Linear Algebra and its Applications 685 (2024) 77–103

Contents lists available at ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

The A_α spectral moments of digraphs with a given dichromatic number ☆

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A R T I C L E   I N F O

Article history:
Received 10 May 2023
Received in revised form 11 October 2023
Accepted 29 December 2023
Available online 5 January 2024
Submitted by R.A. Brualdi

MSC:
05C20
05C35
05C50

Keywords:
A_α spectral moment
Laplacian spectral moment
Dichromatic

A B S T R A C T

The A_α-matrix of a digraph G is defined as $A_\alpha(G) = \alpha D^+(G) + (1-\alpha)A(G)$, where $\alpha \in [0,1)$, $D^+(G)$ is the diagonal outdegree matrix and $A(G)$ is the adjacency matrix. The k-th A_α spectral moment of G is defined as $\sum_{i=1}^{n} \lambda_{\alpha i}^k$, where $\lambda_{\alpha i}$ are the eigenvalues of the A_α-matrix of G, and k is a nonnegative integer. In this paper, we obtain the digraphs which attain the minimal and maximal second A_α spectral moment (also known as the A_α energy) within classes of digraphs with a given 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 are related to earlier results about the second and third Laplacian spectral moments of digraphs.

☆ Supported by the National Natural Science Foundation of China (No. 12271439) and the China Scholarship Council (No. 202106290009).

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https://doi.org/10.1016/j.laa.2023.12.024

1. Preliminaries

Before we start with the necessary terminology and notation, let us first give some general background and motivation for the research that led to this paper. We will give more details and references to related work after we have defined the relevant concepts.

1.1. Background and motivation

Generally speaking, our research is motivated by different variants of the concept of graph energy. This concept was originally introduced by Gutman [8], 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 [25] 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. Following up on this idea, several groups of researchers have studied the properties of this A_α-matrix and its counterpart for digraphs. In this paper, we continue this line of research by determining the digraphs which attain the minimal and maximal second A_α spectral moment within classes of digraphs with a given dichromatic number. We also determine sharp bounds for the third A_α spectral moment within a special subclass which we define as join digraphs. These results are related to our earlier results obtained in [34] about the second and third Laplacian spectral moments of digraphs. Before we can give more details about related work, we need to introduce some terminology and notation.

1.2. Terminology, notation and more background

For the results of this paper we only consider digraphs, but we will also refer to related work on undirected graphs. Let G be a digraph with vertex set $\mathcal{V}(G)$ and arc set $\mathcal{A}(G)$, and let $n = |\mathcal{V}(G)|$ and $e = |\mathcal{A}(G)|$ denote the order and size of G, respectively. We use (u, v) to denote an arc from a vertex u to a vertex v, and we call u the tail and v the head of the arc (u, v). For a vertex $v \in \mathcal{V}(G)$, the outdegree $d_G^+(v)$ is the number of arcs in $\mathcal{A}(G)$ whose tail is v, while the indegree $d_G^-(v)$ is the number of arcs in $\mathcal{A}(G)$ whose head is v. A directed walk π of length ℓ from vertex u to vertex v in G is a sequence of vertices π: $u = v_0, v_1, \dots, v_\ell = v$, 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 we use $P_{\ell+1}$ to denote such a path; 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 use $c_\ell(v)$ to denote the number of directed closed walks of length ℓ starting at vertex v, and $c_\ell = \sum_{v\in\mathcal{V}(G)} c_\ell(v)$ to denote the total number of directed closed walks of length ℓ (clearly involving a lot of double counting).

For a digraph G with vertex set $\{v_1, v_2, \ldots, v_n\}$, 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 diagonal outdegree matrix $D^+(G)$ of G is defined by $D^+(G) = diag(d_1^+, d_2^+, \ldots, d_n^+)$, where $d_i^+ = d_G^+(v_i)$. The Laplacian matrix $L(G)$ and the signless Laplacian matrix $Q(G)$ of G are defined by $L(G) = D^+(G) - A(G)$ and $Q(G) = D^+(G) + A(G)$, respectively. In [22], the A_α-matrix of G is defined by

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

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 $Q(G) = 2A_{\frac{1}{2}}(G)$.

The above definition is the directed counterpart of the concept of the A_α-matrix of an undirected graph we mentioned in the previous subsection. The latter was introduced in 2017 by Nikiforov [25]. Subsequently, many scholars studied the A_α-matrix of undirected graphs (See, e.g., [2,17,19–21,26]). Motivated by the aforementioned work of Nikiforov in [25], the concept of the A_α-matrix of a graph has been extended to digraphs in the above sense by Liu et al. [22]. Very recent work on the A_α-matrix of a digraph can be found in [7,31,33].

Our research is related to graph energy, which is one of the oldest graph concepts motivated by applications in chemistry. The energy of an undirected graph, as introduced by Gutman [8], is defined as $\sum_{i=1}^{n} |\nu_i|$, where ν_i are the eigenvalues of the adjacency matrix of G. In 2006, Gutman and Zhou [11] and Lazić [14] 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. Hence, the latter definition is in fact an extension of what is better known as the second adjacency spectral moment of a graph. This has in turn been extended to the Laplacian matrix of a digraph in [28] and to the A_α-matrix of a digraph in [30]. There exist many alternative definitions for energies of graphs and digraphs. Interested readers are referred to the three monographs [9,10,15]. In this paper, we prefer the use of “second spectral moment” rather than “energy”, to avoid confusion because there exist many different definitions of “energy”.

The k-th adjacency spectral moment of an undirected graph G is defined as $\sum_{i=1}^{n} \nu_i^k$, where ν_i are the eigenvalues of the adjacency matrix of G. We refer to [3,5,6,27] for results on these spectral moments from the last decades. For a digraph G, the k-th adjacency spectral moment of G is defined as $\sum_{i=1}^{n} z_i^k$, where z_i are the eigenvalues of the adjacency matrix of G, and it is known to be equal to the total number of directed closed walks of length k in G. Hence, the interesting cases start with $k = 2$, and the main focus has been on the cases where $k = 2$ or $k = 3$. Since the A_α-matrix is an extension of the adjacency matrix of a digraph, we are also mainly concerned with the second and third A_α spectral moments of digraphs in this paper. 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 $A_\alpha(G)$. Note that the 0-th A_α spectral moment is n, the order of the digraph; and the first A_α spectral moment is αe, where e is the size of the digraph. For the second A_α spectral moment, since $Q(G) = 2A_{\frac{1}{2}}(G)$, one obtains:

$$tr(L(G)^2) = tr(Q(G)^2),$$

if G is a digraph without loops. Hence, the second spectral moments of the Laplacian matrix and the signless Laplacian matrix are equal. Actually, Yang and Wang [35] have shown that results on the second Laplacian spectral moment of a digraph are also applicable to its second signless Laplacian spectral moment.

Our results are closely related to the results we obtained in [34]. In [34], we were dealing with the second and third Laplacian spectral moments of digraphs with a fixed dichromatic number. A key concept in that paper is the dichromatic number of a digraph, which was introduced by Neumann-Lara [24] in 1982. A digraph G is acyclic if it has no directed cycles. A vertex set $F \subseteq \mathcal{V}(G)$ is acyclic if its induced subdigraph $G[F]$ in G is acyclic. A partition of $\mathcal{V}(G)$ into r acyclic sets is called an r-coloring of G. Adopting the definition of [24], the minimum integer r for which there exists an r-coloring of G is the dichromatic number $\chi(G)$ of G. In 2010, Mohar [23] was the first to establish a connection between the dichromatic number and algebraic properties related to eigenvalues of digraphs. Since then, many scholars have paid attention to this topic (See, e.g., [1,4,13,16,18,22,32]).

The rest of the paper is organized as follows. In Section 1.3, we introduce some special classes of digraphs and some lemmas used for our proofs. In Section 2, we determine the digraphs which attain the minimal and maximal second A_α spectral moment among all digraphs with given dichromatic number, as well as for the subclass of join digraphs. In Section 3, we determine sharp bounds for the third A_α spectral moment among all join digraphs with given dichromatic number, and characterize the extremal join digraphs with dichromatic number 2.

1.3. Special digraph classes and auxiliary results

In this section, we first introduce some additional terminology and special classes of digraphs, followed by several auxiliary results that we will need in our proofs.

For a digraph G, its underlying graph is the undirected 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 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. 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.

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

Every undirected graph H determines a bidirected graph $\overleftrightarrow{H}$ that is obtained from H by replacing each edge with two oppositely directed arcs joining the same pair of vertices. We use $\overleftrightarrow{K}_n$ to denote the bidirected complete graph of order n, and we use $\overleftrightarrow{C}_n$ 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 $\mathcal{V}(G_1) \cup \mathcal{V}(G_2)$ and arc set $\mathcal{A}(G_1) \cup \mathcal{A}(G_2) \cup \{(u, v), (v, u) | u \in \mathcal{V}(G_1), v \in \mathcal{V}(G_2)\}$. 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 $\mathcal{G}_{n,r}$ 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 connected acyclic digraphs. In particular, we let $\bigvee_{i=1}^{r} V^i$ denote the join digraph in $\mathcal{G}_{n,r}$ which is isomorphic to $V^1 \vee V^2 \vee \cdots \vee V^r$, in which each V^i is a connected acyclic digraph on n_i vertices, and we assume that $\sum_{i=1}^{r} n_i = n$ and $n_1 \geq n_2 \geq \cdots \geq n_r$.

We also recall Karamata's inequality [12] 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 $x_1 \geq x_2 \geq \cdots \geq x_n$ and $y_1 \geq y_2 \geq \cdots \geq y_n$ are numbers in I such that $(x_1, x_2, \ldots, x_n)$ majorizes $(y_1, y_2, \ldots, y_n)$, then

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

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

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

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

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

In the final part of this section, we list some results on the second and third spectral moment of the Laplacian matrix and the A_α-matrix of a digraph G. Throughout this paper, we only consider connected digraphs without loops or multiple arcs, and we assume that $\mathcal{V}(G) = \{v_1, v_2, \ldots, v_n\}$. Recall that we use d_i^+ as shorthand for $d_G^+(v_i)$ and $c_\ell^{(i)}$ as shorthand for $c_\ell(v_i)$, and we call $\left(c_\ell^{(1)}, c_\ell^{(2)}, \ldots, c_\ell^{(n)}\right)$ the directed closed walk sequence of length ℓ of G. We let $c_\ell = \sum_{i=1}^n c_\ell^{(i)}$ denote the total number of directed closed walks of length ℓ in G.

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 [28], they studied the Laplacian energy (second Laplacian spectral moment) $LE(G)$ of a digraph. This is followed by a result due to Xi. In [30], she defined and studied the A_α energy (second A_α spectral moment) $SM_\alpha^2(G)$ of a digraph.

Lemma 1.1. *([29]) Let G be a digraph of order n. Then*

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

Lemma 1.2. *([30]) Let G be a digraph of order n. Then*

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

Let $LSM_3(G) = \sum_{i=1}^n \lambda_i^3$ be the third Laplacian spectral moment of a digraph, where λ_i are the eigenvalues of $L(G)$. In [34], the authors studied the third Laplacian spectral moment $LSM_3(G)$ of a digraph.

Lemma 1.3. *([34]) Let G be a digraph of order n. Then*

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

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

Lemma 1.4. *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 $A_\alpha(G) = (\alpha_{ij})_{n\times n}$,

Table 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
		$j_3\neq j_1$	$\alpha(1-\alpha)^2\sum_{i=1}^{n}d_i^+c_2^{(i)}$
	$j_2\neq j_3$	$j_3=j_1$	$\alpha(1-\alpha)^2\sum_{i=1}^{n}d_i^+c_2^{(i)}$
		$j_3\neq j_1$	$(1-\alpha)^3c_3$

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

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 1.

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

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

Comparing the expressions for $L(G)$ and $A_\alpha(G)$ in the above Lemmas 1.1-1.4, 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.

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

and

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

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

In this sense, our results are related to the results in [34]. In the next section, we use the above expression for $SM_\alpha^2(G)$ to characterize the digraphs attaining the minimal and maximal second A_α spectral moment among all join digraphs and all digraphs in $\mathcal{G}_{n,r}$.

2. Extremal digraphs for the second A_α spectral moment

In this section, we will characterize the digraphs which attain the minimal and maximal second A_α spectral moment $SM_\alpha^2(G)$ among all join digraphs and all digraphs in $\mathcal{G}_{n,r}$. First, we determine the extremal digraphs for the second A_α spectral moment among all join digraphs $\bigvee_{i=1}^{r} V^i$ in $\mathcal{G}_{n,r}$. We make use of the following earlier result and its consequence for $SM_\alpha^2(G)$.

Lemma 2.1. *([34]) 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.

Since $SM_\alpha^2(G) = \alpha^2 LE(G) + (-2\alpha + 1)c_2$, the following corollary is immediate.

Corollary 2.2. *Let G be an acyclic digraph of order n. Then*

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

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.

We also need the following lemma.

Lemma 2.3. *([34]) 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*

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

In our next result, 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 2.4. *Let $G = \bigvee_{i=1}^{r} V^i$. Then the following inequalities hold:*
(i)

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

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 $r \mid n$,

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

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

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

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 1.2, we have

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

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

$$n_i - 1 \le \sum_{j=1}^{n_i} d^+_{V^i}(v^i_j) \le \frac{n_i(n_i-1)}{2},$$

$$n_i - 1 \le \sum_{j=1}^{n_i} \left(d^+_{V^i}(v^i_j)\right)^2 \le \frac{n_i(n_i-1)(2n_i-1)}{6}.$$

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

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

Let $f(x) = x^2(a - bx)$ and $F(x_1, x_2, \ldots, x_r) = \sum_{i=1}^{r} f(x_i)$, where $\sum_{i=1}^{r} x_i = n$ and $1 \le x_i \le n-r+1$. From Lemma 2.3, 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 $F(x_1, \ldots, x_i - 1, \ldots, x_j + 1, \ldots, x_r) < F(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_r)$.

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 $n_i - n_j \ge 2$, $F_1(n_1, n_2, \ldots, n_r) = \sum_{i=1}^{r} f_1(n_i)$ is maximal when $n_1 = n-r+1$ and $n_2 = \cdots = n_r = 1$. That is, $SM^2_\alpha(G)$ is minimal when $n_1 = n-r+1$ and $n_2 = \cdots = n_r = 1$.

Similarly, for

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

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

let $f_2(n_i) = n_i^2 \left(\alpha^2 \left(n + \frac{1}{2}\right) - 2\alpha + 1 - \frac{1}{3}\alpha^2 n_i\right)$. Since $\frac{\alpha^2(n+\frac{1}{2})-2\alpha+1}{\alpha^2} - 1 = \frac{\alpha^2(n-\frac{1}{2})-2\alpha+1}{\alpha^2} > \frac{n-r}{2} \geq n_j$ 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, $SM_\alpha^2(G)$ is maximal when $n_i = \lceil \frac{n}{r} \rceil$ or $n_i = \lfloor \frac{n}{r} \rfloor$.

Concluding,

(i)

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

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 $r \mid n$,

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

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

(iii) If $r \nmid n$,

$$\begin{aligned} SM_\alpha^2(G) &\leq \left(\alpha^2 \left(n^3 + \frac{n}{6}\right) - 2\alpha n^2 + n^2\right) + \sum_{i=1}^{r} n_i^2 \left(\alpha^2 \left(\frac{1}{3} n_i - n - \frac{1}{2}\right) + 2\alpha - 1\right) \\ &\leq \left(\alpha^2 \left(n^3 + \frac{n}{6}\right) - 2\alpha n^2 + n^2\right) \\ &\quad + \left\lceil \frac{n}{r} \right\rceil^2 \left(n - r \left\lfloor \frac{n}{r} \right\rfloor\right) \left(\alpha^2 \left(\frac{1}{3} \left\lceil \frac{n}{r} \right\rceil - n - \frac{1}{2}\right) + 2\alpha - 1\right) \end{aligned}$$

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

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 $\mathcal{G}_{n,r}$, $SM_\alpha^2(G)$ and $LE(G)$ have the same extremal digraphs by Theorem 2.4 above and Theorems 2.5, 2.6 in [34]. 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 $|n_i - n_j| \leq 1$. Since

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

in case $0 \leq \alpha \leq \frac{1}{2}$, we can deduce that $SM_\alpha^2(G)$ and $LE(G)$ have the same extremal digraphs directly. But when $\frac{1}{2} < \alpha < 1$, we can not directly get the bounds of $SM_\alpha^2(G)$ based on the bounds of $LE(G)$.

Next, we will determine the digraphs which attain the minimal and maximal second A_α spectral moment $SM_\alpha^2(G)$ among all digraphs in $\mathcal{G}_{n,r}$. We first recall some results about r-critical digraphs that were obtained by Mohar [23]. 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 on critical vertices and r-critical digraphs have been obtained in [23].

Lemma 2.5. *([23]) 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 2.6. *([23]) 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 $r \geq 4$.

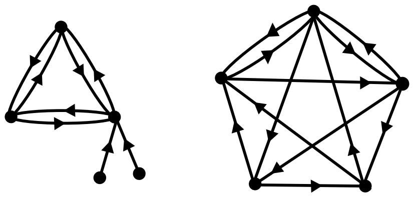

Fig. 1. Different minimal digraphs for $LE(G)$ and $SM^2_\alpha(G)$.

Using the above lemmas, in [34] the authors were able to characterize the digraphs which attain the minimal second Laplacian spectral moment $LE(G)$ among all digraphs in $\mathcal{G}_{n,r}$, as follows.

Lemma 2.7. *([34]) Let G be a digraph in $\mathcal{G}_{n,r}$. 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 $\overleftrightarrow{K}_r$.

From the above results, it is rather natural to expect that the same digraphs attain the minimal second A_α spectral moment among all digraphs in $\mathcal{G}_{n,r}$. However, the following two digraphs illustrated in Fig. 1 show that the minimal digraphs for the second A_α spectral moment and the second Laplacian spectral moment can be different (when α is in some range).

It is easy to check that both digraphs illustrated in Fig. 1 belong to $\mathcal{G}_{5,3}$. From Lemma 2.7, we know that G_1 is an example of a digraph attaining the minimal second Laplacian spectral moment, whereas G_2 is not. But for the second A_α spectral moment, we obtain $SM^2_\alpha(G_1) = 14\alpha^2 + 6(1-\alpha)^2$ and $SM^2_\alpha(G_2) = 30\alpha^2 + 4(1-\alpha)^2$. Hence, $SM^2_\alpha(G_1) \geq SM^2_\alpha(G_2)$ when $\alpha \in [0, \frac{2\sqrt{2}-1}{7}]$, and $SM^2_{\frac{1}{4}}(G_1) > SM^2_{\frac{1}{4}}(G_2)$. Hence, the minimal digraphs for the second A_α spectral moment and the second Laplacian spectral moment 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 second A_α spectral moment and the second Laplacian spectral moment among all digraphs in $\mathcal{G}_{n,r}$ have the same minimal digraphs when $\alpha \in [\frac{1}{2}, 1)$. We need the following earlier result and its straightforward consequence.

Lemma 2.8. *([34]) Let G be a digraph in $\mathcal{G}_{n,r}$, and let G' be an r-critical subdigraph of G. If G attains the minimal second Laplacian spectral moment $LE(G)$ 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 $u \in \mathcal{V}(G')$.*

Using Lemma 2.8, it is easy to prove the following corollary of the above lemma.

Corollary 2.9. *Let G be a digraph in $\mathcal{G}_{n,r}$, and let G' be an r-critical subdigraph of G. If G attains the minimal second A_α spectral moment $SM_\alpha^2(G)$ 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 $u \in \mathcal{V}(G')$.*

Proof. Let G' of order n' be an r-critical subdigraph of G. Then using Lemma 2.8, we know

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

So,

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

Hence, if G attains the minimal second A_α spectral moment $SM_\alpha^2(G)$ 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 $u \in \mathcal{V}(G')$. $\square$

We use the above corollary to prove our next result.

Theorem 2.10. *Let G be a digraph in $\mathcal{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r = 2$, we have

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

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) When $\alpha \in [\frac{1}{2}, 1)$ and $r \geq 3$, we have

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

with equality holding if and only if G contains a bidirected complete graph $\overleftrightarrow{K}_r$ and every component (if any) of $G - \mathcal{V}(\overleftrightarrow{K}_r)$ 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 Corollary 2.9, we obtain that if G attains the minimal second A_α spectral moment $SM_\alpha^2(G)$ 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'. From the proof of Corollary 2.9, we also get

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

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 $SM_\alpha^2(C_2) = 4\alpha^2 - 4\alpha + 2$.

Case 1.2: Suppose $n \geq 3$. Using Lemma 2.5, we get that $d_{G'}^+(u) \geq r - 1 = 1$ for any $u \in \mathcal{V}(G')$. If $d_{G'}^+(u) = 1$ for any $u \in \mathcal{V}(G')$, using Lemma 2.6, we can get $c_2(G') = 0$ if G' is a directed cycle of length $n' \geq 3$. So, we conclude that

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

with equality if and only if G contains a directed cycle $C_{n'}$ ($n' \geq 3$) and every component (if any) of $G - \mathcal{V}(C_{n'})$ 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 $u \in \mathcal{V}(G')$ by Lemma 2.5.

If $n' = r$, then $d^+_{G'}(u) = r - 1$ for any $u \in \mathcal{V}(G')$. From Lemma 2.6, 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 $u \in \mathcal{V}(G')$, $G' = \overset{\leftrightarrow}{K}_r$ of order $r \geq 3$, and

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

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

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

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

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

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 $SM^2_{\frac{1}{2}}(G) = \frac{1}{4}LE(G)$.

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

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

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 $\overleftrightarrow{K}_r$. $\square$

The next result characterizes the digraphs which attain the maximal second A_α spectral moment $SM_\alpha^2(G)$ among all digraphs in $\mathcal{G}_{n,r}$. It is an easy consequence of Theorem 2.4, so we omit the proof.

Theorem 2.11. *Let G be a digraph in $\mathcal{G}_{n,r}$. Then the following inequalities hold:*
(i) If $r \mid n$,

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

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 $r \nmid n$,

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

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. 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 $\mathcal{G}_{n,r}$.

Using the expressions for $LSM_3(G)$ and $SM_\alpha^3(G)$ in Lemmas 1.3 and 1.4, 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.

Lemma 3.1. *([34]) 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 3.2. *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 1.4, we obtain

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

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

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

By Lemma 3.1,

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

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

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

Combining the above equations, we obtain

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

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

Theorem 3.3. *Let $G=\bigvee_{i=1}^{r} V^i$. Then*

(i)
$$SM_\alpha^3(G)\geq -\alpha^3\sum_{i=1}^{r} n_i^4+3\left(\alpha^3(n+1)+\alpha(1-\alpha)^2\right)\sum_{i=1}^{r} n_i^3$$

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

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

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

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

Proof. From Lemma 3.2, since

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

$$
\begin{aligned}
&\sum_{i=1}^{r}\sum_{j=1}^{n_i}\left(n-n_i+d^+_{V^i}(v^i_j)\right)^3 \\
=&\sum_{i=1}^{r}\left[n_i(n-n_i)^3+\sum_{j=1}^{n_i}\left(d^+_{V^i}(v^i_j)\right)^3+3(n-n_i)\sum_{j=1}^{n_i}\left(d^+_{V^i}(v^i_j)\right)^2+3(n-n_i)^2\sum_{j=1}^{n_i} d^+_{V^i}(v^i_j)\right],
\end{aligned}
$$

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

$$
n_i-1\le\sum_{j=1}^{n_i} d^+_{V^i}(v^i_j)\le\frac{n_i(n_i-1)}{2},
$$

$$
n_i-1\le\sum_{j=1}^{n_i}\left(d^+_{V^i}(v^i_j)\right)^2\le\frac{n_i(n_i-1)(2n_i-1)}{6},
$$

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

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

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

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

For the upper bound we obtain

$$\begin{aligned}
SM^3_\alpha(G) \le{}& \alpha^3 \sum_{i=1}^{r} \Bigg[n_i(n-n_i)^3 + \frac{n_i^2(n_i-1)^2}{4} + 3(n-n_i)\frac{n_i(n_i-1)(2n_i-1)}{6} \\
&+ 3(n-n_i)^2 \frac{n_i(n_i-1)}{2}\Bigg] + 3\alpha(1-\alpha)^2 \sum_{i=1}^{r} n_i(n-n_i)^2 \\
&+ 3(1-\alpha)^2 \sum_{i=1}^{r} (n-n_i)\frac{n_i(n_i-1)}{2} + (1-\alpha)^3 \sum_{i=1}^{r} n_i \sum_{s\ne i} n_s(n-n_s-n_i) \\
={}& -\frac{\alpha^3}{4} \sum_{i=1}^{r} n_i^4 + \left(\alpha^3\left(n-\frac{1}{2}\right) + 3\alpha(1-\alpha)^2 - \frac{3}{2}(1-\alpha)^2\right) \sum_{i=1}^{r} n_i^3 \\
&- \left(\alpha^3\left(\frac{3n^2}{2} - \frac{3n}{2} + \frac{1}{4}\right) + 6\alpha(1-\alpha)^2 n - \frac{3}{2}(1-\alpha)^2(n+1)\right) \sum_{i=1}^{r} n_i^2
\end{aligned}$$

$$+ \alpha^3 \left(n^4 - \frac{3n^3}{2} + \frac{n^2}{2} \right) + 3\alpha(1-\alpha)^2 n^3 - (1-\alpha)^2 \frac{3n^2}{2}$$

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

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 2.4. However, we can obtain such tight bounds for $SM_\alpha^3(G)$ among the join digraphs in $\mathcal{G}_{n,2}$.

Corollary 3.4. *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 $n_2 = 1$.*

(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 $n_1 = \lceil \frac{n}{2} \rceil$ and $n_2 = \lfloor \frac{n}{2} \rfloor$.

Proof.
(i) If $r = 2$, $n = n_1 + n_2$. Let $n_2 = x$ and $n_1 = n - x$, where $1 \leq n_2 \leq \lfloor \frac{n}{2} \rfloor$. Using Theorem 3.3, we only need to consider

$$- \alpha^3 \left(x^4 + (n-x)^4\right) + 3\left(\alpha^3(n+1) + \alpha(1-\alpha)^2\right)\left(x^3 + (n-x)^3\right)$$
$$- 3\left(\alpha^3(n^2 + 2n + 2) + 2\alpha(1-\alpha)^2 n + (1-\alpha)^2\right)\left(x^2 + (n-x)^2\right).$$

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 $a = -\alpha^3$, $b = 3\left(\alpha^3(n+1) + \alpha(1-\alpha)^2\right)$ and $c = -3\left(\alpha^3(n^2 + 2n + 2) + 2\alpha(1-\alpha)^2 n + (1-\alpha)^2\right)$. Then

$$f(x) = 2ax^4 - 4anx^3 + (6an^2 + 3bn + 2c)x^2 - (4an^3 + 3bn^2 + 2cn)x + (an^4 + bn^3 + cn^2).$$

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

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

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

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

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 $1 \leq n_2 \leq \lfloor \frac{n}{2} \rfloor$. Using Theorem 3.3, 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 $c = -\Big(\alpha^3\left(\frac{3n^2}{2} - \frac{3n}{2} + \frac{1}{4}\right) + 6\alpha(1-\alpha)^2 n - \frac{3}{2}(1-\alpha)^2(n+1)\Big)$. 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 $1 \leq x \leq \frac{n}{2}$.

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

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

So $g''(x)$ 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, $SM_\alpha^3(G)$ 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,

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

If n is odd,

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

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

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

4. Conclusion

In this paper, we compared the second and third spectral moments of $L(G)$ and $A_\alpha(G)$, and we extended the results we obtained in [34] 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 paper by recalling some of the open problems for future research.

With respect to the lower bounds and minimal digraphs for the second A_α spectral moment, Theorem 2.10 shows that the results for the second A_α spectral moment are the same as for the second Laplacian spectral moment 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 second A_α spectral moment among all digraphs with a given dichromatic number. So we leave this as another open problem.

Declaration of competing interest

No competing interests.

Data availability

No data was used for the research described in the article.

Acknowledgements

The authors would like to thank the anonymous referee for providing valuable comments and suggestions which improved the presentation of this paper.

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