on $[\frac{4}{n+2},1)$. So $h(x)_{min}=h(\frac{4}{n+2})=\frac{n^2+4n-44}{(n+2)^2}>0$ if $n\ge 5$.

Hence, if $n\ge 5$, $g''(\frac{n}{2})\le 0$ since $h(x)>0$, $\alpha^2-6\alpha+12>0$ and $2n-6>0$ when $\alpha\in[0,1)$. So $g'(x)$ is a decreasing function and

$$g'(x)_{min}=g'(\frac{n}{2})=0.$$

Hence, $g'(x)\ge 0$ and $g(x)$ is an increasing function when $1\le x\le \frac{n}{2}$, and consequently $g(x)\le g(\frac{n}{2})$.

Concluding, $SM^3_\alpha(G)$ is maximal when $n_1 = n_2 = \frac{n}{2}$ if n is even, and $n_1 = \frac{n+1}{2}$, $n_2 = \frac{n-1}{2}$ if n is odd. If n is even,

$$g(\frac{n}{2}) = \frac{1}{32}\big[-\alpha^3(17n^4+52n^3+4n^2)+12\alpha^2(13n^3+2n^2) \\ -48\alpha(2n^3+n^2)+12(n^3+2n^2)\big].$$

If n is odd,

$$g(\frac{n}{2}) = \frac{1}{32}\big[-\alpha^3(17n^4+52n^3+10n^2+12n+5)+12\alpha^2(13n^3+2n^2+3n+2) \\ -48\alpha(2n^3+n^2+1)+12(n^3+2n^2-n+2)\big].$$

Thus,

$$SM^3_\alpha(G) \leq \begin{cases} \frac{1}{32}\big[\alpha^3(15n^4-4n^3+12n^2)-12\alpha^2(3n^3+2n^2) & \\ +48\alpha n^2+12(n^3-2n^2)\big], & \text{if } n \text{ is even,} \\ \frac{1}{32}\big[\alpha^3(15n^4-4n^3+6n^2-12n-5) & \\ -12\alpha^2(3n^3+2n^2-3n-2) & \\ +48\alpha(n^2-1)+12(n^3-2n^2-n+2)\big], & \text{if } n \text{ is odd,} \end{cases}$$

with equality holding if and only if V^1 and V^2 are transitive tournaments with $n_1 = \left\lceil \frac{n}{2} \right\rceil$ and $n_2 = \left\lfloor \frac{n}{2} \right\rfloor$. □

3.4 Conclusion

In this chapter, we compared the second and third spectral moments of $L(G)$ and $A_\alpha(G)$, and extended the results we obtained in Chapter 2 for $L(G)$ to $A_\alpha(G)$. There are similarities and differences. Some results for the A_α spectral moments could be obtained directly from similar results for the Laplacian spectral moments. But several results required new proofs, and not all questions have been answered. We like to finish this chapter by recalling some of the open problems for future research.

With respect to the lower bounds and minimal digraphs for the A_α energy, Theorem 3.6 shows that the results for the A_α energy are the same as for the Laplacian energy when $\alpha \in [\frac{1}{2}, 1)$. However, when $\alpha \in [0, \frac{1}{2})$ they might be different, and for the interval $\alpha \in [0, \frac{1}{4}]$ we illustrated the difference by concrete examples. We do not know whether such examples exist for $\alpha \in (\frac{2\sqrt{2}-1}{7}, \frac{1}{2})$, and leave this as an open problem. We also did not obtain a full characterization of the minimal digraphs for the A_α energy among all digraphs with a fixed dichromatic number. So we leave this as another open problem.

Chapter 4

Bounds for the A_α spectral radius of digraphs

In this chapter, we characterize the digraph which has the maximal A_α spectral radius within classes of digraphs with a fixed dichromatic number by using a new method: the equitable quotient matrix. This provides a new proof of the results by Liu et al. [89]. Moreover, we obtain the digraph which has the minimal A_α spectral radius of the join of in-trees with a fixed dichromatic number.

4.1 Introduction

Recall that the A_α-matrix of a digraph G as

$$A_\alpha(G) = \alpha D^+(G) + (1-\alpha)A(G),$$

where $\alpha \in [0,1)$. In 2019, Liu et al. [89] characterized the digraph which has the maximal A_α spectral radius with given dichromatic number. As we know, the A_α-matrix is a natural common extension of the adjacency matrix $A(G) = A_0(G)$ and the signless Laplacian matrix $Q(G) = 2A_{\frac{1}{2}}(G)$. In 2011, Lin and Shu [78] characterized the digraph which has the maximal spectral radius with given dichromatic number. In 2017, Xi and Wang [132], Li and You [74] characterized the extremal digraph which has the maximum signless Laplacian spectral radius of digraphs with given dichromatic number, independently. The maximal digraphs of the above results is the same, and that maximal digraph is the join digraph $G = \bigvee_{i=1}^{r} V^i$ which each V^i is a transitive tournament with $|n_i - n_j| \leq 1$. Moreover, the proof methods in [74, 78, 89, 132] are similar. They both use Perron-Frobenius Theorem.

Recently, Kim et al. [62] proved a tight upper bound for the spectral radius of digraphs in terms of the number of vertices and the dichromatic number. They provided a new proof of the results by Lin and Shu [78] and the new method is equitable quotient matrix. From this, we will wonder whether A_α-matrix can also apply the equitable quotient matrix. Actually, it is true. And we characterize the digraph which has the maximal A_α spectral radius within classes of digraphs in $\mathscr{G}_{n,r}$ by using equitable quotient matrix, which provides a new proof of the results by Liu et al. [89].

All of these are depictions of the upper bound for spectral radius of digraphs in $\mathscr{G}_{n,r}$. On the lower bound, in 2007, Feng et al. [36] proved that, among all graphs with given chromatic numbers, the Turán graph has the maximal spectral radius; and the path P_n if $r = 2$, the cycle C_n if $r = 3$ and n is odd, C_{n-1}^1 if $r = 3$ and n is even, $K_r^{(\ell)}$ if $r \geq 4$ has the minimal spectral radius, where C_{n-1}^1 is obtained from the cycle C_{n-1} by adding one pendent vertex and $K_r^{(\ell)}$ is obtained by joining a path of order ℓ to the complete graph K_r. In 2010, Mohar [96] gave a lower bound on the spectral radius for digraphs with given dichromatic number. He obtained

$$\chi(G) \leq \rho_A(G) + 1,$$

if G is strongly connected, then the equality holds if and only if G is one of the digraphs listed in cases (i)-(iii) in Lemma 1.2 for $r = \chi(G)$. In 2013, Lin and Shu [79] determined the extremal digraph with the minimal distance spectral radius with given dichromatic number. This minimal digraph is also the join digraph $G = \bigvee_{i=1}^{r} V^i$ which each V^i is a transitive tournament with $|n_i - n_j| \leq 1$.

In Chapters 2 and 3, the digraphs attaining the maximal Laplacian energy and maximal A_α energy in $\mathscr{G}_{n,r}$ are the join of transitive tournaments with

$|n_i - n_j| \leq 1$. On the other hand, the digraphs attaining the minimal Laplacian energy and minimal A_α energy in $\mathscr{G}_{n,r}$ are different from the maximal ones. But this minimal digraphs are related to in-trees and the digraphs listed in cases (i)-(iii) in Lemma 1.2. Since we have found the digraph which has the maximal A_α spectral radius among all digraphs in $\mathscr{G}_{n,r}$, we also want to find the digraph which has the minimal A_α spectral radius. But we can not find this extremal digraphs. However, in Chapters 2 and 3, we also determine the minimal join digraphs in $\mathscr{G}_{n,r}$ for the second and third Laplacian spectral moments and A_α spectral moments. And the minimal join digraphs are the join of in-trees. This is another motivation for us to study.

Recall that the in-tree is a directed tree for which the outdegree of each vertex is at most one. And an in-tree has exactly one vertex with outdegree 0, and such a vertex is called the root of the in-tree. This is also a class of digraphs. Especially, the directed path and the in-star are also in-trees. Hence we want to find the digraph which has the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,r}$.

First, we give a small result about A_α eigenvalues of acyclic digraphs.

Theorem 4.1. *Let G be an acyclic digraph of order n. Then $\lambda_{\alpha i} = \alpha d_i^+$ for all $i = 1, 2, \ldots, n$.*

Proof. From Lemma 1.8, any acyclic digraph admits a topological ordering, i.e., an ordering of its vertices $\{v_1, v_2, \ldots, v_n\}$ such that for every arc (v_i, v_j), we have $i < j$. So the A_α-matrix of an acyclic digraph is an upper triangular matrix. Obviously, $|xI_n - A_\alpha(G)| = \Pi_{i=1}^n (x - \alpha d_i^+)$. Then $\lambda_{\alpha i} = \alpha d_i^+$ for all $i = 1, 2, \ldots, n$. $\square$

Since the A_α eigenvalue of an acyclic digraph is $\lambda_{\alpha i} = \alpha d_i^+$, we get $\rho_\alpha(G) = \alpha \Delta^+(G)$ in $\mathscr{G}_{n,1}$. Therefore we only consider the cases when $r \geq 2$.

In this chapter, the organization is as follows. In Section 4.2, we characterize the digraph which has the maximal A_α spectral radius among all digraphs in $\mathscr{G}_{n,r}$ by using the equitable quotient matrix. Note that Liu et al. [89] obtained this results by using the Perron-Frobenius Theorem. In Section 4.3, we obtain the digraph which has the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,r}$.

4.2 The maximal A_α spectral radius of digraphs

In this section, we will consider the maximal A_α spectral radius of digraphs in $\mathscr{G}_{n,r}$. Using the Perron-Frobenius Theorem, this result has been proved by Liu et al. [89], but we give a new proof by using the equitable quotient matrix. First, to finding the maximal A_α spectral radius of join digraphs $\bigvee_{i=1}^{r} V^i$ in $\mathscr{G}_{n,r}$, we also need the following lemma.

Lemma 4.2 (Liu, Wu, Chen and Liu [89])**.** *Let G be a strongly connected digraph with the A_α spectral radius $\rho_\alpha(G)$ and maximal outdegree $\Delta^+(G)$. If G' is a proper subdigraph of G, then $\rho_\alpha(G) > \rho_\alpha(G')$, especially, $\rho_\alpha(G) > \alpha\Delta^+(G)$.*

Theorem 4.3. *Let $G = \bigvee_{i=1}^{r} V^i$. Then $\rho_\alpha(G)$ is maximal if and only if each V^i is a transitive tournament with $|n_i - n_j| \leq 1$.*

Proof. By Lemma 4.2, we know that adding the arcs will increase the A_α spectral radius. So the transitive tournament has the maximum A_α spectral radius in acyclic digraphs. That is, the join digraph $G = \bigvee_{i=1}^{r} V^i$ has the maximal A_α spectral radius in $\mathscr{G}_{n,r}$ if and only if each V^i is a transitive tournament. Hence we only need to consider the size of each n_i.

Let $G^T = \bigvee_{i=1}^{r} V^i$ which each V^i is a transitive tournament with n_i vertices and $n_1 \geq n_2 \geq \cdots \geq n_r$. By Lemma 1.8, we obtain a vertex ordering $\{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ of each transitive tournament V^i such that $(v_s^i, v_t^i) \in \mathscr{A}(G^T)$, for all $s < t$ and $i = 1, 2, \ldots, r$. Then $d_{G^T}^+(v_j^i) = n - j$. For each $j = 1, 2, \ldots, n_1$, let $A_j = \{v_j^i | i = 1, 2, \ldots, r\}$ and $|A_j| = a_j$. Then the vertices in A_j have the same outdegree $n - j$. Let $B = B(G^T)$ be the quotient matrix of $A_\alpha(G^T)$, where B corresponds to the vertex partition $A_1, A_2, \ldots, A_{n_1}$. Then the quotient matrix B is equitable and

$$B_{ij} = \begin{cases} \alpha(n-j) + (1-\alpha)(a_j - 1), & \text{if } i = j, \\ (1-\alpha)a_j, & \text{if } i < j, \\ (1-\alpha)(a_j - 1), & \text{if } i > j. \end{cases}$$

The characteristic polynomial of B is

$$|xI_{n_1} - B| = \prod_{i=1}^{n_1}(x-\alpha(n-i)) - \sum_{j=1}^{n_1}\left((1-\alpha)(a_j-1)\prod_{i=1}^{j-1}(x-\alpha(n-i))\prod_{i=j+1}^{n_1}((1-\alpha)+x-\alpha(n-i))\right).$$

Note: if $j = n_1$, let $\prod_{i=j+1}^{n_1}((1-\alpha)+x-\alpha(n-i)) = 1$. (See Appendix 4.4 for detailed calculation.)

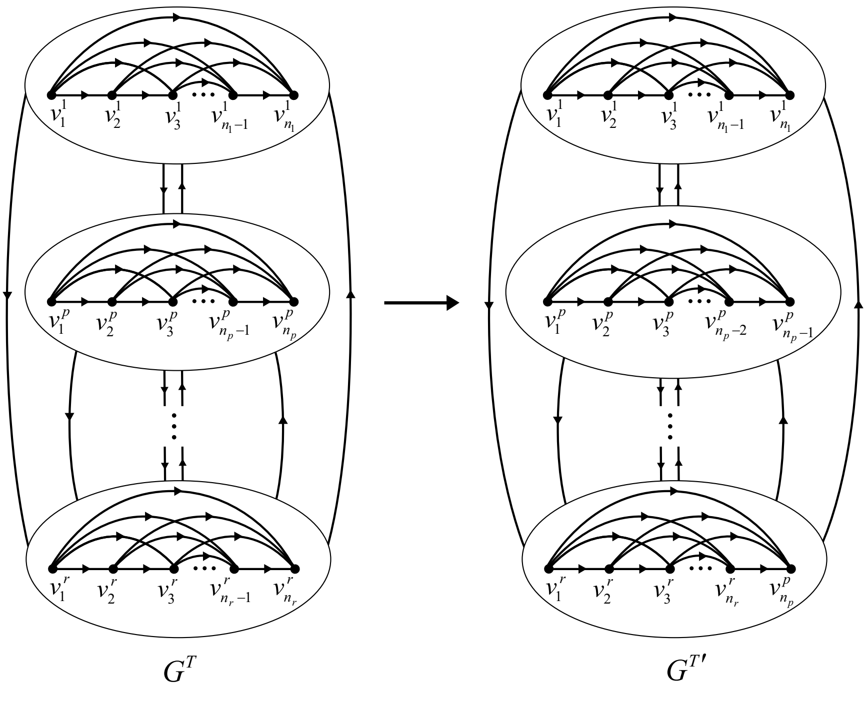


Figure 4.1: The digraphs G^T and $G^{T\prime}$.

Let

$$f(x) = f(x; n_1, \ldots, n_r) = \prod_{i=1}^{n_1}(x-\alpha(n-i)) - \sum_{j=1}^{n_1}\left((1-\alpha)(a_j-1)\prod_{i=1}^{j-1}(x-\alpha(n-i))\prod_{i=j+1}^{n_1}((1-\alpha)+x-\alpha(n-i))\right).$$

By Lemma 1.5, $\rho_\alpha(G^T)$ is an eigenvalue (multiplicity one) of $A_\alpha(G^T)$ and there is a corresponding eigenvector whose coordinates are all positive. And from Lemma 1.7, $\rho_\alpha = \rho_\alpha(G^T)$ is the root of $f(x)$ with the largest modulus. From Lemma 4.2, we know $\rho_\alpha > \alpha\Delta^+(G^T) = \alpha(n-1)$. For convenience, let

$$X_j^{n_1}(x) = \prod_{i=1}^{j-1}(x-\alpha(n-i)) \prod_{i=j+1}^{n_1}((1-\alpha)+x-\alpha(n-i)).$$

Let $G^{T*} = \bigvee_{i=1}^{r} V^i$ which each V^i is a transitive tournament with $|n_i - n_j| \leq 1$. Next we prove $\rho_\alpha(G^T) \leq \rho_\alpha(G^{T*})$. We assume that $G^T \neq G^{T*}$, then we have $n_1 \geq n_r + 2$. Let p be the largest index such that $n_1 = \cdots = n_p > n_{p+1} \geq \cdots \geq n_r$. See Figure 4.1, we do the following operation:

$$G^{T'} = G^T + \{(v_{n_p}^p, v_i^p) | i = 1,2,\ldots,n_p - 1\} - \{(v_{n_p}^p, v_j^r) | j = 1,2,\ldots,n_r\}.$$

Let $\rho'_\alpha = \rho_\alpha(G^{T'})$ be the root of $\tilde{f}(x)$ with the largest modulus, where $\tilde{f}(x) = f(x; n_1, \ldots, n_p - 1, \ldots, n_r + 1)$. Next, we will prove $\tilde{f}(\rho_\alpha) < 0$ by the following two cases.

Case 1. If $p \geq 2$, that is $n_1 = n_2 = \cdots = n_p$. Let

$$\begin{aligned}\tilde{f}(x) &= f(x; n_1, \ldots, n_p - 1, \ldots, n_r + 1)\\ &= \prod_{i=1}^{n_1}(x-\alpha(n-i)) - \sum_{j=1}^{n_1}\Big((1-\alpha)(a'_j - 1)X_j^{n_1}(x)\Big),\end{aligned}$$

where

$$a'_j = \begin{cases} a_j + 1, & \text{if } j = n_r + 1, \\ a_j - 1, & \text{if } j = n_1, \\ a_j, & \text{otherwise.}\end{cases}$$

Then

$$\begin{aligned}\tilde{f}(\rho_\alpha) = &\prod_{i=1}^{n_1}(\rho_\alpha - \alpha(n-i)) - \sum_{j=1, j\neq n_r+1}^{n_1-1}\Big((1-\alpha)(a_j-1)X_j^{n_1}(\rho_\alpha)\Big)\\ &-(1-\alpha)(a_{n_r+1}+1-1)X_{n_r+1}^{n_1}(\rho_\alpha) - (1-\alpha)(a_{n_1}-1-1)X_{n_1}^{n_1}(\rho_\alpha)\end{aligned}$$

$$
\begin{aligned}
&= \prod_{i=1}^{n_1}(\rho_\alpha - \alpha(n-i)) - \sum_{j=1}^{n_1}\Big((1-\alpha)(a_j-1)X_j^{n_1}(\rho_\alpha)\Big) \\
&- (1-\alpha)X_{n_r+1}^{n_1}(\rho_\alpha) + (1-\alpha)X_{n_1}^{n_1}(\rho_\alpha) \\
&= f(\rho_\alpha) - (1-\alpha)\left(X_{n_r+1}^{n_1}(\rho_\alpha) - X_{n_1}^{n_1}(\rho_\alpha)\right).
\end{aligned}
$$

Next,

$$
\begin{aligned}
& X_{n_r+1}^{n_1}(\rho_\alpha) - X_{n_1}^{n_1}(\rho_\alpha) \\
&= \prod_{i=1}^{n_r}(\rho_\alpha - \alpha(n-i)) \prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha - \alpha(n-i)) \\
&- \prod_{i=1}^{n_1-1}(\rho_\alpha - \alpha(n-i)) \prod_{i=n_1+1}^{n_1}((1-\alpha)+\rho_\alpha - \alpha(n-i)) \\
&= \prod_{i=1}^{n_r}(\rho_\alpha - \alpha(n-i)) \left(\prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha - \alpha(n-i)) - \prod_{i=n_r+1}^{n_1-1}(\rho_\alpha - \alpha(n-i))\right).
\end{aligned}
$$

Since $n_1 \geq n_r + 2$, we have

$$\rho_\alpha - \alpha(n-i) > \alpha\Delta^+(G^T) - \alpha(n-i) = \alpha(n-1) - \alpha(n-i) = \alpha(i-1) \geq 0 \; (i \geq 1),$$

$$(1-\alpha)+\rho_\alpha - \alpha(n-i) > (1-\alpha)+\alpha(i-1) = \alpha(i-2)+1 \geq 1 \; (i \geq n_r+2),$$

and

$$((1-\alpha)+\rho_\alpha - \alpha(n-n_1)) - (\rho_\alpha - \alpha(n-(n_r+1))) = \alpha(n_1 - n_r - 2) + 1 \geq 1.$$

Obviously,

$$(1-\alpha)+\rho_\alpha - \alpha(n-i) > \rho_\alpha - \alpha(n-i).$$

Then

$$
\begin{aligned}
& \prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha - \alpha(n-i)) - \prod_{i=n_r+1}^{n_1-1}(\rho_\alpha - \alpha(n-i)) \\
&= \prod_{i=n_r+2}^{n_1-1}((1-\alpha)+\rho_\alpha - \alpha(n-i)) - \prod_{i=n_r+2}^{n_1-1}(\rho_\alpha - \alpha(n-i))
\end{aligned}
$$

$$
\begin{aligned}
&+((1-\alpha)+\rho_\alpha-\alpha(n-n_1))-(\rho_\alpha-\alpha(n-(n_r+1))) \\
&>0.
\end{aligned}
$$

Hence $X_{n_r+1}^{n_1}(\rho_\alpha)-X_{n_1}^{n_1}(\rho_\alpha)>0$. Since $f(\rho_\alpha)=0$, we have $\tilde{f}(\rho_\alpha)<0$.

Case 2. If $p=1$, that is $n_1>n_2$. Let

$$
\begin{aligned}
\tilde{f}(x) &= f(x;n_1-1,\ldots,n_r+1) \\
&= \prod_{i=1}^{n_1-1}(x-\alpha(n-i))-\sum_{j=1}^{n_1-1}\left((1-\alpha)(a'_j-1)X_j^{n_1-1}(x)\right),
\end{aligned}
$$

where

$$
a'_j=\begin{cases} a_j+1, & \text{if } j=n_r+1,\\ a_j, & \text{otherwise.}\end{cases}
$$

Then

$$
\begin{aligned}
\tilde{f}(\rho_\alpha) = &\prod_{i=1}^{n_1-1}(\rho_\alpha-\alpha(n-i))-\sum_{j=1,j\neq n_r+1}^{n_1-1}\left((1-\alpha)(a_j-1)X_j^{n_1-1}(\rho_\alpha)\right) \\
&-(1-\alpha)(a_{n_r+1}+1-1)X_{n_r+1}^{n_1-1}(\rho_\alpha) \\
=&\prod_{i=1}^{n_1-1}(\rho_\alpha-\alpha(n-i))-\sum_{j=1}^{n_1-1}\left((1-\alpha)(a_j-1)X_j^{n_1-1}(\rho_\alpha)\right) \\
&-(1-\alpha)X_{n_r+1}^{n_1-1}(\rho_\alpha).
\end{aligned}
$$

Since

$$
f(\rho_\alpha)=\prod_{i=1}^{n_1}(\rho_\alpha-\alpha(n-i))-\sum_{j=1}^{n_1}\left((1-\alpha)(a_j-1)X_j^{n_1}(\rho_\alpha)\right),
$$

and

$$
X_j^{n_1}(\rho_\alpha)=((1-\alpha)+\rho_\alpha-\alpha(n-n_1))X_j^{n_1-1}(\rho_\alpha),
$$

we have

$$\begin{aligned}
&\tilde{f}(\rho_\alpha)\big((1-\alpha)+\rho_\alpha-\alpha(n-n_1)\big)\\
&=f(\rho_\alpha)+(1-\alpha)\prod_{i=1}^{n_1-1}(\rho_\alpha-\alpha(n-i))\\
&+(1-\alpha)(a_{n_1}-1)X_{n_1}^{n_1}(\rho_\alpha)-(1-\alpha)X_{n_r+1}^{n_1}(\rho_\alpha)\\
&=f(\rho_\alpha)+(1-\alpha)\prod_{i=1}^{n_1-1}(\rho_\alpha-\alpha(n-i))\\
&-(1-\alpha)\prod_{i=1}^{n_r}(\rho_\alpha-\alpha(n-i))\prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha-\alpha(n-i))\\
&=f(\rho_\alpha)+(1-\alpha)\prod_{i=1}^{n_r}(\rho_\alpha-\alpha(n-i))\\
&\left(\prod_{i=n_r+1}^{n_1-1}(\rho_\alpha-\alpha(n-i))-\prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha-\alpha(n-i))\right).
\end{aligned}$$

Since $n_1 \geq n_r+2$, we have

$$(\rho_\alpha-\alpha(n-n_r-1))-((1-\alpha)+\rho_\alpha-\alpha(n-n_1))=\alpha(n_r+2-n_1)-1<0.$$

Then we have

$$\begin{aligned}
&\prod_{i=n_r+1}^{n_1-1}(\rho_\alpha-\alpha(n-i))-\prod_{i=n_r+2}^{n_1}((1-\alpha)+\rho_\alpha-\alpha(n-i))\\
&=\prod_{i=n_r+2}^{n_1-1}(\rho_\alpha-\alpha(n-i))-\prod_{i=n_r+2}^{n_1-1}((1-\alpha)+\rho_\alpha-\alpha(n-i))\\
&+(\rho_\alpha-\alpha(n-n_r-1))-((1-\alpha)+\rho_\alpha-\alpha(n-n_1))\\
&<0.
\end{aligned}$$

So $\tilde{f}(\rho_\alpha)<0$.

As both $f(x)$ and $\tilde{f}(x)$ have the positive leading coefficients, $\tilde{f}(\rho_\alpha)<0$ implies that $\rho_\alpha<\rho'_\alpha$. We perform the above operation as many times as possible until $|n_1 - n_r| \leq 1$, which means that $\rho_\alpha(G)$ is maximal if and only if each V^i is a transitive tournament with $|n_i - n_j| \leq 1$. This completes the proof. $\square$

The next result characterizes the digraph which attains the maximal A_α spectral radius among all digraphs in $\mathscr{G}_{n,r}$. It is an easy consequence of Theorem 4.3.

Theorem 4.4. *Let G be a digraph in $\mathscr{G}_{n,r}$. Then $\rho_\alpha(G)$ is maximal if and only if $G = \bigvee_{i=1}^r V^i$ and each V^i is a transitive tournament with $|n_i - n_j| \leq 1$.*

4.3 The minimal A_α spectral radius of the join of in-trees

In this section, we will consider the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,r}$.

Theorem 4.5. *Let $G = \bigvee_{i=1}^r V^i$ be a join digraph in $\mathscr{G}_{n,r}$, which each V^i is an in-tree with n_i vertices. Then $\rho_\alpha(G)$ is minimal if and only if each V^i is an in-star with n_i vertices.*

Proof. Let $G^\star = \bigvee_{i=1}^r V^{i^\star}$ be a join digraph in $\mathscr{G}_{n,r}$, which each $V^{i^\star}$ is an in-star with n_i vertices. Let $\mathscr{V}(V^{i^\star}) = \{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ such that $(v_j^i, v_{n_i}^i) \in \mathscr{A}(G^\star)$, for all $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, n_i - 1$. Then $d_{G^\star}^+(v_j^i) = n - n_i + 1$ and $d_{G^\star}^+(v_{n_i}^i) = n - n_i$. Suppose that

$$\mathbf{x} = (x_1^1, x_2^1, \ldots, x_{n_1}^1, x_1^2, x_2^2, \ldots, x_{n_2}^2, \ldots, x_1^r, x_2^r, \ldots, x_{n_r}^r)^T$$

is a Perron vector of $G^\star$ corresponding to the A_α spectral radius $\rho_\alpha^\star = \rho_\alpha(G^\star)$, where x_j^i is the characteristic component corresponding to v_j^i for each $1 \leq i \leq r$ and $1 \leq j \leq n_i$.

Since $A_\alpha(G^\star)\mathbf{x} = \rho_\alpha^\star \mathbf{x}$, we have

$$\begin{cases} \alpha(n - n_i + 1)x_j^i + (1-\alpha)x_{n_i}^i + (1-\alpha)\sum_{s=1, s\neq i}^r \sum_{t=1}^{n_s} x_t^s = \rho_\alpha^\star x_j^i, \\ \alpha(n - n_i)x_{n_i}^i + (1-\alpha)\sum_{s=1, s\neq i}^r \sum_{t=1}^{n_s} x_t^s = \rho_\alpha^\star x_{n_i}^i, \end{cases}$$

where $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, n_i - 1$. Then we have

$$((1-\alpha) + \rho_\alpha^\star - \alpha(n - n_i))x_{n_i}^i = (\rho_\alpha^\star - \alpha(n - n_i + 1))x_j^i.$$

Obviously, $x_{n_i}^i < x_1^i = x_2^i = \cdots = x_{n_i-1}^i$ for all $i = 1, 2, \ldots, r$.

Next we prove $\rho_\alpha(G) \geq \rho_\alpha(G^\star)$. Suppose that $G \neq G^\star$, we can get the digraph G by changing many arcs in $G^\star$. We first consider the transformation of one arc. We do the transformation of an arbitrary arc $(v_j^i, v_{n_i}^i) \in \mathscr{A}(G^\star)$ for all $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, n_i - 1$. Without loss of generality, we consider the arc $(v_j^1, v_{n_1}^1)$. Let

$$G = G^\star - (v_j^1, v_{n_1}^1) + (v_s^1, v_t^1).$$

By the structural property of directed trees, the arc (v_s^1, v_t^1) only has three cases: $(v_s^1, v_t^1) = (v_j^1, v_t^1)$ or $(v_s^1, v_t^1) = (v_{n_1}^1, v_j^1)$ or $(v_s^1, v_t^1) = (v_s^1, v_j^1)$, where $s, t = 1, 2, \ldots, n_1 - 1$. Since the outdegree sequence of the in-tree is (1,1,...,1,0), the case $(v_s^1, v_t^1) = (v_s^1, v_j^1)$ is impossible. So we only discuss the two cases: $(v_j^1, v_{n_1}^1) \to (v_j^1, v_t^1)$ or $(v_j^1, v_{n_1}^1) \to (v_{n_1}^1, v_j^1)$.

Case 1. If $(v_j^1, v_{n_1}^1) \to (v_j^1, v_t^1)$. Since $x_{n_1}^1 < x_j^1 = x_t^1$, we obtain

$$(A_\alpha(G) - A_\alpha(G^\star))\mathbf{x} = (0, \ldots, 0, (1-\alpha)(x_t^1 - x_{n_1}^1), 0, \ldots, 0)^T > 0.$$

That is $A_\alpha(G)\mathbf{x} > A_\alpha(G^\star)\mathbf{x} = \rho_\alpha(G^\star)\mathbf{x}$. By Lemma 1.6, $\rho_\alpha(G) > \rho_\alpha(G^\star)$.

Case 2. If $(v_j^1, v_{n_1}^1) \to (v_{n_1}^1, v_j^1)$. We can find a digraph G' such that $G' \cong G$. Without loss of generality, let $v_j^1 = v_1^1$. Then we have $d_G^+(v_1^1) = n - n_1$ and $d_{G^\star}^+(v_{n_1}^1) = n - n_1$. Let G' be a digraph which switch the index of $v_{n_1}^1$ and v_1^1 in G. Then

$$\begin{aligned} G' = G &- (v_{n_1}^1, v_1^1) - \{(v_i^1, v_{n_1}^1) | i = 2, 3, \ldots, n_1 - 1\} \\ &+ (v_1^1, v_{n_1}^1) + \{(v_i^1, v_1^1) | i = 2, 3, \ldots, n_1 - 1\}. \end{aligned}$$

Obviously, $G' \cong G$ and

$$G' = G^\star - \{(v_i^1, v_{n_1}^1) | i = 2, 3, \ldots, n_1 - 1\} + \{(v_i^1, v_1^1) | i = 2, 3, \ldots, n_1 - 1\}.$$

Then we obtain

$$(A_\alpha(G')-A_\alpha(G^\star))\mathbf{x} = (0,(1-\alpha)(x_1^1-x_{n_1}^1),\dots,(1-\alpha)(x_1^1-x_{n_1}^1),0,\dots,0)^T > 0.$$

That is $A_\alpha(G')\mathbf{x} > A_\alpha(G^\star)\mathbf{x} = \rho_\alpha(G^\star)\mathbf{x}$. By Lemma 1.6, $\rho_\alpha(G') > \rho_\alpha(G^\star)$. So we have $\rho_\alpha(G) = \rho_\alpha(G') > \rho_\alpha(G^\star)$.

For the transformation of many arcs, similar to Case 2, we can find a digraph G such that $d_G^+(v_{n_i}^i) = n - n_i$ and $d_G^+(v_j^i) = n - n_i + 1$ for all $i = 1, 2, \dots, r$ and $j = 1, 2, \dots, n_i - 1$. Then the components of $(A_\alpha(G) - A_\alpha(G^\star))\mathbf{x}$ are 0 or $(1-\alpha)(x_j^i - x_{n_i}^i)$. So $(A_\alpha(G) - A_\alpha(G^\star))\mathbf{x} > 0$ always holds and $\rho_\alpha(G) > \rho_\alpha(G^\star)$.

To sum up the above, we have $\rho_\alpha(G) \geq \rho_\alpha(G^\star)$ with equality holding if and only if $G \cong G^\star$. □

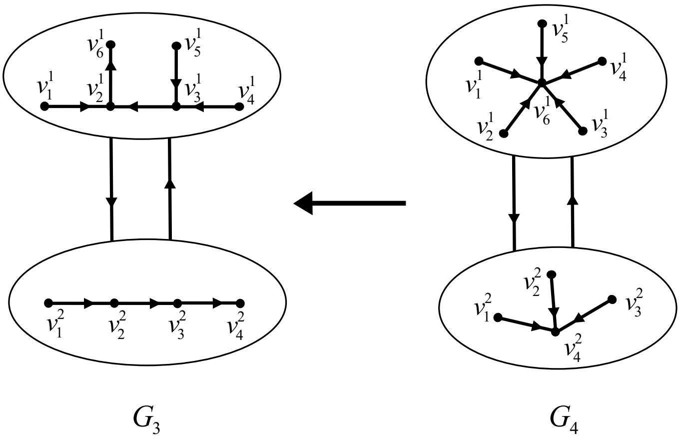


Figure 4.2: The digraphs G_3 and G_4.

To illustrate the transformation for Theorem 4.5 better, we give the following example.

Let $G_3 = V^1 \vee V^2$ and $G_4 = V^{1\star} \vee V^{2\star}$ be two digraphs shown in Figure 4.2. Then we can get the digraph G_3 by changing many arcs in the digraph G_4: $(v_1^1, v_6^1) \to (v_1^1, v_2^1)$, $(v_3^1, v_6^1) \to (v_3^1, v_2^1)$, $(v_4^1, v_6^1) \to (v_4^1, v_3^1)$, $(v_5^1, v_6^1) \to (v_5^1, v_3^1)$, $(v_1^2, v_4^2) \to (v_1^2, v_2^2)$, $(v_2^2, v_4^2) \to (v_2^2, v_3^2)$. From Theorem 4.5, we have $(A_\alpha(G_3) - A_\alpha(G_4))\mathbf{x} = \{(1-\alpha)(x_2^1 - x_6^1), 0, (1-\alpha)(x_2^1 - x_6^1), (1-\alpha)(x_3^1 -$

$x_6^1), (1-\alpha)(x_3^1 - x_6^1), 0, (1-\alpha)(x_2^2 - x_4^2), (1-\alpha)(x_3^2 - x_4^2), 0, 0\} > 0$. So $\rho_\alpha(G_3) > \rho_\alpha(G_4)$.

Unfortunately, we can not get a concrete digraph which has the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,r}$, liking Theorem 4.3. We also can not get this minimal digraph in $\mathscr{G}_{n,2}$. But we obtain the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,2}$ when $\alpha = 0$ or $\alpha = \frac{1}{2}$. Notice, the A_0 spectral radius is adjacency spectral radius and the $A_{\frac{1}{2}}$ spectral radius is the half of signless Laplacian spectral radius.

Theorem 4.6. *Let $G = V^1 \vee V^2$ be a join digraph in $\mathscr{G}_{n,2}$ which each V^i is an in-tree with n_i vertices. Then $\rho_0(G)$ is minimal if and only if V^1 and V^2 are in-stars with $n_1 = n-1$ and $n_2 = 1$.*

Proof. Let $G^\star = V^{1^\star} \vee V^{2^\star}$ which $V^{1^\star}$ and $V^{2^\star}$ are in-stars and $n_1 \geq n_2$. By Theorem 4.5, we know that the digraph which has the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,2}$ if and only if each V^i is an in-star with n_i vertices. So we only need to consider the size of n_i of $G^\star$. Obviously, $\left\lceil \frac{n}{2} \right\rceil \leq n_1 \leq n-1$, $1 \leq n_2 \leq \left\lfloor \frac{n}{2} \right\rfloor$. And $d^+_{G^\star}(v^i_j) = n - n_i + 1$ and $d^+_{G^\star}(v^i_{n_i}) = n - n_i$, where $i = 1,2$ and $j = 1,2,\ldots,n_i - 1$. Let $A_{11} = \{v^1_j | j = 1,2,\ldots,n_1 - 1\}$, $A_{12} = \{v^1_{n_1}\}$, $A_{21} = \{v^2_j | j = 1,2,\ldots,n_2 - 1\}$ and $A_{22} = \{v^2_{n_2}\}$. Let $B_A = B_A(G^\star)$ be the quotient matrix of $A(G^\star)$, where B_A corresponds to the vertex partition $A_{11}, A_{12}, A_{21}, A_{22}$. Then the quotient matrix B_A is equitable. Next we consider the cases when $n_1 > n_2 > 1$, $n_1 = n_2$ and $n_1 = n-1$, $n_2 = 1$.

Case 1. If $n_1 > n_2 > 1$, then the equitable quotient matrix B_A as follows:

$$B_A = \begin{pmatrix} 0 & 1 & n_2 - 1 & 1 \\ 0 & 0 & n_2 - 1 & 1 \\ n_1 - 1 & 1 & 0 & 1 \\ n_1 - 1 & 1 & 0 & 0 \end{pmatrix}.$$

The characteristic polynomial of B_A is

$$|xI_4 - B_A| = x^4 - n_1 n_2 x^2 + (n - 2n_1 n_2)x + (n - n_1 n_2 - 1).$$

Let

$$f_A(x) = f_A(x; n_1, n_2) = x^4 - n_1 n_2 x^2 + (n - 2n_1 n_2)x + (n - n_1 n_2 - 1).$$

By using the Perron-Frobenius Theorem, $\rho_A(G^\star)$ is an eigenvalue (multiplicity one) of $A(G^\star)$ and there is a corresponding eigenvector whose coordinates are all positive. And from Lemma 1.7, $\rho_A^\star = \rho_A(G^\star)$ is the root of $f_A(x)$ with the largest modulus.

Next we prove $\rho_A(G^\star)$ is minimal if and only if $V^{1^\star}$ and $V^{2^\star}$ are in-stars with $n_1 = n - 1$ and $n_2 = 1$. We move one of the vertices in $V^{1^\star}$ (except for the vertex $v^1_{n_1}$) to $V^{2^\star}$. Without loss of generality, let that vertex be v^1_1. That is

$$\begin{aligned} G' = & G^\star - (v^1_1, v^1_{n_1}) - \{(v^1_1, v^2_s) | s = 1, 2, \ldots, n_2\} - \{(v^2_s, v^1_1) | s = 1, 2, \ldots, n_2\} \\ & + (v^1_1, v^2_{n_2}) + \{(v^1_t, v^1_1) | t = 2, \ldots, n_1\} + \{(v^1_1, v^1_t) | t = 2, \ldots, n_1\}. \end{aligned}$$

Let $\rho'_A = \rho_A(G')$ be the root of $\tilde{f}_A(x)$ with the largest modulus, where $\tilde{f}_A(x) = f_A(x; n_1 - 1, n_2 + 1) = x^4 - (n_1 - 1)(n_2 + 1)x^2 + (n - 2(n_1 - 1)(n_2 + 1))x + (n - (n_1 - 1)(n_2 + 1) - 1)$. Then

$$\tilde{f}_A(\rho^\star_A) = f_A(\rho^\star_A) + (n_2 + 1 - n_1)\left(\rho^\star_A + 1\right)^2.$$

We know $f_A(\rho^\star_A) = 0$ and $n_1 > n_2 > 1$. If $n_2 + 1 - n_1 = 0$, then $n > 2$ is odd and $n_1 = \frac{n+1}{2}$, $n_2 = \frac{n-1}{2}$. That is $G' = G^\star$. If $n_2 + 1 - n_1 < 0$, then $\tilde{f}_A(\rho^\star_A) < 0$.

As both $f_A(x)$ and $\tilde{f}_A(x)$ have the positive leading coefficients, $\tilde{f}_A(\rho^\star_A) < 0$ implies that $\rho^\star_A < \rho'_A$. So the A_0 spectral radius with n_1 and n_2 is smaller than the A_0 spectral radius with $n_1 - 1$ and $n_2 + 1$. That is when $n_1 = n - 2$ and $n_2 = 2$, the A_0 spectral radius is minimal.

Case 2. If $n_1 = n_2 > 1$, then $n > 2$ is even and $n_1 = n_2 = \frac{n}{2}$. By Case 1, we know the A_0 spectral radius with $n_1 = n_2 = \frac{n}{2}$ is bigger than the A_0 spectral radius with $n_1 = \frac{n}{2} + 1$ and $n_2 = \frac{n}{2} - 1$. So when $n_1 = n - 2$ and $n_2 = 2$, the A_0 spectral radius is minimal.

Case 3. If $n_1 = n-1$ and $n_2 = 1$, then the equitable quotient matrix B'_A is

$$B'_A = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ n-2 & 1 & 0 \end{pmatrix}.$$

From Lemma 1.3, we have $\rho(B'_A) = \rho(B''_A) < \rho(B_A)$, where B_A with $n_1 = n-1$, $n_2 = 1$ and

$$B''_A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ n-2 & 1 & 0 & 0 \end{pmatrix}.$$

By Case 1, the A_0 spectral radius with $n_1 = n-2$ and $n_2 = 2$ is bigger than the A_0 spectral radius with $n_1 = n-1$ and $n_2 = 1$. So when $n_1 = n-1$ and $n_2 = 1$, the A_0 spectral radius is minimal.

Hence, $\rho_0(G)$ is minimal if and only if V^1 and V^2 are in-stars with $n_1 = n-1$ and $n_2 = 1$. □

Theorem 4.7. *Let $G = V^1 \vee V^2$ be a join digraph in $\mathcal{G}_{n,2}$ which each V^i is an in-tree with n_i vertices. Then $\rho_{\frac{1}{2}}(G)$ is minimal if and only if V^1 and V^2 are in-stars with $n_1 = n-1$ and $n_2 = 1$.*

Proof. Similar to the proof of Theorem 4.6, we only need to consider the size of n_i of $G^\star$. Let $B_Q = B_Q(G^\star)$ be the equitable quotient matrix of $Q(G^\star)$, where B_Q corresponds to the vertex partition $A_{11}, A_{12}, A_{21}, A_{22}$. We also omit the category discussion about n_1 and n_2.

If $n_1 > n_2 > 1$, then the equitable quotient matrix B_Q as follows:

$$B_Q = \begin{pmatrix} n_2+1 & 1 & n_2-1 & 1 \\ 0 & n_2 & n_2-1 & 1 \\ n_1-1 & 1 & n_1+1 & 1 \\ n_1-1 & 1 & 0 & n_1 \end{pmatrix}.$$

The characteristic polynomial of B_Q is

$$\begin{aligned}|xI_4 - B_Q| = x^4 &- (2+2n)x^3 + (1+3n+n^2+n_1n_2)x^2 \\ &+ (n-n^2-4n_1n_2-n_1n_2n)x \\ &+ (-4+2n-4n_1n_2+2n_1n_2n).\end{aligned}$$

Let

$$\begin{aligned}f_Q(x) = f_Q(x;n_1,n_2) = x^4 - (2+2n)x^3 + (1+3n+n^2+n_1n_2)x^2 \\ + (n-n^2-4n_1n_2-n_1n_2n)x + (-4+2n-4n_1n_2+2n_1n_2n).\end{aligned}$$

By the Perron-Frobenius Theorem, $\rho_Q(G^\star)$ is an eigenvalue (multiplicity one) of $Q(G^\star)$ and there is a corresponding eigenvector whose coordinates are all positive. And from Lemma 1.7, $\rho_Q^\star = \rho_Q(G^\star)$ is the root of $f_Q(x)$ with the largest modulus.

Next we prove $\rho_Q(G^\star)$ is minimal if and only if $V^{1^\star}$ and $V^{2^\star}$ are in-stars with $n_1 = n-1$ and $n_2 = 1$. We move one of the vertices in $V^{1^\star}$ (except for the vertex $v^1_{n_1}$) to $V^{2^\star}$. The operation is same to the Theorem 4.6, so we omit it. Let $\rho'_Q = \rho_Q(G')$ be the root of $\tilde{f}_Q(x)$ with the largest modulus, where

$$\begin{aligned}\tilde{f}_Q(x) &= f_Q(x;n_1-1,n_2+1) \\ &= x^4 - (2+2n)x^3 + (1+3n+n^2+(n_1-1)(n_2+1))x^2 \\ &+ (n-n^2-4(n_1-1)(n_2+1)-(n_1-1)(n_2+1)n)x \\ &+ (-4+2n-4(n_1-1)(n_2+1)+2(n_1-1)(n_2+1)n).\end{aligned}$$

Then

$$\tilde{f}_Q(\rho_Q^\star) = f_Q(\rho_Q^\star) + (n_1-n_2-1)\left((\rho_Q^\star)^2 - (4+n)\rho_Q^\star + 2(n-2)\right).$$

Since $n_1 > n_2 > 1$ and $f_Q(\rho_Q^\star) = 0$, to prove $\tilde{f}_Q(\rho_Q^\star) < 0$ implies that $(\rho_Q^\star)^2 - (4+n)\rho_Q^\star + 2(n-2) < 0$. That is

$$\frac{4+n-\sqrt{32+n^2}}{2} < \rho_Q^\star < \frac{4+n+\sqrt{32+n^2}}{2}.$$

Since $f_Q(n+2) = 4(3n + n_1^2 + n_2^2) > 0$ and $f_Q(n) = -2(n+2)(n_1 - 1)(n_2 - 1) < 0$, we get $n < \rho_Q^\star < n+2$. Because $\frac{4+n-\sqrt{32+n^2}}{2} < n$ and $n+2 < \frac{4+n+\sqrt{32+n^2}}{2}$ are always true, $\tilde{f}_Q(\rho_Q^\star) < 0$. Then $\rho_Q' > \rho_Q^\star$.

Therefore, similar to the proof of Theorem 4.6, when $n_1 = n-1$ and $n_2 = 1$, the $A_{\frac{1}{2}}$ spectral radius is minimal. That is, $\rho_{\frac{1}{2}}(G)$ is minimal if and only if V^1 and V^2 are in-stars with $n_1 = n-1$ and $n_2 = 1$. $\square$

From the proof of Theorems 4.6 and 4.7, we know the equitable quotient matrix B_α of A_α matrix of the join of in-stars in $\mathscr{G}_{n,2}$ as follows:

$$B_\alpha = \begin{pmatrix} \alpha(n_2+1) & 1-\alpha & (1-\alpha)(n_2-1) & 1-\alpha \\ 0 & n_2\alpha & (1-\alpha)(n_2-1) & 1-\alpha \\ (1-\alpha)(n_1-1) & 1-\alpha & \alpha(n_1+1) & 1-\alpha \\ (1-\alpha)(n_1-1) & 1-\alpha & 0 & \alpha n_1 \end{pmatrix}.$$

From Tables 4.1 and 4.2, we take two examples about the A_α spectral radius of the join of in-stars in $\mathscr{G}_{7,2}$ and $\mathscr{G}_{10,2}$ when $\alpha = \frac{1}{6}, \frac{3}{10}, \frac{1}{2}, \frac{11}{20}, \frac{3}{5}, \frac{8}{11}, \frac{6}{7}$.

From Table 4.1, with n_1 increases and n_2 decreases, the A_α spectral radius of the join of in-stars is decreasing when $\alpha = \frac{1}{6}, \frac{3}{10}, \frac{1}{2}, \frac{11}{20}$. But when $\alpha = \frac{3}{5}, \frac{8}{11}, \frac{6}{7}$, it has no such property. From Table 4.2, with n_1 increases and n_2 decreases, the A_α spectral radius of the join of in-stars is decreasing when $\alpha = \frac{1}{6}, \frac{3}{10}, \frac{1}{2}$. But when $\alpha = \frac{11}{20}, \frac{3}{5}, \frac{8}{11}, \frac{6}{7}$, it has no such property. So we give the following problem.

Problem 4.1. Characterize the minimal digraphs for A_α spectral radius of the join of in-trees with a fixed dichromatic number.

Furthermore, from Theorem 4.5, we only find the digraph which has the minimal A_α spectral radius of the join of in-trees in $\mathscr{G}_{n,r}$. But for the join of any directed trees, whether the same conclusion can be obtained. So we give the following problem.

Problem 4.2. Characterize the minimal digraphs for A_α spectral radius of the join of directed trees with a fixed dichromatic number.

Table 4.1: The A_α spectral radius of the join of in-stars in $\mathcal{G}_{7,2}$.

$n=n_1+n_2=7$		$n_1=4, n_2=3$	$n_1=5, n_2=2$	$n_1=6, n_2=1$
ρ_α	$\alpha=\frac{1}{6}$	4.0838	3.7847	2.9626
	$\alpha=\frac{3}{10}$	4.1024	3.8660	3.1616
	$\alpha=\frac{1}{2}$	4.1475	4.0685	3.6309
	$\alpha=\frac{11}{20}$	4.1646	4.1463	3.85
	$\alpha=\frac{3}{5}$	4.1856	4.2420	4.2
	$\alpha=\frac{8}{11}$	4.2699	4.6040	5.0909
	$\alpha=\frac{6}{7}$	4.4674	5.1892	6

Table 4.2: The A_α spectral radius of the join of in-stars in $\mathcal{G}_{10,2}$.

$n=n_1+n_2=10$		$n_1=5$ $n_2=5$	$n_1=6$ $n_2=4$	$n_1=7$ $n_2=3$	$n_1=8$ $n_2=2$	$n_1=9$ $n_2=1$
ρ_α	$\alpha=\frac{1}{6}$	5.7080	5.6181	5.3333	4.7906	3.7203
	$\alpha=\frac{3}{10}$	5.7152	5.6472	5.4314	5.0168	4.1378
	$\alpha=\frac{1}{2}$	5.7321	5.7183	5.6715	5.5649	5.0958
	$\alpha=\frac{11}{20}$	5.7382	5.7454	5.7615	5.7619	5.5
	$\alpha=\frac{3}{5}$	5.7457	5.7789	5.8704	5.9916	6
	$\alpha=\frac{8}{11}$	5.7737	5.9142	6.2727	6.7479	7.2727
	$\alpha=\frac{6}{7}$	5.8307	6.2256	6.9544	7.7523	8.5714

4.4 Appendix

Let $b_i = x - \alpha(n-i)$, $c_i = -(1-\alpha)(a_i - 1)$, $d = b_{n_1} + c_{n_1} = x - \alpha(n-n_1) - (1-\alpha)(a_{n_1} - 1)$, $\beta = -(1-\alpha)$ and $\gamma = -b_{n_1} + \beta = -x + \alpha(n-n_1) - (1-\alpha)$, where $i = 1, 2, \ldots, n_1$. Let

$$Q_{n_1} = \begin{vmatrix} b_1 & \beta & \beta & \cdots & \beta & \gamma \\ 0 & b_2 & \beta & \cdots & \beta & \gamma \\ 0 & 0 & b_3 & \cdots & \beta & \gamma \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & b_{n_1-1} & \gamma \\ c_1 & c_2 & c_3 & \cdots & c_{n_1-1} & d \end{vmatrix}, \; P_{n_1-1} = \begin{vmatrix} \beta & \beta & \cdots & \beta & \gamma \\ b_2 & \beta & \cdots & \beta & \gamma \\ 0 & b_3 & \cdots & \beta & \gamma \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & b_{n_1-1} & \gamma \end{vmatrix},$$

and Q_{n_1-i} be the determinant obtained by deleting the pre-i rows and the pre-i columns of Q_{n_1}, P_{n_1-1-i} be the determinant obtained by deleting the pre-i rows and the pre-i columns of P_{n_1-1}.

Then

$$|xI_{n_1} - B| = \begin{vmatrix} b_1+c_1 & c_2+\beta & c_3+\beta & \cdots & c_{n_1-1}+\beta & c_{n_1}+\beta \\ c_1 & b_2+c_2 & c_3+\beta & \cdots & c_{n_1-1}+\beta & c_{n_1}+\beta \\ c_1 & c_2 & b_3+c_3 & \cdots & c_{n_1-1}+\beta & c_{n_1}+\beta \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ c_1 & c_2 & c_3 & \cdots & b_{n_1-1}+c_{n_1-1} & c_{n_1}+\beta \\ c_1 & c_2 & c_3 & \cdots & c_{n_1-1} & b_{n_1}+c_{n_1} \end{vmatrix}$$

$$
\begin{aligned}
&= \begin{vmatrix} b_1 & \beta & \beta & \cdots & \beta & \gamma \\ 0 & b_2 & \beta & \cdots & \beta & \gamma \\ 0 & 0 & b_3 & \cdots & \beta & \gamma \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & b_{n_1-1} & \gamma \\ c_1 & c_2 & c_3 & \cdots & c_{n_1-1} & d \end{vmatrix} \\
&= b_1 \begin{vmatrix} b_2 & \beta & \cdots & \beta & \gamma \\ 0 & b_3 & \cdots & \beta & \gamma \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & b_{n_1-1} & \gamma \\ c_2 & c_3 & \cdots & c_{n_1-1} & d \end{vmatrix} + (-1)^{n_1+1} c_1 \begin{vmatrix} \beta & \beta & \cdots & \beta & \gamma \\ b_2 & \beta & \cdots & \beta & \gamma \\ 0 & b_3 & \cdots & \beta & \gamma \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & b_{n_1-1} & \gamma \end{vmatrix} \\
&= b_1 Q_{n_1-1} + (-1)^{n_1+1} c_1 P_{n_1-1} \\
&= b_1 Q_{n_1-1} + (-1)^{n_1+1} c_1 (\beta - b_2) P_{n_1-2} \\
&= b_1 Q_{n_1-1} + (-1)^{n_1+1} c_1 \prod_{i=2}^{n_1-1} (\beta - b_i)\gamma \\
&= b_1 \left(b_2 Q_{n_1-2} + (-1)^{n_1} c_2 \prod_{i=3}^{n_1-1} (\beta - b_i)\gamma \right) + (-1)^{n_1+1} c_1 \prod_{i=2}^{n_1-1} (\beta - b_i)\gamma \\
&= \prod_{i=1}^{2} b_i Q_{n_1-2} + b_1 (-1)^{n_1} c_2 \prod_{i=3}^{n_1-1} (\beta - b_i)\gamma + (-1)^{n_1+1} c_1 \prod_{i=2}^{n_1-1} (\beta - b_i)\gamma \\
&= \prod_{i=1}^{2} b_i \left(b_3 Q_{n_1-3} + (-1)^{n_1-1} c_3 \prod_{i=4}^{n_1-1} (\beta - b_i)\gamma \right) \\
&+ b_1 (-1)^{n_1} c_2 \prod_{i=3}^{n_1-1} (\beta - b_i)\gamma + (-1)^{n_1+1} c_1 \prod_{i=2}^{n_1-1} (\beta - b_i)\gamma \\
&= \prod_{i=1}^{3} b_i Q_{n_1-3} + \prod_{i=1}^{2} b_i (-1)^{n_1-1} c_3 \prod_{i=4}^{n_1-1} (\beta - b_i)\gamma \\
&+ b_1 (-1)^{n_1} c_2 \prod_{i=3}^{n_1-1} (\beta - b_i)\gamma + (-1)^{n_1+1} c_1 \prod_{i=2}^{n_1-1} (\beta - b_i)\gamma
\end{aligned}
$$

$$
\begin{aligned}
&= \prod_{i=1}^{3} b_i Q_{n_1-3} + \sum_{t=0}^{2} \left(\prod_{i=1}^{t} b_i (-1)^{n_1+1-t} c_{t+1} \prod_{i=t+2}^{n_1-1} (\beta - b_i)\gamma \right) \\
&= \prod_{i=1}^{n_1-1} b_i d + \sum_{t=0}^{n_1-2} \left((-1)^{n_1+1-t} c_{t+1} \gamma \prod_{i=1}^{t} b_i \prod_{i=t+2}^{n_1-1} (\beta - b_i) \right).
\end{aligned}
$$

Note: if $t = 0$, let $\prod_{i=1}^{t} b_i = 1$; if $t = n_1 - 2$, let $\prod_{i=t+2}^{n_1-1} (\beta - b_i) = 1$.

Hence, we get

$$
\begin{aligned}
|xI_{n_1} - B| = \prod_{i=1}^{n_1} (x - \alpha(n-i)) - \sum_{j=1}^{n_1} \Bigg(&(1-\alpha)(a_j - 1) \\
&\prod_{i=1}^{j-1} (x - \alpha(n-i)) \prod_{i=j+1}^{n_1} ((1-\alpha) + x - \alpha(n-i)) \Bigg).
\end{aligned}
$$

Note: if $j = n_1$, let $\prod_{i=j+1}^{n_1} ((1-\alpha) + x - \alpha(n-i)) = 1$.

Chapter 5

Bounds for the eccentricity spectral radius of digraphs

In this final chapter, we consider another type of matrix which is known as the eccentricity matrix or the earlier term D_{MAX}-matrix. Just like in the previous chapters, we focus on extremal problems related to invariants which are based on the eigenvalues of this matrix. In particular, we obtain lower bounds for the eccentricity spectral radius among all join digraphs with a fixed dichromatic number. Analogous upper bounds seem to be difficult to obtain. However, we obtain upper bounds for the eccentricity spectral radius of some more special join digraphs with a fixed dichromatic number.

5.1 Introduction

We refer to Chapter 1 for general terminology and notation, as well as for the relevant definitions regarding digraphs, their associated matrices and related eigenvalue invariants, and the dichromatic number. Here we recall some of the background that motivated our work. More on the background and related work can be found in Subsection 1.2.3 of Chapter 1.

Scholars in spectral graph theory have often focused their study on the adjacency matrix, the Laplacian matrix, the signless Laplacian matrix, and the distance matrix, among others. Interested readers can find a lot of information on these matrices in the monographs [13, 28, 118]. As we mentioned before, without doubt most of the earlier work has been done on the adjacency matrix, after its introduction by Poincaré in order to characterize labyrinths [109]. In a sense, the adjacency matrix can be considered as a simplification of the distance matrix which was introduced by Harary [49]. The adjacency matrix can be obtained from the distance matrix by only keeping the smallest positive distances 1 in each row and each column, and setting the other entries to 0.

In this view, the adjacency matrix can be renamed as a D_{MIN}-matrix, and one may wonder whether there is a useful concept of a D_{MAX}-matrix. Such considerations have led to the introduction of a novel distance-type graph matrix, as a kind of opposite of the adjacency matrix. The natural idea is to maintain only the largest distances of the distance matrix in each row and each column, and setting the other entries to 0.

In 2013, this concept of the D_{MAX}-matrix was introduced by Randić [113]. This matrix differs from most of the above mentioned matrices in that it is very sensitive to the pattern of branching in a graph. Randić [113] confined attention mostly to the D_{MAX}-matrix of trees, notably because in case of trees it is sufficient to know all the distances between its terminal vertices (leaves). More details about this matrix and the various Randić-type descriptors can be found in [31, 91, 114].

In 2018, the D_{MAX}-matrix was renamed to eccentricity matrix by Wang et al. [120]. So, the eccentricity matrix is obtained from the distance matrix by keeping the largest distances in each row and each column, and putting 0 in the remaining entries. For more studies and details about this matrix for undirected graphs we refer the reader to [51, 67, 92–94, 104, 111, 121–125]. However, there is still little research on the eccentricity matrix of digraphs. In 2022, Yang and Wang [137] first extended the concept of eccentricity matrix from graphs to digraphs. Recall that the eccentricity matrix $\varepsilon(G)$ of a strongly connected digraph G is defined as

$$\varepsilon(G)_{ij} = \begin{cases} d(v_i, v_j), & \text{if } d(v_i, v_j) = \min\{e^+(v_i), e^-(v_j)\}, \\ 0, & \text{otherwise.} \end{cases}$$

With the above motivation, our aim was to extend our results and techniques, and to continue studying analogous extremal problems associated with the eccentricity matrix of digraphs.

Following up on the early work of Randić [113], research on the eccentricity matrix has often been focused on the eccentricity matrix of trees. Randić [113] focused on the D_{MAX}-matrix of trees. Wang et al. [120] showed that the eccentricity matrices of trees are irreducible. Mahato et al. [93] provided an alternate proof of the result that the eccentricity matrix of a tree is irreducible. Wei et al. [124] characterized the extremal trees of given diameter having the minimum ε-spectral radius. He and Lu [51] determined the trees with the smallest ε-eigenvalues in $[-2-\sqrt{13}, -2\sqrt{2})$. Mahato and Kannan [94] showed that any tree with even diameter, except the star, has the same number of positive and negative ε-eigenvalues. Besides, they proved that the ε-eigenvalues of a tree are symmetric with respect to the origin if and only if the tree has odd diameter.

Since the eccentricity matrix of a digraph only makes sense for strongly connected digraphs, this matrix is not defined for directed trees. In a recent paper, Yang and Wang [137] focused on the eccentricity matrix of digraphs with diameter 2. They considered the irreducibility, lower bounds for the ε-energy, and lower bounds for the eccentricity spectral radius of digraphs with diameter 2. One of the main reasons for studying the eccentricity matrix of digraphs with diameter 2, is that they have a nice property, which we are going to show next.

Let $\overline{G}$ be the *complement* of a digraph G, i.e., with the same vertices as G, and for which (u,v) is an arc in $\overline{G}$ if and only if (u,v) is not an arc in G. For a digraph G with diameter 2, the distance matrix $D(G)$ is $D(G)=A(G)+2A(\overline{G})$, and the eccentricity matrix $\varepsilon(G)$ has the following property.

Lemma 5.1 (Yang and Wang [137]). *Let G be a strongly connected digraph of order n with $diam(G)=2$.*
(i) If $\Delta^+(G)\neq n-1$ and $\Delta^-(G)\neq n-1$, then $\varepsilon(G)=2A(\overline{G})$.
(ii) If $\Delta^+(G)=n-1$ or $\Delta^-(G)=n-1$, then $\varepsilon(G)=2A(\overline{G})+A(G')$, where G' is the subdigraph of G obtained by deleting the arcs (v_i,v_j) with $d_G^+(v_i)\neq n-1$ and $d_G^-(v_j)\neq n-1$, for all $i,j=1,2,\ldots,n$.

As an illustration of the above lemma, we give some examples, as shown in Figure 5.1.

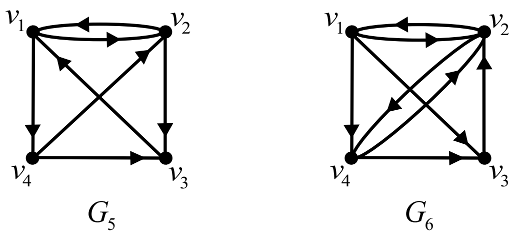


Figure 5.1: The strongly connected digraphs G_5 and G_6.

The digraph G_5 is a strongly connected digraph with diameter 2 and $\Delta^+(G_5) < 3$, $\Delta^-(G_5) < 3$. The digraph G_6 is a strongly connected digraph with diameter 2 and $\Delta^+(G_6) = \Delta^-(G_6) = 3$. Then

$$\varepsilon(G_5) = \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 2 & 0 & 2 \\ 2 & 0 & 0 & 0 \end{pmatrix} = 2A(\overline{G}_5).$$

And

$$\varepsilon(G_6) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 0 \\ 2 & 1 & 0 & 2 \\ 2 & 1 & 0 & 0 \end{pmatrix} = 2A(\overline{G}_6) + A(G_6'),$$

where G_6' is the subdigraph of G_6 obtained by deleting the arcs (v_2, v_1), (v_2, v_4) and (v_4, v_3).

As in the previous chapters, we focus on digraphs with a fixed dichromatic number. Lin and Shu [78] characterized the digraph which has the maximal adjacency spectral radius among all digraphs with a given dichromatic number. And, recalling earlier definitions, the maximal digraph for the spectral radius among all these digraphs is the join digraph $G = \bigvee_{i=1}^{r} V^i$, in which each V^i is a transitive tournament and $|n_i - n_j| \leq 1$ for all orders of the V^i and V^j. Liu et al. [89] characterized the digraph which has the maximal A_α spectral radius with given dichromatic number, and the maximal digraph is identical to the above digraph. Recall that in Chapter 4, we obtain this maximal digraph for the A_α spectral radius by using another method: the equitable quotient matrix. Moreover, in Chapters 2 and 3, we obtain the digraphs which attain the maximal Laplacian energy and maximal A_α energy with a fixed dichromatic number. Also in these cases, the maximal digraphs are still identical to the above digraph. So, a natural question is whether the maximal digraphs for the eccentricity spectral radius are the same as in all of the above cases. Actually, these maximal digraphs turn out to be very different from those in the other chapters. Based on this, we want to study bounds and extremal digraphs for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$.

For the join digraph $G = \bigvee_{i=1}^{r} V^i$ in $\mathscr{G}_{n,r}$, we know that each V^i is an acyclic digraph. If $r = 1$, then G is an acyclic digraph. But we know the eccentricity matrix is only defined if G is strongly connected. If $r = n$, then $G = \overleftrightarrow{K}_n$ and $\rho_\varepsilon(\overleftrightarrow{K}_n) = \rho_A(\overleftrightarrow{K}_n) = n - 1$. Therefore, we only consider digraphs in $\mathscr{G}_{n,r}$ for $2 \leq r \leq n-1$.

Before we are going to consider lower bounds for the eccentricity spectral radius in the next section, we finish this section by introducing a useful digraph for our purposes.

Let G^ε denote the digraph, the adjacency matrix $A(G^\varepsilon)$ of which is obtained from $\varepsilon(G)$ by setting the nonzero elements of $\varepsilon(G)$ are equal to 1. The motivation for this is the known fact that adjacency matrices of strongly connected digraphs are irreducible. Because a lot of properties of spectral radii involve irreducibility of matrices, when studying the spectral radius of eccentricity matrices, it is often worthwhile to consider the digraph G^ε that corresponds to the eccentricity matrix.

The remainder of this chapter is organized as follows. In Section 5.2, we obtain lower bounds for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$. In Section 5.3, we derive upper bounds for the eccentricity spectral radius of some more special join digraphs in $\mathscr{G}_{n,r}$.

5.2 Lower bounds for the eccentricity spectral radius

In this section, we obtain lower bounds for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$, and we characterize the corresponding minimal digraphs. First, we present some lemmas that we use in our proofs. The first lemma is a recent result due to Yang and Wang [137].

Lemma 5.2 (Yang and Wang [137]). *Let G be a strongly connected digraph of order n with $diam(G) = 2$. If $\Delta^+(G) = n-1$ or $\Delta^-(G) = n-1$, then*

$$\rho_\varepsilon(G) > 2.$$

The second lemma is closely related to the above lemma and easy to prove.

Lemma 5.3. *Let G be a strongly connected digraph of order $n \geq 4$ with $diam(G) = 2$. If G has $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, and*
(i) there are at least two vertices with outdegree $n-1$; or
(ii) there are at least two vertices with indegree $n-1$; or
(iii) there is one vertex with outdegree $n-1$ and indegree $n-1$, then

$$\rho_\varepsilon(G) \geq 3.$$

Proof. Since $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, we assume that u is a vertex with $d_G^+(u) = n-1$, v is a vertex with $d_G^-(v) = n-1$, and w is a vertex with $d_G^+(w) \neq n-1$ and $d_G^-(w) \neq n-1$. By the definition of eccentricity matrix, we have the following:
(a) except for the diagonal element, the elements of the row of $\varepsilon(G)$ corresponding to u are all 1, and the column of $\varepsilon(G)$ corresponding to u has at least one entry 2 or all elements are 1;
(b) except for the diagonal element, the elements of the column of $\varepsilon(G)$ corresponding to v are all 1, and the row of $\varepsilon(G)$ corresponding to v has at least one entry 2 or all elements are 1;
(c) the row (and column) of $\varepsilon(G)$ corresponding to w has at least one entry 2 and one entry 1.

Suppose that there are at least two vertices with outdegree $n-1$, without loss of generality, let $d_G^+(u_1)=n-1$ and $d_G^+(u_2)=n-1$. Then by (a), the column sum of $\varepsilon(G)$ corresponding to u_1 (u_2) is at least 3. By (b) and (c), the column sums of $\varepsilon(G)$ corresponding to other vertices are also at least 3. So all the column sums of $\varepsilon(G)$ are at least 3.

Suppose that there are at least two vertices with indegree $n-1$, without loss of generality, let $d_G^-(v_1)=n-1$ and $d_G^-(v_2)=n-1$. Similarly, by (b), the row sum of $\varepsilon(G)$ corresponding to v_1 (v_2) is at least 3. By (a) and (c), the row sums of $\varepsilon(G)$ corresponding to other vertices are also at least 3. So all the row sums of $\varepsilon(G)$ are at least 3.

Suppose that there is one vertex with outdegree $n-1$ and indegree $n-1$, without loss of generality, let $d_G^+(u)=n-1$ and $d_G^-(u)=n-1$. Then by (a)-(c), all the row (column) sums of $\varepsilon(G)$ are at least 3.

Hence, using Lemma 1.4, if G has $\Delta^+(G)=n-1$ and $\Delta^-(G)=n-1$, and satisfies (i) or (ii) or (iii), we obtain that $\rho_\varepsilon(G)\geq 3$. $\square$

From Lemma 5.1, for the join digraphs $G=\bigvee_{i=1}^r V^i$ with $\Delta^+(G)\neq n-1$ and $\Delta^-(G)\neq n-1$, we get

$$\rho_\varepsilon(G)=2\rho_A(\overline{G}).$$

Hence, in order to get the digraphs which attain the lower bounds for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$, it is sufficient to consider the adjacency spectral radius of the complement of the join digraph.

For this purpose, as illustrated in Figure 5.2, we define a class of digraphs of order n, denoted by $\mathscr{T}_{n,k}^2$ which satisfies the following:
(1) $\mathscr{V}(\mathscr{T}_{n,k}^2)$ has a partition $\{\mathscr{V}(G_1),\mathscr{V}(G_2),\ldots,\mathscr{V}(G_k)\}$ such that $G_i=K_1$ or $G_i=2K_1$ for any $1\leq i\leq k$;
(2) for any two parts G_i and G_j with $1\leq i<j\leq k$, $G_i\mapsto G_j$.

The just defined class of digraphs is relevant in the light of the following result.

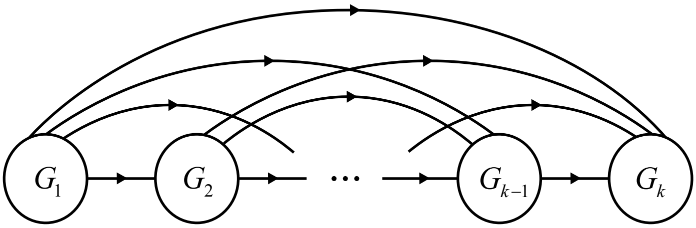


Figure 5.2: A class of digraphs $\mathcal{T}^2_{n,k}$.

Theorem 5.4. *Let G be an acyclic digraph of order n (possibly disconnected).*
(i) If $\Delta^+(G) \neq n-1$ and $\Delta^-(G) \neq n-1$, then

$$\rho_A(\overline{G}) \geq 1,$$

with equality holding if and only if $G \in \mathcal{T}^2_{n,k}$ with $G_1 = G_k = 2K_1$. Especially, when $n = 3$,

$$\rho_A(\overline{G}) = \rho_A(\overline{P_3}) = \sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}}.$$

(ii) If $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, then

$$\rho_A(\overline{G}) \geq 0,$$

with equality holding if and only if G is a transitive tournament.
(iii) If $\Delta^+(G) = n-1$ and $\Delta^-(G) \neq n-1$, then

$$\rho_A(\overline{G}) \geq 1,$$

with equality holding if and only if $G \in \mathcal{T}^2_{n,k}$ with $G_1 = K_1$ and $G_k = 2K_1$.
(iv) If $\Delta^+(G) \neq n-1$ and $\Delta^-(G) = n-1$, then

$$\rho_A(\overline{G}) \geq 1,$$

with equality holding if and only if $G \in \mathcal{T}^2_{n,k}$ with $G_1 = 2K_1$ and $G_k = K_1$.

Proof. If $n = 2$, then G is either $G = 2K_1$ or $G = P_2$. And $\rho_A(\overline{2K_1}) = \rho_A(C_2) =$

1, $\rho_A(\overline{P_2}) = \rho_A(P_2) = 0$. Next we consider the lower bounds for $\rho_A(\overline{G})$ when $n \geq 3$.

Case 1. $\Delta^+(G) \neq n-1$ and $\Delta^-(G) \neq n-1$.

If $n = 3$, then $G = P_3$ or $G = P_2 \cup K_1$ or $G = 3K_1$. Obviously,

$$\rho_A(\overline{G}) \geq \rho_A(\overline{P_3}) = \sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}} \approx 1.32.$$

If $n \geq 4$, then $d^+_{\overline{G}}(v) > 0$ and $d^-_{\overline{G}}(v) > 0$ for any $v \in G$. So there must exist directed cycles in $\overline{G}$. Then

$$\rho_A(\overline{G}) \geq 1.$$

Next we prove that if $\rho_A(\overline{G}) = 1$, then $G \in \mathscr{T}^2_{n,k}$ with $G_1 = G_k = 2K_1$.

If $\rho_A(\overline{G}) = 1$, then any two directed cycles in $\overline{G}$ are vertex-disjoint. If $\overline{G}$ is a strongly connected digraph, $\rho_A(\overline{G}) = 1$ if and only if $\overline{G} = C_n$, and then $G = \overline{C_n}$, a contradiction. So $\overline{G}$ is not strongly connected.

Let $\overline{G_1}, \overline{G_2}, \ldots, \overline{G_k}$ be the strong components of $\overline{G}$. Then $\overline{G_i} \nrightarrow \overline{G_j}$ or $\overline{G_j} \nrightarrow \overline{G_i}$ for any $1 \leq i < j \leq k$. Otherwise, we can get a new strong component constructed by $\overline{G_i}$ and $\overline{G_j}$. If there exist two vertices $u, v \in \mathscr{V}(\overline{G})$ such that $(u,v) \notin \mathscr{A}(\overline{G})$ and $(v,u) \notin \mathscr{A}(\overline{G})$, then $C_2 \subseteq G$. Since G is acyclic, this is a contradiction. Then there is at least one arc between any two vertices in $\overline{G}$. So, without loss of generality, we get $\overline{G_i} \nrightarrow \overline{G_j}$ and $\overline{G_j} \rightarrow \overline{G_i}$ in $\overline{G}$. Then $\overline{G_j} \mapsto \overline{G_i}$ in $\overline{G}$. Hence $G_i \mapsto G_j$ in G for any $1 \leq i < j \leq k$.

Since

$$\rho_A(\overline{G}) = \max_{1 \leq i \leq k} \left\{ \rho_A(\overline{G_i}) \right\} = 1,$$

we obtain $\rho_A(\overline{G_i}) = 0$ or $\rho_A(\overline{G_i}) = 1$, and there is at least one $\overline{G_i}$ with $\rho_A(\overline{G_i}) = 1$ for any $i = 1, 2, \ldots, k$. If $\rho_A(\overline{G_i}) = 0$, then $\overline{G_i} = K_1$. So $G_i = K_1$. If $\rho_A(\overline{G_i}) = 1$, then $\overline{G_i}$ is a directed cycle. So $\overline{G_i} = C_2$ and $G_i = 2K_1$. Otherwise, G is not acyclic. Then in G, we obtain $G_i = K_1$ or $G_i = 2K_1$, and $G_i \mapsto G_j$ for any $1 \leq i < j \leq k$. Since $\Delta^+(G) \neq n-1$ and $\Delta^-(G) \neq n-1$, we get $G_1 \neq K_1$ and $G_k \neq K_1$.

Hence, for the vertex set $\mathscr{V}(G)$ of G, we get

$$\mathscr{V}(G) = \{\mathscr{V}(G_1), \mathscr{V}(G_2), \dots, \mathscr{V}(G_k)\}$$

such that

$$G_1 = G_k = 2K_1, \ G_i = K_1 \ or \ G_i = 2K_1$$

for any $1 < i < k$. And for any two parts G_i and G_j with $1 \le i < j \le k$,

$$G_i \mapsto G_j.$$

That is, if $\rho_A(\overline{G}) = 1$, then $G \in \mathscr{T}^2_{n,k}$ with $G_1 = G_k = 2K_1$.

Case 2. $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$.

Since G is an acyclic digraph with $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, there exists only one vertex $u \in \mathscr{V}(G)$ with $d^+_G(u) = n-1$, one vertex $v \in \mathscr{V}(G)$ with $d^-_G(v) = n-1$ and $u \neq v$. Otherwise, G is not acyclic.

If G has none of the arcs (u,v) and (v,u) for $u,v \in \mathscr{V}(G)$, then $C_2 \subseteq \overline{G}$ and $\rho_A(\overline{G}) \ge 1$.

If G has one of (u,v) and (v,u) for each $u,v \in \mathscr{V}(G)$, then G is a transitive tournament. So $\overline{G}$ is also a transitive tournament and $\rho_A(\overline{G}) = 0$.

Case 3. $\Delta^+(G) = n-1$ and $\Delta^-(G) \neq n-1$.

Since G is an acyclic digraph with $\Delta^+(G) = n-1$, similar as in the proof of Case 2, there exists only one vertex $u \in \mathscr{V}(G)$ with $d^+_G(u) = n-1$ and $d^-_G(u) = 0$.

Since $\Delta^-(G) \neq n-1$, there are at least two vertices $u,v \in \mathscr{V}(G)$ such that $(u,v) \notin \mathscr{A}(G)$ and $(v,u) \notin \mathscr{A}(G)$. Otherwise, G is a transitive tournament, a contradiction. So $C_2 \subseteq \overline{G}$ and $\rho_A(\overline{G}) \ge 1$.

If $\rho_A(\overline{G}) = 1$, then any two directed cycles in $\overline{G}$ are vertex-disjoint. Similar as in the proof of Case 1, if $\rho_A(\overline{G}) = 1$, then $G \in \mathscr{T}^2_{n,k}$ with $G_1 = K_1$ and $G_k = 2K_1$.

Case 4. $\Delta^+(G) \neq n-1$ and $\Delta^-(G) = n-1$.

Similar as in the proof of Case 3, we get $\rho_A(\overline{G}) \ge 1$. And if $\rho_A(\overline{G}) = 1$, then $G \in \mathscr{T}^2_{n,k}$ with $G_1 = 2K_1$ and $G_k = K_1$.

Actually, the transitive tournament belongs to $\mathscr{T}_{n,k}^2$ with $G_i = K_1$ for all $i = 1, 2, \ldots, n$. Also $2K_1 \in \mathscr{T}_{n,k}^2$ and P_2 is a transitive tournament. By calculation,

$$\rho_A(\mathscr{T}_{n,k}^2) = \begin{cases} 0, & \text{if } G_i = K_1 \text{ for all } i = 1, 2, \ldots, n, \\ 1, & \text{otherwise.} \end{cases}$$

This completes the proof. □

In our next results we turn back to $\rho_\varepsilon(G)$ for digraphs $G = \bigvee_{i=1}^{r} V^i$. We start with a lemma before we state and prove our main result.

Lemma 5.5. *Let $G = \bigvee_{i=1}^{r} V^i$ which each V^i with $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$.*
(i) If $n \geq 2r$ and $n \neq 2r + 1$, then

$$\rho_\varepsilon(G) \geq 2,$$

with equality holding if and only if each $V^i \in \mathscr{T}_{n_i,k_i}^2$ with $G_1 = G_{k_i} = 2K_1$, where $i = 1, 2, \ldots, r$.
(ii) If $n = 2r + 1$, then

$$\rho_\varepsilon(G) \geq 2\left(\sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}}\right),$$

with equality holding if and only if $V^1 = P_3$ and $V^i = 2K_1$, where $i = 2, 3, \ldots, r$.

Proof. Since $G = \bigvee_{i=1}^{r} V^i$ in which each V^i is an acyclic digraph of order n_i with $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, we get $n_i \geq 2$, $diam(G) = 2$, $\Delta^+(G) \neq n - 1$ and $\Delta^-(G) \neq n - 1$. By Lemma 5.1, $\varepsilon(G) = 2A(\overline{G})$ and $\overline{G} = \bigcup_{i=1}^{r} \overline{V^i}$. So

$$\rho_\varepsilon(G) = 2\rho_A(\overline{G}) = 2 \max_{1 \leq i \leq k} \left\{\rho_A(\overline{V^i})\right\}.$$

From Theorem 5.4, we get

$$\rho_A(\overline{V^i}) \geq 1,$$

with equality holding if and only if $V^i \in \mathcal{T}^2_{n_i,k_i}$ with $G_1 = G_{k_i} = 2K_1$. Especially, when $n_i = 3$,

$$\rho_A(\overline{V^i}) = \rho_A(\overline{P_3}) = \sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}}.$$

(i) If $n \geq 2r$ and $n \neq 2r+1$, then we can find a suitable n_i such that $n_i \geq 2$ and $n_i \neq 3$ for all $i = 1, 2, \ldots, r$. Hence, we obtain

$$\rho_\varepsilon(G) \geq 2,$$

with equality holding if and only if each $V^i \in \mathcal{T}^2_{n_i,k_i}$ with $G_1 = G_{k_i} = 2K_1$.
(ii) If $n = 2r+1$, then there is only one V^s with $n_s = 3$, and all other V^i have $n_i = 2$ for $i \neq s$. Without loss of generality, let $n_1 = 3$ and $n_i = 2$, where $i = 2, 3, \ldots, r$. Hence, we obtain

$$\rho_\varepsilon(G) \geq 2\left(\sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}}\right),$$

with equality holding if and only if $V^1 = P_3$ and $V^i = 2K_1$, where $i = 2, 3, \ldots, r$. $\square$

Now, we finally present our main result of this section.

Theorem 5.6. *Let* $G = \bigvee_{i=1}^r V^i$.
(i) If $n \geq 2r$ *and* $n \neq 2r+1$, *then*

$$\rho_\varepsilon(G) \geq 2,$$

with equality holding if and only if each $V^i \in \mathcal{T}^2_{n_i,k_i}$ *with* $G_1 = G_{k_i} = 2K_1$, *where* $i = 1, 2, \ldots, r$.

(ii) If $n = 2r + 1$, then

$$\rho_\varepsilon(G) \geq 2\left(\sqrt[3]{\frac{1}{2}+\sqrt{\frac{23}{108}}}+\sqrt[3]{\frac{1}{2}-\sqrt{\frac{23}{108}}}\right),$$

with equality holding if and only if $V^1 = P_3$ and $V^i = 2K_1$, where $i = 2, 3, \ldots, r$.

Proof. Since $G = \bigvee_{i=1}^{r} V^i$, $diam(G) = 2$. From Lemma 5.2, we get $\rho_\varepsilon(G) > 2$ if $\Delta^+(G) = n-1$ or $\Delta^-(G) = n-1$. We consider two cases to derive lower bounds for $\rho_\varepsilon(G)$.

Case 1. $n \geq 2r$ and $n \neq 2r+1$.

If there exists at least one V^i with $\Delta^+(V^i) = n_i - 1$ or $\Delta^-(V^i) = n_i - 1$, then $\Delta^+(G) = n-1$ or $\Delta^-(G) = n-1$, and $\rho_\varepsilon(G) > 2$. From Lemma 5.5, if each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, then

$$\rho_\varepsilon(G) \geq 2,$$

with equality holding if and only if each $V^i \in \mathscr{T}^2_{n_i,k_i}$ with $G_1 = G_{k_i} = 2K_1$, where $i = 1, 2, \ldots, r$. So (i) holds.

Case 2. $n = 2r+1$.

If there exists V^i with $n_i = 1$, then $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, and G has one vertex with outdegree $n-1$ and indegree $n-1$. From (iii) in Lemma 5.3, we get $\rho_\varepsilon(G) \geq 3$. If there is no V^i with $n_i = 1$, without loss of generality, we get $n_1 = 3$ and $n_i = 2$, where $i = 2, 3, \ldots, r$.

When $n_i = 2$, $V^i = 2K_1$ or $V^i = P_2$. If $V^i = P_2$, we also have $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$. If there exist at least two $V^i = P_2$, then from (i) and (ii) in Lemma 5.3, we get $\rho_\varepsilon(G) \geq 3$. If there exists only one $V^i = P_2$, then $\varepsilon(G)$

contains a principal submatrix ε', where

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

From Lemma 1.3, we get $\rho_\varepsilon(G) \geq \rho(\varepsilon') \approx 2.73$.

When $n_1 = 3$, we consider the following cases.

Case 2.1. If $\Delta^+(V^1) \neq 2$ and $\Delta^-(V^1) \neq 2$, by the proof of Theorem 5.4 and Lemma 5.5, we get

$$\rho_\varepsilon(G) \geq 2\left(\sqrt[3]{\frac{1}{2}+\sqrt{\frac{23}{108}}}+\sqrt[3]{\frac{1}{2}-\sqrt{\frac{23}{108}}}\right) \approx 2.65,$$

with equality holding if and only if $V^1 = P_3$ and $V^i = 2K_1$, where $i = 2, 3, \ldots, r$.

Case 2.2. If $\Delta^+(V^1) = 2$ and $\Delta^-(V^1) = 2$, then $V^1 = B_3$. $\varepsilon(G)$ contains a principal submatrix ε'', where

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

From Lemma 1.3, we get $\rho_\varepsilon(G) \geq \rho(\varepsilon'') \approx 2.85$.

Case 2.3. If $\Delta^+(V^1) = 2$ and $\Delta^-(V^1) \neq 2$, then $V^1 = \overrightarrow{K}_{1,2}$. $\varepsilon(G)$ contains a principal submatrix ε''', where

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

From Lemma 1.3, we get $\rho_\varepsilon(G) \geq \rho(\varepsilon''') \approx 3.24$.

Case 2.4. If $\Delta^+(V^1) \neq 2$ and $\Delta^-(V^1) = 2$, then $V^1 = \overleftarrow{K}_{1,2}$. Similar to Case 2.3, we get $\rho_\varepsilon(G) \geq 3.24$.

Hence, we obtain

$$\rho_\varepsilon(G) \geq 2\left(\sqrt[3]{\frac{1}{2} + \sqrt{\frac{23}{108}}} + \sqrt[3]{\frac{1}{2} - \sqrt{\frac{23}{108}}}\right) \approx 2.65,$$

with equality holding if and only if $V^1 = P_3$ and $V^i = 2K_1$, where $i = 2, 3, \ldots, r$. So (ii) holds.

This completes the proof. $\square$

To illustrate Lemma 5.5 and Theorem 5.6 better, we give some examples, as shown in Figures 5.3 and 5.4.

5.3 Upper bounds for the eccentricity spectral radius

In this section, we give upper bounds for the eccentricity spectral radius of some special join digraphs in $\mathcal{G}_{n,r}$. Recall that for the join digraph $G = \bigvee_{i=1}^{r} V^i$, in which each V^i is an acyclic digraph, we let

$$\varepsilon(G) = \begin{pmatrix} \varepsilon^{11} & \varepsilon^{12} & \cdots & \varepsilon^{1r} \\ \varepsilon^{21} & \varepsilon^{22} & \cdots & \varepsilon^{2r} \\ \vdots & \vdots & & \vdots \\ \varepsilon^{r1} & \varepsilon^{r2} & \cdots & \varepsilon^{rr} \end{pmatrix},$$

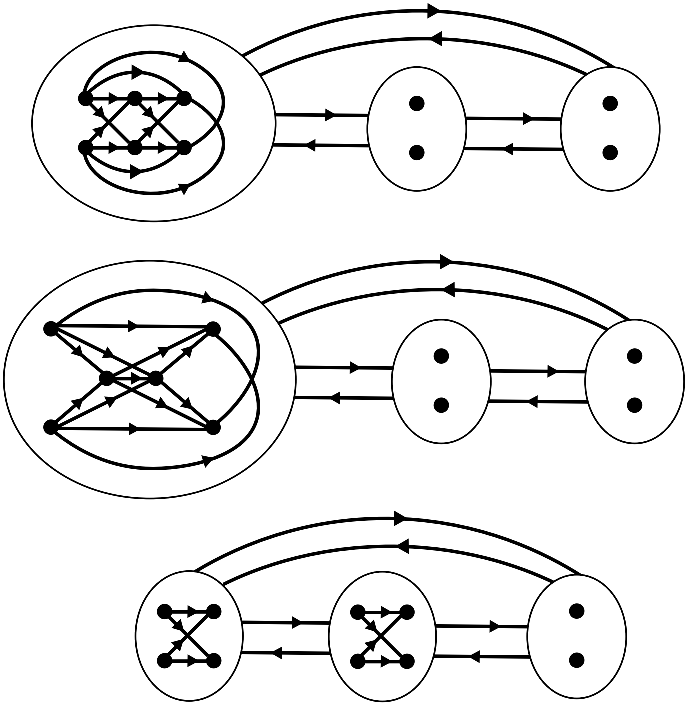


Figure 5.3: The digraphs in $\mathcal{G}_{10,3}$ with the minimal eccentricity spectral radius.

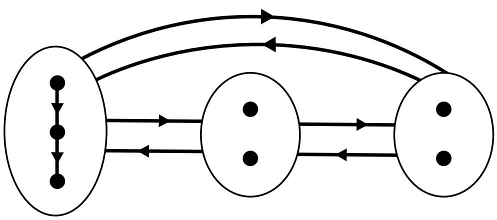


Figure 5.4: The digraph in $\mathcal{G}_{7,3}$ with the minimal eccentricity spectral radius.

where each ε^{ii} is a principal submatrix of $\varepsilon(G)$ corresponding to V^i.

Next, we are going to state and prove a number of results for special choices of the maximum outdegree (and indegree) of the V^i. We gather the obtained results at the end of this chapter.

Theorem 5.7. *Let $G = \bigvee_{i=1}^{r} V^i$. If each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, then*

$$\rho_\varepsilon(G) \leq 2(n - 2r + 1),$$

with equality holding if and only if $G = \overleftrightarrow{K}_{n-2r+2,2,\ldots,2}$.

Proof. From the proof of Lemma 5.5, we get

$$\rho_\varepsilon(G) = 2\rho_A(\overline{G}) = 2 \max_{1 \leq i \leq k} \left\{ \rho_A(\overline{V^i}) \right\}.$$

For $\overline{V^i}$, we know

$$\rho_A(\overline{V^i}) \leq n_i - 1,$$

with equality holding if and only if $\overline{V^i} = \overleftrightarrow{K}_{n_i}$. That is, $V^i = n_i K_1$.

Without loss of generality, let $n_1 \geq n_2 \geq \cdots \geq n_r$. Since $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, we have $n_i \geq 2$ and $n_1 \leq n - 2(r-1)$. So $\rho_A(\overline{V^i}) \leq n_i - 1 \leq n - 2r + 1$. Then when $n_1 = n - 2(r-1)$,

$$\rho_\varepsilon(G) = 2 \max_{1 \leq i \leq k} \left\{ \rho_A(\overline{V^i}) \right\} \leq 2\rho_A(\overleftrightarrow{K}_{n-2r+2}) = 2(n - 2r + 1).$$

That means, when $G = (n - 2r + 2)K_1 \vee \underbrace{2K_1 \vee \ldots \vee 2K_1}_{r-1} = \overleftrightarrow{K}_{n-2r+2,2,\ldots,2}$,

$$\rho_\varepsilon(G) \leq \rho_\varepsilon(\overleftrightarrow{K}_{n-2r+2,2,\ldots,2}) = 2(n - 2r + 1),$$

with equality holding if and only if $G = \overleftrightarrow{K}_{n-2r+2,2,\ldots,2}$. □

Theorem 5.8. *Let $G = \bigvee_{i=1}^{r} V^i$. If each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, then*

$$\rho_\varepsilon(G) \leq \rho_\varepsilon(B_{n-r+1} \vee \overleftrightarrow{K}_{r-1}),$$

with equality holding if and only if $G = B_{n-r+1} \vee \overleftrightarrow{K}_{r-1}$.

Proof. Since $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, there is only one vertex with outdegree $n_i - 1$ in V^i and one vertex with indegree $n_i - 1$ in V^i. Without loss of generality, we let $\mathscr{V}(V^i) = \{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ with $d_{V^i}^+(v_1^i) = n_i - 1$ and $d_{V^i}^-(v_{n_i}^i) = n_i - 1$.

From Lemma 5.1, if $\Delta^+(G) = n-1$ and $\Delta^-(G) = n-1$, then

$$\varepsilon(G) = 2A(\overline{G}) + A(G'),$$

where G' is the subdigraph of G obtained by deleting the arcs (v_i, v_j) with $d_G^+(v_i) \neq n-1$ and $d_G^-(v_j) \neq n-1$, for all $i, j = 1, 2, \ldots, n$. By the definition of $\varepsilon(G)$, we have

$$\varepsilon^{ii} = 2A(\overline{V^i}) + A(B_{n_i})$$

and

$$\varepsilon^{is} = \begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 0 & 0 & \cdots & 0 & 1 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}_{n_i \times n_s},$$

where $i, s = 1, 2, \ldots, r$ and $i \neq s$. Obviously, when $V^i = B_{n_i}$, $A(\overline{V^i})$ is maximal. That is,

$$\varepsilon^{ii} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 & 1 \\ 2 & 0 & 2 & \cdots & 2 & 1 \\ 2 & 2 & 0 & \cdots & 2 & 1 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & 2 & \cdots & 0 & 1 \\ 2 & 2 & 2 & \cdots & 2 & 0 \end{pmatrix}_{n_i \times n_i}.$$

Let $G^B = \bigvee_{i=1}^{r} B_{n_i}$. If $G \neq G^B$, then we have $0 < \varepsilon(G) < \varepsilon(G^B)$. Since G^{B^ε} is strongly connected, $\varepsilon(G^B)$ is irreducible. From Lemma 1.3, $\rho_\varepsilon(G) < \rho_\varepsilon(G^B)$. Hence, $\rho_\varepsilon(G) \leq \rho_\varepsilon(G^B)$, with equality holding if and only if $G = G^B$. Without loss of generality, let $n_1 \geq n_2 \geq \cdots \geq n_r$. Next we prove that when $n_1 = n - r + 1$, $n_2 = n_3 = \cdots = n_r = 1$, $\rho_\varepsilon(G^B)$ is maximal.

Suppose that

$$\mathbf{x} = (x_1^1, x_2^1, \ldots, x_{n_1}^1, x_1^2, x_2^2, \ldots, x_{n_2}^2, \ldots, x_1^r, x_2^r, \ldots, x_{n_r}^r)^T$$

is a Perron vector of $\varepsilon(G^B)$ corresponding to the eccentricity spectral radius $\rho_\varepsilon = \rho_\varepsilon(G^B)$, where x_j^i is the characteristic component corresponding to v_j^i of B_{n_i} for each $1 \leq i \leq r$ and $1 \leq j \leq n_i$.

Since $\varepsilon(G^B)\mathbf{x} = \rho_\varepsilon \mathbf{x}$, we have

$$\begin{cases} \sum_{s=1}^{r} \sum_{t=1}^{n_s} x_t^s - x_1^i = \rho_\varepsilon x_1^i, \\ \sum_{t=1}^{n_i-1} 2x_t^i - 2x_j^i + \sum_{s=1}^{r} x_{n_s}^s = \rho_\varepsilon x_j^i, \\ \sum_{t=1}^{n_i-1} 2x_t^i - x_{n_i}^i + \sum_{s=1}^{r} x_{n_s}^s = \rho_\varepsilon x_{n_i}^i, \end{cases}$$

where $i = 1, 2, \ldots, r$ and $j = 2, 3, \ldots, n_i - 1$. Since each $V^i = B_{n_i}$, we get $x_2^i = x_3^i = \cdots = x_{n_i-1}^i$. So we have

$$\begin{cases} \sum_{s=1}^{r} \sum_{t=1}^{n_s} x_t^s = (\rho_\varepsilon + 1)x_1^i, \\ 2x_1^i + \sum_{s=1}^{r} x_{n_s}^s = (\rho_\varepsilon - 2n_i + 6)x_2^i, \\ (\rho_\varepsilon + 2)x_2^i = (\rho_\varepsilon + 1)x_{n_i}^i. \end{cases}$$

From Lemma 1.5 (Perron-Frobenius Theorem), then $x_1^1 = x_1^2 = \cdots = x_1^r = \frac{1}{\rho_\varepsilon + 1}$, $x_{n_i}^i > x_{n_s}^s$ and $x_j^i > x_t^s$ for $1 \leq i < s \leq r$, $j = 2, 3, \ldots, n_i - 1$ and $t = 2, 3, \ldots, n_s - 1$.

We assume that $n_1 \geq \cdots \geq n_s \geq 2 > 1 = n_{s+1} = \cdots = n_r$. Let $G^{B'} = \bigvee_{i=2, i \neq s}^{r} B_{n_i} \vee B_{n_1+n_s-1} \vee K_1$, see Figure 5.5. Then

$$\begin{aligned} G^{B'} = G^B &- \{(v_j^1, v_t^s) | j = 2, 3, \ldots, n_1,\ t = 2, 3, \ldots, n_s\} \\ &- \{(v_t^s, v_j^1) | j = 1, 2, \ldots, n_1 - 1,\ t = 2, 3, \ldots, n_s\} \end{aligned}$$

$$- \{(v_t^s, v_{n_s}^s) | t = 2, 3, \ldots, n_s - 1\}$$
$$+ \{(v_t^s, v_1^s) | t = 2, 3, \ldots, n_s\}.$$

Now we prove $\rho_\varepsilon(G^{B'}) > \rho_\varepsilon(G^B)$.

We get

$$\varepsilon(G^{B'})\mathbf{x} - \varepsilon(G^B)\mathbf{x} = \left(0, \underbrace{y_1, \ldots, y_1}_{n_1-1}, \underbrace{0, \ldots, 0}_{\sum_{i=2}^{s-1} n_i+1}, \underbrace{y_2, \ldots, y_2}_{n_s-2}, y_3, \underbrace{0, \ldots, 0}_{\sum_{i=s+1}^{r} n_i}\right)^T,$$

where $y_1 = x_1^s + 2\sum_{t=2}^{n_s-1} x_t^s + x_{n_s}^s$, $y_2 = 2\sum_{j=1}^{n_1-1} x_j^1 - x_1^s + x_{n_s}^s$ and $y_3 = 2\sum_{j=1}^{n_1-1} x_j^1 - x_1^s$.

Since $x_1^1 = x_1^s$, we have $y_2 \geq y_3 \geq 0$. Obviously, $y_1 > 0$. So we get

$$\varepsilon(G^{B'})\mathbf{x} - \varepsilon(G^B)\mathbf{x} > 0.$$

That is,

$$\varepsilon(G^{B'})\mathbf{x} > \varepsilon(G^B)\mathbf{x} = \rho_\varepsilon(G^B)\mathbf{x}.$$

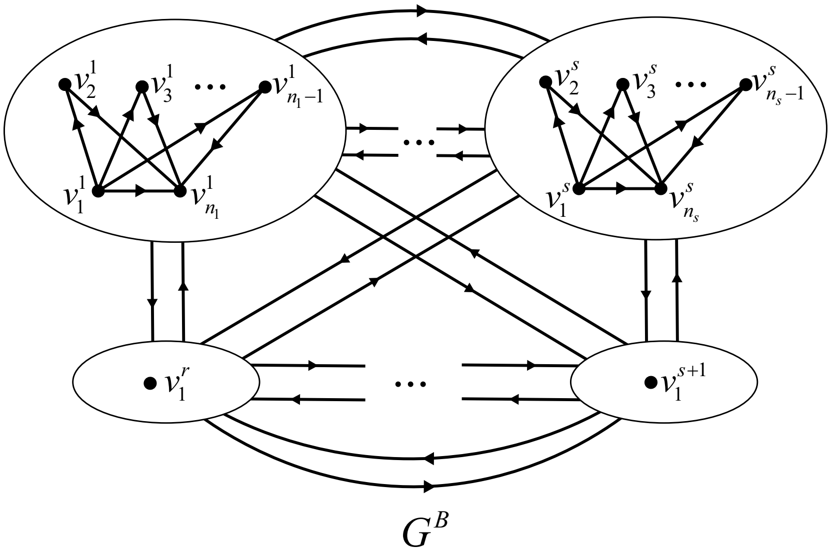
From Lemma 1.6, we obtain $\rho_\varepsilon(G^{B'}) > \rho_\varepsilon(G^B)$.

We perform the above operation as many times as possible until $n_1 = n - r + 1 > 1 = n_2 = \cdots = n_r$. Finally, we get $B_{n-r+1} \vee \overleftrightarrow{K}_{r-1}$ attaining the maximal eccentricity spectral radius of $G = \bigvee_{i=1}^r V^i$ if each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) = n_i - 1$. $\square$

Theorem 5.9. *Let $G = \bigvee_{i=1}^r V^i$. If each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, then*

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}).$$

Proof. Similar to the proof of Theorem 5.8, since $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, there is only one vertex with outdegree $n_i - 1$ in V^i, and we let $\mathcal{V}(V^i) = \{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ with $d_{V^i}^+(v_1^i) = n_i - 1$. And $\varepsilon(G)$ is maximal when each $V^i = \overrightarrow{K}_{1,n_i-1}$.



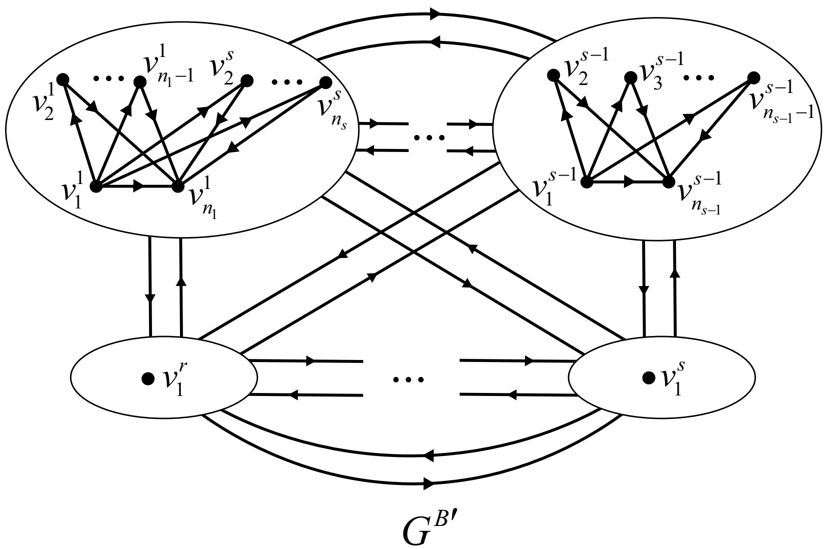


Figure 5.5: The digraphs G^B and $G^{B\prime}$.

Let $G^{\overrightarrow{K}} = \bigvee_{i=1}^{r} \overrightarrow{K}_{1,n_i-1}$ with $n_1 \geq n_2 \geq \cdots \geq n_r \geq 3$. For $\varepsilon(G^{\overrightarrow{K}}) = [\varepsilon^{is}]_{r\times r}$, we get

$$\varepsilon^{is} = \begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{n_i\times n_s} \quad \text{and } \varepsilon^{ii} = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 & 1 \\ 2 & 0 & 2 & \cdots & 2 & 2 \\ 2 & 2 & 0 & \cdots & 2 & 2 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 2 & 2 & 2 & \cdots & 0 & 2 \\ 2 & 2 & 2 & \cdots & 2 & 0 \end{pmatrix}_{n_i\times n_i},$$

where $i, s = 1, 2, \ldots, r$ and $i \neq s$.

Since $G^{\overrightarrow{K}^{\varepsilon}}$ is strongly connected, $\varepsilon(G^{\overrightarrow{K}})$ is an irreducible and nonnegative matrix. Similarly, we get $\rho_\varepsilon(G) \leq \rho_\varepsilon(G^{\overrightarrow{K}})$, with equality holding if and only if $G = G^{\overrightarrow{K}}$. Next we prove $\rho_\varepsilon(G^{\overrightarrow{K}}) < \rho_\varepsilon(\overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1})$.

Similar to the proof of Theorem 5.8, suppose that

$$\mathbf{x} = (x_1^1, x_2^1, \ldots, x_{n_1}^1, x_1^2, x_2^2, \ldots, x_{n_2}^2, \ldots, x_1^r, x_2^r, \ldots, x_{n_r}^r)^T$$

is a Perron vector of $G^{\overrightarrow{K}}$ corresponding to the eccentricity spectral radius $\rho_\varepsilon = \rho(\varepsilon(G^{\overrightarrow{K}}))$, where x_j^i is the characteristic component corresponding to v_j^i of $\overrightarrow{K}_{1,n_i-1}$ for each $1 \leq i \leq r$ and $1 \leq j \leq n_i$.

Since $\varepsilon(G^{\overrightarrow{K}})\mathbf{x} = \rho_\varepsilon \mathbf{x}$, we have

$$\begin{cases} \sum_{s=1}^{r} \sum_{t=1}^{n_s} x_t^s - x_1^i = \rho_\varepsilon x_1^i, \\ \sum_{t=1}^{n_i} 2x_t^i - 2x_j^i = \rho_\varepsilon x_j^i, \end{cases}$$

where $i = 1, 2, \ldots, r$ and $j = 2, 3, \ldots, n_i$. From Lemma 1.5 (Perron-Frobenius Theorem), $x_1^1 = x_1^2 = \cdots = x_1^r = \frac{1}{\rho_\varepsilon + 1}$ and $x_j^i = \frac{2}{\rho_\varepsilon - 2n_i + 4} x_1^i$.

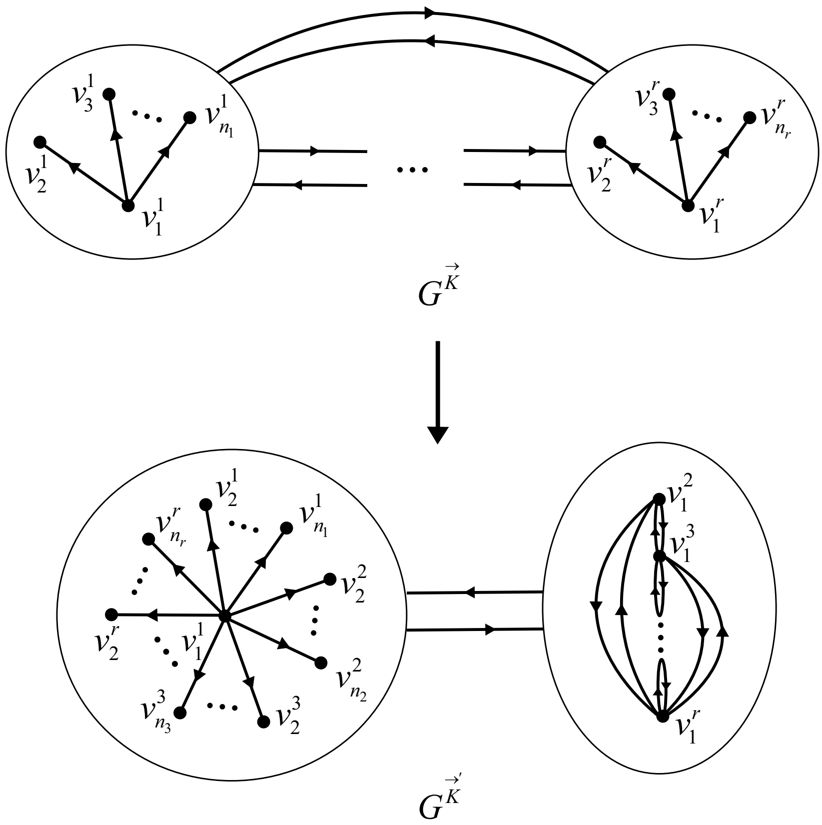


Figure 5.6: The digraphs $G^{\vec{K}}$ and $G^{\vec{K}'}$.

Let $\overrightarrow{G^{K}}' = \overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}$. That is, see Figure 5.6, $\overrightarrow{G^{K}}' = \bigvee_{i=1}^{r} V^i$ with $V^1 = \overrightarrow{K}_{1,n-r}$ and $V^2 = V^3 = \cdots = V^r = K_1$. Then we get

$$\varepsilon(\overrightarrow{G^{K}}')\mathbf{x} - \varepsilon(\overrightarrow{G^{K}})\mathbf{x} = \left(0, \underbrace{y_1, \ldots, y_1}_{n_1-1}, 0, \underbrace{y_2, \ldots, y_2}_{n_2-2}, 0, \underbrace{y_3, \ldots, y_3}_{n_3-1}, \ldots, 0, \underbrace{y_r, \ldots, y_r}_{n_r-1}\right)^T,$$

where $y_1 = \sum_{s=2}^{r}(x_1^s + 2\sum_{t=2}^{n_s} x_t^s)$, $y_i = 2\sum_{t=1}^{n_1} x_t^1 + \sum_{s=2}^{r}(x_1^s + 2\sum_{t=2}^{n_s} x_t^s) - (x_1^i + 2\sum_{t=2}^{n_i} x_t^i) - x_1^i$ for $i = 2, 3, \ldots, r$.

Since $x_1^1 = x_1^i$, we have $y_i \geq 0$ for $i = 2, 3, \ldots, r$. Obviously, $y_1 > 0$. So we get

$$\varepsilon(\overrightarrow{G^{K}}')\mathbf{x} > \varepsilon(\overrightarrow{G^{K}})\mathbf{x} = \rho(\varepsilon(\overrightarrow{G^{K}}))\mathbf{x}.$$

From Lemma 1.6, we obtain $\rho(\varepsilon(\overrightarrow{G^{K}}')) > \rho(\varepsilon(\overrightarrow{G^{K}}))$.

Hence, we obtain

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}),$$

if each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$. $\square$

Theorem 5.10. *Let $G = \bigvee_{i=1}^{r} V^i$. If each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, then*

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}).$$

Proof. Similar to the proof of Theorem 5.8, since $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, there is only one vertex with indegree $n_i - 1$ in V^i, and we let $\mathcal{V}(V^i) = \{v_1^i, v_2^i, \ldots, v_{n_i}^i\}$ with $d_{V^i}^-(v_1^i) = n_i - 1$. And $\varepsilon(G)$ is maximal when each $V^i = \overleftarrow{K}_{1,n_i-1}$.

Let $G^{\overleftarrow{K}} = \bigvee_{i=1}^{r} \overleftarrow{K}_{1,n_i-1}$ with $n_1 \geq n_2 \geq \cdots \geq n_r \geq 3$. For $\varepsilon(G^{\overleftarrow{K}}) = [\varepsilon^{is}]_{r\times r}$, we get

$$\varepsilon^{is} = \begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}_{n_i\times n_s} \quad \text{and } \varepsilon^{ii} = \begin{pmatrix} 0 & 2 & 2 & \cdots & 2 & 2 \\ 1 & 0 & 2 & \cdots & 2 & 2 \\ 1 & 2 & 0 & \cdots & 2 & 2 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 1 & 2 & 2 & \cdots & 0 & 2 \\ 1 & 2 & 2 & \cdots & 2 & 0 \end{pmatrix}_{n_i\times n_i},$$

where $i,s = 1,2,\ldots,r$ and $i \neq s$.

Since $G^{\overleftarrow{K}^{\varepsilon}}$ is strongly connected, $\varepsilon(G^{\overleftarrow{K}})$ is an irreducible and nonnegative matrix. Similarly, we get $\rho_\varepsilon(G) \leq \rho_\varepsilon(G^{\overleftarrow{K}})$, with equality holding if and only if $G = G^{\overleftarrow{K}}$. Next we prove $\rho_\varepsilon(G^{\overleftarrow{K}}) < \rho_\varepsilon(\overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1})$.

Let $G^{\overleftarrow{K}'} = \overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}$. That is, see Figure 5.7, $G^{\overleftarrow{K}'} = \bigvee_{i=1}^{r} V^i$ with $V^1 = \overleftarrow{K}_{1,n-r}$ and $V^2 = V^3 = \cdots = V^r = K_1$.

Actually, $\varepsilon(G^{\overleftarrow{K}}) = \left(\varepsilon(G^{\overrightarrow{K}})\right)^T$. So $\rho_\varepsilon(\bigvee_{i=1}^{r} \overleftarrow{K}_{1,n_i-1}) = \rho_\varepsilon(\bigvee_{i=1}^{r} \overrightarrow{K}_{1,n_i-1})$. Also, $\overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1} = \left(\overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}\right)^T$. Hence, we obtain

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}),$$

if each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) = n_i - 1$. □

Theorem 5.11. *Let $G = V \vee \overleftrightarrow{K}_{r-1}$, in which V is an acyclic digraph of order $n - r + 1$. Then*

$$\rho_\varepsilon(G) \leq \frac{2n - r - 2 + \sqrt{4n^2 + 4n - 4r - 8nr + 5r^2}}{2},$$

with equality holding if and only if $G = \overleftrightarrow{K}_{n-r+1,1,\ldots,1}$.

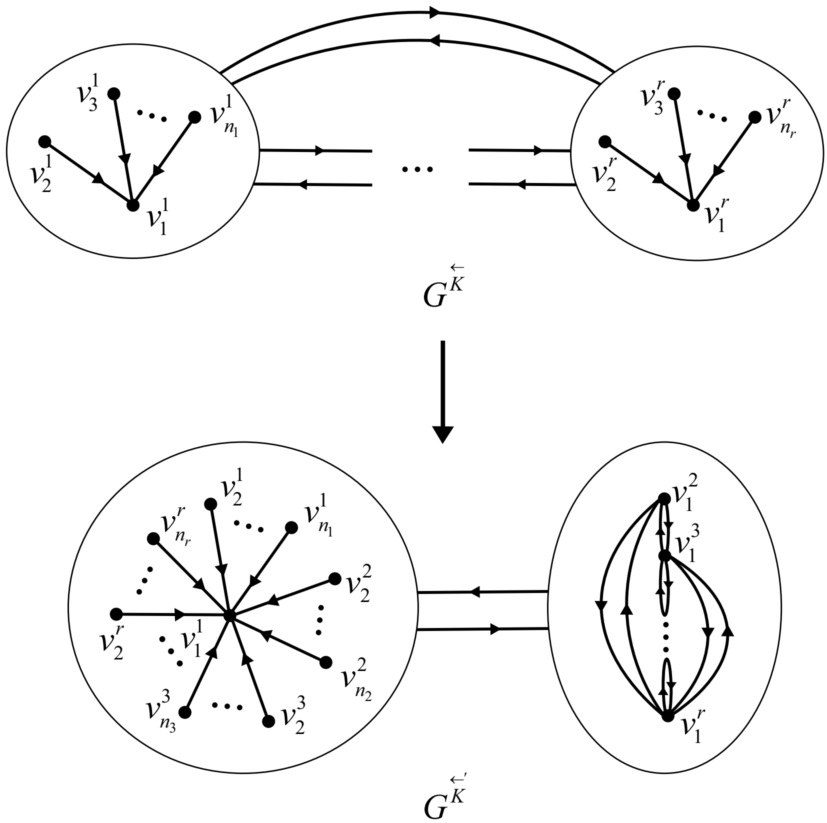


Figure 5.7: The digraphs $\overleftarrow{G^K}$ and $\overleftarrow{G^K}'$.

Proof. Since $G = V \vee \overleftrightarrow{K}_{r-1}$, for any $u \in \overleftrightarrow{K}_{r-1}$, we get that the elements of the row and column of vertex u of $\varepsilon(G)$ are all 1, except for the diagonal element. Then

$$\varepsilon(G) = \varepsilon(V \vee \overleftrightarrow{K}_{r-1}) = \begin{pmatrix} \varepsilon^* & J_{(n-r+1)\times(r-1)} \\ J_{(r-1)\times(n-r+1)} & J_{r-1} - I_{r-1} \end{pmatrix}.$$

By the definition of eccentricity matrix, $\varepsilon^* \leq 2(J_{n-r+1} - I_{n-r+1})$. By the proof of Theorems 5.7-5.10, $\varepsilon^* = 2(J_{n-r+1} - I_{n-r+1})$ if and only if $V = (n-r+1)K_1$. So we obtain

$$\rho_\varepsilon(G) \leq \rho_\varepsilon((n-r+1)K_1 \vee \overleftrightarrow{K}_{r-1}) = \rho_\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\dots,1}).$$

Since

$$\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\dots,1}) = \begin{pmatrix} 2(J_{n-r+1} - I_{n-r+1}) & J_{(n-r+1)\times(r-1)} \\ J_{(r-1)\times(n-r+1)} & J_{r-1} - I_{r-1} \end{pmatrix},$$

we get that the equitable quotient matrix of $\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\dots,1})$ is

$$B(\overleftrightarrow{K}_{n-r+1,1,\dots,1}) = \begin{pmatrix} 2(n-r) & r-1 \\ n-r+1 & r-2 \end{pmatrix}.$$

By Lemma 1.7, we obtain

$$\begin{aligned} \rho_\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\dots,1}) &= \rho(B(\overleftrightarrow{K}_{n-r+1,1,\dots,1})) \\ &= \frac{2n - r - 2 + \sqrt{4n^2 + 4n - 4r - 8nr + 5r^2}}{2}. \end{aligned}$$

□

From Theorems 5.7-5.10, for $G = \bigvee_{i=1}^{r} V^i$, we get:

(i) if each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, then

$$\rho_\varepsilon(G) \leq \rho_\varepsilon(\overleftrightarrow{K}_{n-2r+2,2,\ldots,2}) < \rho_\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\ldots,1});$$

(ii) if each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, then

$$\rho_\varepsilon(G) \leq \rho_\varepsilon(B_{n-r+1} \vee \overleftrightarrow{K}_{r-1});$$

(iii) if each V^i has $\Delta^+(V^i) = n_i - 1$ and $\Delta^-(V^i) \neq n_i - 1$, then

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overrightarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1});$$

(v) if each V^i has $\Delta^+(V^i) \neq n_i - 1$ and $\Delta^-(V^i) = n_i - 1$, then

$$\rho_\varepsilon(G) < \rho_\varepsilon(\overleftarrow{K}_{1,n-r} \vee \overleftrightarrow{K}_{r-1}).$$

From Theorem 5.11, for $G = V \vee \overleftrightarrow{K}_{r-1}$, in which V is an acyclic digraph of order $n - r + 1$, we get

$$\rho_\varepsilon(G) \leq \rho_\varepsilon(\overleftrightarrow{K}_{n-r+1,1,\ldots,1}).$$

So we guess that $\overleftrightarrow{K}_{n-r+1,1,\ldots,1}$ attains the upper bound for the eccentricity spectral radius among all join digraphs in $\mathscr{G}_{n,r}$. Since we were unable to prove or refute this, we leave it as a challenging open problem.

Problem 5.1. Find the upper bound and characterize the maximal digraphs for the eccentricity spectral radius among all join digraphs with a fixed dichromatic number.

Summary

The research that led to this thesis is of a pure theoretical nature, and part of the general area within mathematics which is commonly referred to as algebraic graph theory. One of the mainstreams in this area is the study of eigenvalues of certain matrices associated with graphs, as well as their significance for the structure and properties of the graphs. As such, these eigenvalues are closely related to other graph invariants, and have proved to be relevant in applications such as chemical graph theory. However, the results reported here are mainly of theoretical interest.

This thesis contains a number of new contributions to the research field that studies the spectral properties of graphs, involving the eigenvalues of different types of matrices associated with these graphs. One of the central problems in this area is the problem of finding the extremal values and characterizing the extremal graphs for invariants involving the eigenvalues of the graph matrix. In this thesis, we restrict ourselves to studying the spectral properties of digraphs, since results on digraphs in this area are relatively scarce.

Commonly studied concepts related to the eigenvalues of digraph matrices are the spectral radius, the k-th spectral moment, the spread, and the sum of k largest eigenvalues. In such studies, one of the approaches is to restrict the attention to digraph classes for which a certain graph parameter is fixed. In this thesis we focus on digraphs with a fixed dichromatic number. With respect to the choice of particular matrices, in this thesis we focus on the spectral properties for the Laplacian matrix, the A_α-matrix, and the eccentricity matrix.

In Chapters 2 and 3, we focus on studying the k-th spectral moment. In

Chapters 4 and 5, we focus on studying the spectral radius. In particular, in Chapter 2 we study the k-th spectral moment of the Laplacian matrix of digraphs. In Chapters 3 and 4, we study the k-th spectral moment and spectral radius of the A_α-matrix of digraphs, respectively. In Chapter 5, we study the spectral radius of the eccentricity matrix of digraphs. Our main new contributions to the field can be described as follows.

In Chapter 2, we characterize the digraphs which attain the minimal and maximal Laplacian energy among all digraphs with a fixed dichromatic number. We also determine sharp bounds for the third Laplacian spectral moment among all join digraphs.

In Chapter 3, we obtain the digraphs which attain the minimal and maximal A_α energy among all digraphs with a fixed dichromatic number. We also determine sharp bounds for the third A_α spectral moment among all join digraphs. These results generalize the results about the second and third Laplacian spectral moments of digraphs in Chapter 2.

We find that the Laplacian matrix and the A_α-matrix have much in common with respect to the second and third spectral moments. In particular, the second spectral moments of the Laplacian matrix and the $A_{\frac{1}{2}}$-matrix are the same. Concerning the spectral radius, scholars often study the spectral radius of the adjacency matrix, signless Laplacian matrix and A_α-matrix. But scholars rarely study the spectral radius of the Laplacian matrix, since the Laplacian matrix is not a nonnegative matrix. Also, the extremal digraphs for the Laplacian spectral radius may be very different from that of the A_α-matrix.

In Chapter 4, we characterize the digraph which has the maximal A_α spectral radius among all digraphs with a fixed dichromatic number, by using the equitable quotient matrix. This provides a new proof of the results by Liu et al. [89]. Moreover, we obtain the digraph which has the minimal A_α spectral radius of the join of in-trees with a fixed dichromatic number.

In Chapter 5, we consider bounds for the spectral radius of the eccentricity matrix of join digraphs with a fixed dichromatic number. We attain lower bounds for the eccentricity spectral radius among all join digraphs with a fixed dichromatic number, and give upper bounds for the eccentricity spectral radius of some special join digraphs with a fixed dichromatic number. These extremal digraphs for the eccentricity spectral radius are very different from those in the other chapters.

The eccentricity matrix of a graph is a relatively new matrix. Although there are already several results on eccentricity matrices of graphs, the study regarding eccentricity matrices of digraphs has just begun. The eccentricity matrix seems to be difficult to study. In particular, the eccentricity matrix of a digraph has the additional difficulty of being asymmetric. This is reflected by the complex structure of the extremal digraphs, complicating their characterization.

The asymmetric nature of the matrices associated with digraphs poses a great difficulty for solving problems of the above type. However, since undirected graphs can be considered as a special type of digraphs, results on digraphs are more general, and therefore studying them is worthwhile. Throughout this thesis, we present several open problems that remain unsolved. This shows that there is still much to be explored in this fascinating area of algebraic graph theory.

Samenvatting

Het onderzoek dat heeft geleid tot dit proefschrift is puur theoretisch van aard, en deel van het algemene gebied binnen de wiskunde dat meestal wordt aangeduid als algebraïsche grafentheorie. Eén van de hoofdrichtingen binnen dit gebied is de studie van eigenwaarden van bepaalde met grafen geassocieerde matrices, en hun belang voor de structuur en eigenschappen van die grafen. Als zodanig zijn deze eigenwaarden nauw verbonden met andere invarianten van grafen, en hebben ze hun belang in toepassingen zoals chemische grafentheorie bewezen. De hier gerapporteerde resultaten zijn echter hoofdzakelijk van theoretische betekenis.

Dit proefschrift bevat een aantal nieuwe bijdragen op het gebied van de spectrale grafentheorie. Dit deelgebied van de grafentheorie richt zich op het bestuderen van structurele eigenschappen van grafen die verband houden met de eigenwaarden van bepaalde matrices die aan de hand van die grafen gedefinieerd kunnen worden. In dit proefschrift richten we ons met name op gerichte grafen en het bepalen van de extreme waarden van invarianten die gebaseerd zijn op de eigenwaarden van drie typen matrices, alsmede het karakteriseren van de structuur van de bijbehorende gerichte grafen. De drie typen matrices waartoe we ons beperken zijn de Laplacian matrix, de A_α-matrix en de excentriciteitsmatrix.

In Hoofdstuk 2 en 3 bestuderen we de extreme waarden en extremale gerichte grafen van het k-de spectrale moment. In Hoofdstuk 4 en 5 richten we ons op het bestuderen van de spectrale straal. Daarbij gaat het in Hoofdstuk 2 om het k-de spectrale moment van de Laplacian matrix van gerichte grafen. In Hoofdstuk 3 en 4 richten we ons respectievelijk op het k-de spectrale moment en de spectrale straal van de A_α-matrix van gerichte grafen. In Hoofdstuk 5 bestuderen we de spectrale straal van de excentriciteitsmatrix van gerichte grafen.

In het bijzonder bepalen we in Hoofdstuk 2 de gerichte grafen met de minimale en maximale Laplacian energie, onder alle gerichte grafen met een vast dichromatisch getal. We bepalen tevens scherpe grenzen voor het derde Laplacian spectrale moment voor alle gerichte grafen met een vast dichromatisch getal.

In Hoofdstuk 3 doen we hetzelfde, maar dan voor de minimale en maximale energie behorend by de A_α-matrix, wederom onder alle gerichte grafen met een vast dichromatisch getal. We bepalen ook wederom scherpe grenzen voor het derde spectrale moment van deze A_α-matrix onder alle gerichte grafen met een vast dichromatisch getal. Deze resultaten veralgemeniseren de resultaten betreffende het tweede en derde Laplacian spectrale moment van gerichte grafen uit Hoofdstuk 2.

We constateren dat de Laplacian matrix en de A_α-matrix veel overeenkomsten vertonen wat betreft het tweede en derde spectrale moment. Met name de tweede spectrale momenten van de Laplacian matrix en de $A_{\frac{1}{2}}$-matrix komen overeen. Voor wat betreft de spectrale straal bestuderen deskundigen vaak de spectrale straal van de buurmatrix, de tekenloze Laplacian matrix en de A_α-matrix. Maar wetenschappers bestuderen in veel mindere mate de spectrale straal van de Laplacian matrix, omdat de Laplacian matrix geen niet-negatieve matrix is. Ook kunnen de extremale grafen voor de spectrale straal van de Laplacian matrix sterk verschillen van die van de A_α-matrix.

In Hoofdstuk 4 bepalen we de gerichte graaf die de maximale spectrale straal van de A_α-matrix aanneemt, onder alle gerichte grafen met een vast dichromatisch getal, door gebruik te maken van de 'equitable quotient' matrix. Dit levert een nieuw bewijs op van de resultaten van Liu et al. [89]. Bovendien bepalen we de gerichte graaf met de minimale spectrale straal van de A_α-matrix onder de 'join' van in-bomen met een vast dichromatisch getal. Tenslotte bepalen we in dit hoofdstuk de maximale gerichte graaf voor de spectrale straal van de A_α-matrix onder alle 'joins' als de gerichte graaf $G = \bigvee_{i=1}^{r} V^i$ waarbij elke V^i een transitief toernooi is met

$|\mathscr{V}(V^i) - \mathscr{V}(V^j)| \leq 1$.

In Hoofdstuk 5 beschouwen we de grenzen voor de spectrale straal van de excentriciteitsmatrix van 'joins' met een vast dichromatisch getal. We stellen de ondergrenzen vast voor de spectrale straal van de excentriciteitsmatrix onder alle 'joins' met een vast dichromatisch getal en geven bovengrenzen voor de spectrale straal van de excentriciteitsmatrix van enkele speciale 'joins' met een vast dichromatisch getal. Deze extremale gerichte grafen voor de excentriciteitsmatrix verschillen sterk van die uit de andere hoofdstukken.

De excentriciteitsmatrix van grafen is een relatief nieuwe matrix. Hoewel er al een aantal resultaten bekend zijn voor de excentriciteitsmatrix van ongerichte grafen, is de studie naar eigenschappen van de excentriciteitsmatrix van gerichte grafen nog maar net begonnen. Deze excentriciteitsmatrix lijkt een stuk moeilijker te bestuderen, en de extremale grafen zien er complexer uit waardoor ze moeilijker te karakteriseren zijn.

Daarbij komt het probleem van de asymmetrie van dit soort matrices voor gerichte grafen. Die asymmetrie bemoeilijkt de studie naar de eigenschappen van die matrices en in het bijzonder het bepalen van hun extreme waarden wat betreft invarianten van hun eigenwaarden. Aangezien ongerichte grafen als een speciaal type gerichte grafen kunnen worden opgevat, zijn studies naar gerichte grafen meer omvattend en zeer de moeite waard.

Naast de nieuwe bijdragen presenteren we in dit proefschrift tevens verschillende open problemen die onopgelost blijven. Dit toont onder andere aan dat er nog veel diepgaand onderzoek met betrekking tot gerichte grafen mogelijk is, met name binnen het fascinerende gebied van de algebraïsche grafentheorie.

Bibliography

[1] B. Afshari, M.T. Saadati, R. Saadati, Lower bounds for the Laplacian spectral radius of graphs, *Linear Algebra Appl.* **631** (2021) 136–142.

[2] N. Agudelo, J. Rada, M. Rivera, Upper bound for the trace norm of the Laplacian matrix of a digraph and normally regular digraphs, *Linear Algebra Appl.* **552** (2018) 194–209.

[3] D. Al-Mniny, Subdivisions of four blocks cycles in digraphs with large chromatic number, *Discrete Appl. Math.* **305** (2021) 71–75.

[4] M. Baghipur, H.A. Ganie, M. Ghorbani, E. Andrade, On the spectral radius of the generalized adjacency matrix of a digraph, *Linear Algebra Appl.* **653** (2022) 287–313.

[5] W. Barrett, T.R. Cameron, E. Evans, H.T. Hall, M. Kempton, On the Laplacian spread of digraphs, *Linear Algebra Appl.* **664** (2023) 126–146.

[6] A. Berman, R.J. Plemmons, Nonnegative matrices in the mathematical sciences, Computer Science and Applied Mathematics, *Academic Press, New York*, 1979.

[7] D. Bokal, G. Fijavž, M. Juvan, P.M. Kayll, B. Mohar, The circular chromatic number of a digraph, *J. Graph Theory* **46** (2004) 227–240.

[8] J.A. Bondy, U.S.R. Murty, Graph theory, Graduate Texts in Mathematics, 244, *Springer, New York*, 2008.

[9] S.S. Bose, M. Nath, S. Paul, On the maximal distance spectral radius of graphs without a pendent vertex, *Linear Algebra Appl.* **438** (2013) 4260–4278.

[10] Ş.B. Bozkurt, D. Bozkurt, On the signless Laplacian spectral radius of digraphs, *Ars Combin.* **108** (2013) 193–200.

[11] Ş.B. Bozkurt, D. Bozkurt, X.D. Zhang, On the spectral radius and the energy of a digraph, *Linear Multilinear Algebra* **63** (2015) 2009–2016.

[12] A.E. Brondani, F.A.M. França, C.S. Oliveira, Positive semidefiniteness of $A_\alpha(G)$ on some families of graphs, *Discrete Appl. Math.* **323** (2022) 113–123.

[13] A.E. Brouwer, W.H. Haemers, Spectra of graphs, *Springer, New York*, 2012.

[14] R.A. Brualdi, Spectra of digraphs, *Linear Algebra Appl.* **432** (2010) 2181–2213.

[15] X.D. Chen, On Brouwer's conjecture for the sum of k largest Laplacian eigenvalues of graphs, *Linear Algebra Appl.* **578** (2019) 402–410.

[16] X.D. Chen, K.C. Das, Some results on the Laplacian spread of a graph, *Linear Algebra Appl.* **505** (2016) 245–260.

[17] Q.Q. Chen, Q.X. Huang, The maximal A_α-spectral radius of graphs with given matching number, *Linear Multilinear Algebra* **70** (2022) 5193–5206.

[18] Y.Q. Chen, L.G. Wang, The Laplacian spread of tricyclic graphs, *Electron. J. Combin.* **16** (2009) Paper 80, 18 pp.

[19] W.W. Chen, B. Wang, M.Q. Zhai, Signless Laplacian spectral radius of graphs without short cycles or long cycles, *Linear Algebra Appl.* **645** (2022) 123–136.

[20] M.Z. Chen, X.D. Zhang, On the signless Laplacian spectral radius of $K_{s,t}$-minor free graphs, *Linear Multilinear Algebra* **69** (2021) 1922–1934.

[21] B. Cheng, B.L. Liu, J.X. Liu, On the spectral moments of unicyclic graphs with fixed diameter, *Linear Algebra Appl.* **437** (2012) 1123–1131.

[22] S.M. Cioabǎ, E.R. van Dam, J.H. Koolen, J.H. Lee, A lower bound for the spectral radius of graphs with fixed diameter, *European J. Combin.* **31** (2010) 1560–1566.

[23] N. Cohen, F. Havet, W. Lochet, R. Lopes, Bispindles in strongly connected digraphs with large chromatic number, *Electron. J. Combin.* **25** (2018) Paper No. 2.39, 19 pp.

[24] N. Cohen, F. Havet, W. Lochet, N. Nisse, Subdivisions of oriented cycles in digraphs with large chromatic number, *J. Graph Theory* **89** (2018) 439–456.

[25] D.M. Cvetković, M. Doob, I. Gutman, A. Torgašev, Recent results in the theory of graph spectra, Annals of Discrete Mathematics, 36, *North-Holland Publishing Co., Amsterdam*, 1988.

[26] D.M. Cvetković, M. Doob, H. Sachs, Spectra of graphs. Theory and application, Pure and Applied Mathematics, 87, *Academic press, New York*, 1980.

[27] D.M. Cvetković, M. Doob, H. Sachs, Spectra of graphs. Theory and Application, third ed. *Johann Ambrosius Barth Verlag, Heidelberg*, 1995.

[28] D.M. Cvetković, P. Rowlinson, S. Simić, An introduction to the theory of graph spectra, London Mathematical Society Student Texts, 75, *Cambridge University Press, Cambridge*, 2010.

[29] D.M. Cvetković, D. Stevanović, Spectral moments of fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 63–72.

[30] P. Dankelmann, Distance and size in digraphs, *Discrete Math.* **338** (2015) 144–148.

[31] M. Dehmer, Y.T. Shi, The uniqueness of D_{MAX}-matrix graph invariants, *PLoS One* **9** (2014) e83868.

[32] S. Drury, H.Q. Lin, Colorings and spectral radius of digraphs, *Discrete Math.* **339** (2016) 327–332.

[33] Z.B. Du, B. Zhou, Upper bounds for the sum of Laplacian eigenvalues of graphs, *Linear Algebra Appl.* **436** (2012) 3672–3683.

[34] L.F. Fang, B. Wang, M.Q. Zhai, On the spectral moment of quasi-bicyclic graphs, *Appl. Math. Comput.* **363** (2019) 124601.

[35] L.F. Fang, M.Q. Zhai, B. Wang, Complete subgraphs in connected graphs and its application to spectral moment, *Discrete Appl. Math.* **291** (2021) 36–42.

[36] L.H. Feng, Q. Li, X.D. Zhang, Spectral radii of graphs with given chromatic number, *Appl. Math. Lett.* **20** (2007) 158–162.

[37] H.A. Ganie, On the A_α-spectrum of joined union of digraphs, *Discrete Math. Algorithms Appl.* **14** (2022) 2150086.

[38] H.A. Ganie, A.M. Alghamdi, S. Pirzada, On the sum of the Laplacian eigenvalues of a graph and Brouwer's conjecture, *Linear Algebra Appl.* **501** (2016) 376–389.

[39] H.A. Ganie, M. Baghipur, Bounds for the A_α-spectral radius of a digraph, *Mat. Vesnik* **74** (2022) 119–129.

[40] H.A. Ganie, M. Baghipur, On the generalized adjacency spectral radius of digraphs, *Linear Multilinear Algebra* **70** (2022) 3497–3510.

[41] H.A. Ganie, J.R. Carmona, An (increasing) sequence of lower bounds for the spectral radius and energy of digraphs, *Discrete Math.* **346** (2023) 113118.

[42] A.L. Gavrilyuk, A. Munemasa, Maximal digraphs whose Hermitian spectral radius is at most 2, *Linear Algebra Appl.* **658** (2023) 331–349.

[43] D. González-Moreno, R. Hernández-Ortiz, B. Llano, M. Olsen, The dichromatic polynomial of a digraph, *Graphs Combin.* **38** (2022) Paper No. 85, 16 pp.

[44] R.L. Graham, A.J. Hoffman, H. Hosoya, On the distance matrix of a directed graph, *J. Graph Theory* **1** (1977) 85–88.

[45] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sekt. Forsch. Graz* **103** (1978) 1–22.

[46] I. Gutman, The energy of a graph: old and new results, *Algebraic Combinatorics and Applications, Springer, Berlin* (2001) 196–211.

[47] I. Gutman, X.L. Li, Energies of graphs-theory and applications, in: Mathematical Chemistry Monographs, No. 17, *University of Kragujevac, Kragujevac*, 2016.

[48] I. Gutman, B. Zhou, Laplacian energy of a graph, *Linear Algebra Appl.* **414** (2006) 29–37.

[49] F. Harary, Graph Theory, *Addison-Wesley, Reading*, 1969.

[50] A. Harutyunyan, B. Mohar, Two results on the digraph chromatic number, *Discrete Math.* **312** (2012) 1823–1826.

[51] X.C. He, L. Lu, On the largest and least eigenvalues of eccentricity matrix of trees, *Discrete Math.* **345** (2022) 112662.

[52] C. Helmberg, V. Trevisan, Spectral threshold dominance, Brouwer's conjecture and maximality of Laplacian energy, *Linear Algebra Appl.* **512** (2017) 18–31.

[53] L. Hogben, C. Reinhart, Spectra of variants of distance matrices of graphs and digraphs: a survey, *Matematica* **1** (2022) 186–224.

[54] Y. Hong, J.L. Shu, K.F. Fang, A sharp upper bound of the spectral radius of graphs, *J. Combin. Theory Ser. B* **81** (2001) 177–183.

[55] W.X. Hong, L.H. You, Spectral radius and signless Laplacian spectral radius of strongly connected digraphs, *Linear Algebra Appl.* **457** (2014) 93–113.

[56] R.A. Horn, C.R. Johnson, Matrix Analysis, *Cambridge University Press, New York*, 1985.

[57] P. Huang, J.X. Li, W.C. Shiu, Maximizing the A_α-spectral radius of graphs with given size and diameter, *Linear Algebra Appl.* **651** (2022) 116–130.

[58] A. Jahanbani, S.M. Sheikholeslami, On the spectral radius of the adjacency matrix and signless Laplacian matrix of a graph, *Linear Multilinear Algebra* **70** (2022) 6846–6851.

[59] Y.L. Jin, X.D. Zhang, On the spectral radius of simple digraphs with prescribed number of arcs, *Discrete Math.* **338** (2015) 1555–1564.

[60] A. Joó, Uncountable dichromatic number without short directed cycles, *J. Graph Theory* **94** (2020) 113–116.

[61] P. Keevash, Z.T. Li, B. Mohar, B. Reed, Digraph girth via chromatic number, *SIAM J. Discrete Math.* **27** (2013) 693–696.

[62] J. Kim, S. Kim, S. O, S. Oh, A Cvetković-type theorem for coloring of digraphs, *Linear Algebra Appl.* **634** (2022) 30–36.

[63] J. Kim, A.V. Kostochka, S. O, Y.T. Shi, Z.W. Wang, A sharp lower bound for the spectral radius in K_4-saturated graphs, *Discrete Math.* **346** (2023) 113231.

[64] J. Kwapisz, On the spectral radius of a directed graph, *J. Graph Theory* **23** (1996) 405–411.

[65] W.W. Lang, L.G. Wang, Sharp bounds for the signless Laplacian spectral radius of digraphs, *Appl. Math. Comput.* **238** (2014) 43–49.

[66] M. Lazić, On the Laplacian energy of a graph, *Czechoslovak Math. J.* **56** (2006) 1207–1213.

[67] X.Y. Lei, J.F. Wang, G.Z. Li, On the eigenvalues of eccentricity matrix of graphs, *Discrete Appl. Math.* **295** (2021) 134–147.

[68] X.L. Li, Y.T. Shi, I. Gutman, Graph energy, *Springer, New York*, 2012.

[69] S.C. Li, W.T. Sun, Some spectral inequalities for connected bipartite graphs with maximum A_α-index, *Discrete Appl. Math.* **287** (2020) 97–109.

[70] S.C. Li, W.T. Sun, Some bounds on the A_α-index of connected graphs with fixed order and size, *Linear Multilinear Algebra* **70** (2022) 5859–5878.

[71] D. Li, G.P. Wang, J.X. Meng, On the distance signless Laplacian spectral radius of graphs and digraphs, *Electron. J. Linear Algebra* **32** (2017) 438–446.

[72] X.H. Li, L.G. Wang, S.Y. Zhang, The signless Laplacian spectral radius of some strongly connected digraphs, *Indian J. Pure Appl. Math.* **49** (2018) 113–127.

[73] K. Li, L.G. Wang, G.P. Zhao, The signless Laplacian spectral radius of unicyclic and bicyclic graphs with a given girth, *Electron. J. Combin.* **18** (2011) Paper 183, 10 pp.

[74] J.X. Li, L.H. You, The (distance) signless Laplacian spectral radii of digraphs with given dichromatic number, *Ars Combin.* **132** (2017) 257–267.

[75] S.C. Li, Y.T. Yu, On A_α spectral extrema of graphs forbidding even cycles, *Linear Algebra Appl.* **668** (2023) 11–27.

[76] H.Q. Lin, X. Huang, J. Xue, A note on the A_α-spectral radius of graphs, *Linear Algebra Appl.* **557** (2018) 430–437.

[77] H.Q. Lin, X.G. Liu, J. Xue, Graphs determined by their A_α-spectra, *Discrete Math.* **342** (2019) 441–450.

[78] H.Q. Lin, J.L. Shu, Spectral radius of digraphs with given dichromatic number, *Linear Algebra Appl.* **434** (2011) 2462–2467.

[79] H.Q. Lin, J.L. Shu, The distance spectral radius of digraphs, *Discrete Appl. Math.* **161** (2013) 2537–2543.

[80] H.Q. Lin, J.L. Shu, Y.R. Wu, G.L. Yu, Spectral radius of strongly connected digraphs, *Discrete Math.* **312** (2012) 3663–3669.

[81] H.Q. Lin, J. Xue, J.L. Shu, On the A_α-spectra of graphs, *Linear Algebra Appl.* **556** (2018) 210–219.

[82] H.Q. Lin, W.H. Yang, H.L. Zhang, J.L. Shu, Distance spectral radius of digraphs with given connectivity, *Discrete Math.* **312** (2012) 1849–1856.

[83] H.Q. Lin, L.W. Zhang, J. Xue, Majorization, degree sequence and A_α-spectral characterization of graphs, *Discrete Math.* **343** (2020) 112132.

[84] X.X. Liu, H. Broersma, L.G. Wang, On a conjecture of Nikiforov involving a spectral radius condition for a graph to contain all trees, *Discrete Math.* **345** (2022) 113112.

[85] S.T. Liu, K.C. Das, J.L. Shu, On the eigenvalues of A_α-matrix of graphs, *Discrete Math.* **343** (2020) 111917.

[86] X.G. Liu, S.Y. Liu, On the A_α-characteristic polynomial of a graph, *Linear Algebra Appl.* **546** (2018) 274–288.

[87] H.Q. Liu, M. Lu, Bounds for the Laplacian spectral radius of graphs, *Linear Multilinear Algebra* **58** (2010) 113–119.

[88] Y. Liu, Y.Q. Sun, On the second Laplacian spectral moment of a graph, *Czechoslovak Math. J.* **60** (2010) 401–410.

[89] J.P. Liu, X.Z. Wu, J.S. Chen, B.L. Liu, The A_α spectral radius characterization of some digraphs, *Linear Algebra Appl.* **563** (2019) 63–74.

[90] C. Liu, Z.M. Yan, J.P. Li, The maximum A_α-spectral radius of t-connected graphs with bounded matching number, *Discrete Math.* **346** (2023) 113447.

[91] Y.D. Ma, S.J. Cao, Y.T. Shi, I. Gutman, M. Dehmer, B. Furtula, From the connectivity index to various Randić-type descriptors, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 85–106.

[92] I. Mahato, R. Gurusamy, M.R. Kannan, S. Arockiaraj, Spectra of eccentricity matrices of graphs, *Discrete Appl. Math.* **285** (2020) 252–260.

[93] I. Mahato, R. Gurusamy, M.R. Kannan, S. Arockiaraj, On the spectral radius and the energy of eccentricity matrices of graphs, *Linear Multilinear Algebra* **71** (2023) 5–15.

[94] I. Mahato, M.R. Kannan, On the eccentricity matrices of trees: inertia and spectral symmetrys, *Discrete Math.* **345** (2022) 113067.

[95] S.J. Miao, S.C. Li, Characterizing star factors via the size, the spectral radius or the distance spectral radius of graphs, *Discrete Appl. Math.* **326** (2023) 17–32.

[96] B. Mohar, Eigenvalues and colorings of digraphs, *Linear Algebra Appl.* **432** (2010) 2273–2277.

[97] R. Nasiri, H.R. Ellahi, A. Gholami, Ordering c-cyclic graphs with respect to signless Laplacian spectral moments, *Ars Combin.* **140** (2018) 293–300.

[98] V. Neumann-Lara, The dichromatic number of a digraph, *J. Combin. Theory Ser. B* **33** (1982) 265–270.

[99] V. Nikiforov, Merging the A- and Q-spectral theories, *Appl. Anal. Discrete Math.* **11** (2017) 81–107.

[100] V. Nikiforov, G. Pastén, O. Rojo, R.L. Soto, On the A_α-spectra of trees, *Linear Algebra Appl.* **520** (2017) 286–305.

[101] V. Nikiforov, O. Rojo, A note on the positive semidefiniteness of $A_\alpha(G)$, *Linear Algebra Appl.* **519** (2017) 156–163.

[102] M.R. Oboudi, Distance spectral radius of complete multipartite graphs and majorization, *Linear Algebra Appl.* **583** (2019) 134–145.

[103] X.F. Pan, X.G. Liu, H.Q. Liu, On the spectral moment of quasi-trees, *Linear Algebra Appl.* **436** (2012) 927–934.

[104] A.K. Patel, L. Selvaganesh, S.K. Pandey, Energy and inertia of the eccentricity matrix of coalescence of graphs, *Discrete Math.* **344** (2021) 112591.

[105] J.A. de la Peña, L. Mendoza, J. Rada, Comparing momenta and π-electron energy of benzenoid molecules, *Discrete Math.* **302** (2005) 77–84.

[106] I. Peña, J. Rada, Energy of digraphs, *Linear Multilinear Algebra* **56** (2008) 565–579.

[107] K. Perera, Y. Mizoguchi, Laplacian energy of directed graphs and minimizing maximum outdegree algorithms, *MI Preprint Series* (2010) 2010-35.

[108] S. Pirzada, H.A. Ganie, On the Laplacian eigenvalues of a graph and Laplacian energy, *Linear Algebra Appl.* **486** (2015) 454–468.

[109] H. Poincaré, Second Complement a l'Analysis Situs, *Proc. Lond. Math. Soc.* **32** (1900) 277–308.

[110] X.Q. Qi, E. Fuller, R. Luo, G.D. Guo, C.Q. Zhang, Laplacian energy of digraphs and a minimum Laplacian energy algorithm, *Internat. J. Found. Comput. Sci.* **26** (2015) 367–380.

[111] Z.P. Qiu, Z.K. Tang, On the eccentricity spectra of threshold graphs, *Discrete Appl. Math.* **310** (2022) 75–85.

[112] J. Rada, Lower bounds for the energy of digraphs, *Linear Algebra Appl.* **432** (2010) 2174–2180.

[113] M. Randić, D_{MAX}-Matrix of dominant distances in a graph, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 221–238.

[114] M. Randić, R. Orel, A.T. Balaban, D_{MAX} Matrix invariants as graph descriptors. Graphs having the same Balaban index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 239–258.

[115] H.Y. Shan, F.F. Wang, C.X. He, Some α-spectral extremal results for some digraphs, *Linear Multilinear Algebra* **70** (2022) 7493–7513.

[116] C. Soh, The circular chromatic numbers of planar digraphs, *J. Graph Theory* **55** (2007) 14–26.

[117] R. Steiner, On coloring digraphs with forbidden induced subgraphs, *J. Graph Theory* **103** (2023) 323–339.

[118] D. Stevanović, Spectral radius of graphs, *Academic Press, Amsterdam*, 2015.

[119] G.X. Tian, S.Y. Cui, On upper bounds for the energy of digraphs, *Linear Algebra Appl.* **438** (2013) 4742–4749.

[120] J.F. Wang, M. Lu, F. Belardo, M. Randić, The anti-adjacency matrix of a graph: Eccentricity matrix, *Discrete Appl. Math.* **251** (2018) 299–309.

[121] J.F. Wang, M. Lu, M. Brunetti, L. Lu, X.Y. Huang, Spectral determinations and eccentricity matrix of graphs, *Adv. in Appl. Math.* **139** (2022) 102358.

[122] J.F. Wang, M. Lu, L. Lu, F. Belardo, Spectral properties of the eccentricity matrix of graphs, *Discrete Appl. Math.* **279** (2020) 168–177.

[123] J.F. Wang, L. Lu, M. Randić, G.Z. Li, Graph energy based on the eccentricity matrix, *Discrete Math.* **342** (2019) 2636–2646.

[124] W. Wei, X.C. He, S.C. Li, Solutions for two conjectures on the eigenvalues of the eccentricity matrix, and beyond, *Discrete Math.* **343** (2020) 111925.

[125] W. Wei, S.C. Li, L.C. Zhang, Characterizing the extremal graphs with respect to the eccentricity spectral radius, and beyond, *Discrete Math.* **345** (2022) 112686.

[126] Y.P. Wu, H.Q. Liu, Q. Fan, On the spectral moments of signless Laplacian matrix of trees and unicyclic graphs, *Ars Combin.* **141** (2018) 345–351.

[127] W.G. Xi, On the A_α spectral radius and A_α energy of digraphs, 2021. Available at https://arxiv.org/abs/2107.06470v1.

[128] W.G. Xi, W. So, L.G. Wang, The (distance) signless Laplacian spectral radius of digraphs with given arc connectivity, *Linear Algebra Appl.* **581** (2019) 85–111.

[129] W.G. Xi, W. So, L.G. Wang, On the distance spectral radius of digraphs with given diameter, *Linear Multilinear Algebra* **69** (2021) 2547–2557.

[130] W.G. Xi, W. So, L.G. Wang, On the A_α spectral radius of digraphs with given parameters, *Linear Multilinear Algebra* **70** (2022) 2248–2263.

[131] W.G. Xi, L.G. Wang, Sharp upper bounds on the signless Laplacian spectral radius of strongly connected digraphs, *Discuss. Math. Graph Theory* **36** (2016) 977–988.

[132] W.G. Xi, L.G. Wang, The signless Laplacian and distance signless Laplacian spectral radius of digraphs with some given parameters, *Discrete Appl. Math.* **227** (2017) 136–141.

[133] W.G. Xi, L.G. Wang, The A_α spectral radius and maximum outdegree of irregular digraphs, *Discrete Optim.* **38** (2020) 100592.

[134] W.G. Xi, L.G. Wang, On the A_α spectral radius of strongly connected digraphs, *Oper. Matrices* **16** (2022) 1005–1026.

[135] J. Xue, H.Q. Lin, S.T. Liu, J.L. Shu, On the A_α-spectral radius of a graph, *Linear Algebra Appl.* **550** (2018) 105–120.

[136] X.W. Yang, L.G. Wang, Extremal Laplacian energy of directed trees, unicyclic digraphs and bicyclic digraphs, *Appl. Math. Comput.* **366** (2020) 124737.

[137] X.W. Yang, L.G. Wang, The eccentricity matrix of a digraph, *Discrete Appl. Math.* **322** (2022) 61–73.

[138] L.H. You, M. Yang, W. So, W.G. Xi, On the spectrum of an equitable quotient matrix and its application, *Linear Algebra Appl.* **577** (2019) 21–40.

[139] Q.X. Yuan, R.F. Liu, J.J. Yuan, The A_α-spectral radius of nonregular graphs (digraphs) and maximum degree (outdegree), *Discrete Optim.* **47** (2023) 100758.

[140] M.Q. Zhai, Y.R. Wu, J.L. Shu, Maximizing the spectral radius of bicyclic graphs with fixed girth, *Linear Algebra Appl.* **431** (2009) 716–723.

[141] X.L. Zhang, On the distance spectral radius of unicyclic graphs with perfect matchings, *Electron. J. Linear Algebra* **27** (2014) 569–587.

[142] H.H. Zhang, S.C. Li, On the Laplacian spectral radius of bipartite graphs with fixed order and size, *Discrete Appl. Math.* **229** (2017) 139–147.

[143] Y.K. Zhang, H.Q. Lin, Perfect matching and distance spectral radius in graphs and bipartite graphs, *Discrete Appl. Math.* **304** (2021) 315–322.

[144] X.L. Zhang, H.P. Zhang, The Laplacian spectral radius of some bipartite graphs, *Linear Algebra Appl.* **428** (2008) 1610–1619.

[145] X.L. Zhang, H.P. Zhang, Some results on Laplacian spectral radius of graphs with cut vertices, *Discrete Math.* **310** (2010) 3494–3505.

[146] B. Zhou, I. Gutman, J.A. de la Peña, J. Rada, L. Mendoza, On spectral moments and energy of graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 183–191.

[147] B.X. Zhu, On the signless Laplacian spectral radius of graphs with cut vertices, *Linear Algebra Appl.* **433** (2010) 928–933.

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Xiuwen Yang
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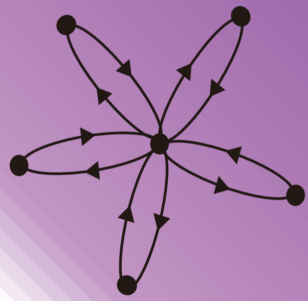
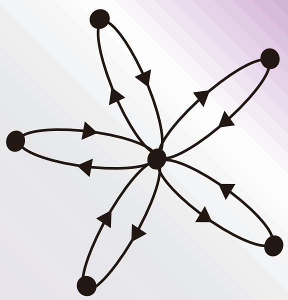
About the Author

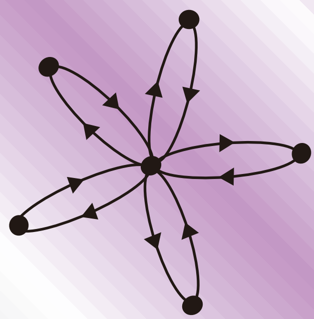
Xiuwen Yang was born on April 14, 1995 in Xingtai City, Hebei Province, P.R. China. From 2001 to 2007, Xiuwen Yang studied in an elementary education in her city. From 2007 to 2010, she completed her junior middle school education in Xingtai Foreign Language School. From 2010 to 2013, she completed her senior middle school education in NO.1 High School of Xingtai.

In September 2013, she stared her college life at Yunnan Normal University (YNNU). In June 2017, she received her bachelor degree, and she was recommended for exemption to graduate school at Northwestern Polytechnical University (NPU) with the first ranking in her major in YNNU. Since then, she started to study the spectral properties of digraphs under the supervision of Professor Ligong Wang.

After obtaining her master degree in March 2020, she chose to continue her PhD education in NPU with the same supervisor. Starting from December 2021, she visited the group of Formal Methods and Tools, University of Twente as a joint PhD student to perform research on the spectral properties of digraphs under the supervision of Professor Hajo Broersma. The research has been sponsored by the China Scholarship Council. The main results obtained from her research during her PhD work have been collected in the current thesis.







This thesis focuses on the study of the spectral properties of digraphs with a fixed dichromatic number. This study involves different types of matrices associated with the digraph, such as the Laplacian matrix, the A_α matrix and the eccentricity matrix.