

On the A_α -index of graphs with given order and dissociation number*

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Abstract: Given a graph G , a subset of vertices is called a maximum dissociation set of G if it induces a subgraph with vertex degree at most 1, and the subset has maximum cardinality. The cardinality of a maximum dissociation set is called the dissociation number of G . The adjacency matrix and the degree diagonal matrix of G are denoted by $A(G)$ and $D(G)$, respectively. In 2017, Nikiforov proposed the A_α -matrix: $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$, where $\alpha \in [0, 1]$. The largest eigenvalue of this novel matrix is called the A_α -index of G . In this paper, we firstly determine the connected graph (resp. bipartite graph, tree) having the largest A_α -index over all connected graphs (resp. bipartite graphs, trees) with fixed order and dissociation number. Secondly, we describe the structure of all the n -vertex graphs having the minimum A_α -index with dissociation number τ , where $\tau \geq \lceil \frac{2}{3}n \rceil$. Finally, we identify all the connected n -vertex graphs with dissociation number $\tau \in \{2, \lceil \frac{2}{3}n \rceil, n-1, n-2\}$ having the minimum A_α -index.

Keywords: A_α -index; Dissociation number; Bipartite graph; Tree

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1. Introduction

In this section, we introduce some definitions that will help the reader to build up the necessary background for the main results.

1.1. Background and definitions

Given a graph G , its *adjacency matrix* $A(G)$ is an $n \times n$ 0-1 square matrix whose (u, v) -entry is 1 if and only if $u \sim v$ in G . Let $D(G) = \text{diag}(d_1, \dots, d_n)$ be the diagonal matrix of vertex degrees in a graph G . The matrix $Q(G) = D(G) + A(G)$ is called the *signless Laplacian matrix* of G ; see [8]. Nikiforov [22] introduced the A_α -matrix of a graph G , which is a convex combination of $D(G)$ and $A(G)$, i.e.,

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G), \quad 0 \leq \alpha \leq 1.$$

Note that $A_\alpha(G)$ is real symmetric. Hence its eigenvalues are real, and so we may display the eigenvalues of $A_\alpha(G)$ as $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$. For short, the A_α spectral radius of G (i.e. the largest eigenvalue of $A_\alpha(G)$), denoted by $\lambda_\alpha(G) = \lambda_1(G)$, is called the A_α -index of G . Notice that

$$A(G) = A_0(G), \quad Q(G) = 2A_{1/2}(G) \quad \text{and} \quad D(G) = A_1(G). \quad (1.1)$$

Recently, more and more people studied the A_α -spectra of graphs. Nikiforov et al. [23] gave some bounds on the A_α -index of a graph, and they determined the unique tree with maximum (resp. minimum) A_α -index among n -vertex trees. Nikiforov and Rojo [24] determined the graph of order n and diameter at least d having the largest A_α -index. Xue et al. [33] determined the graphs with the maximum (resp. minimum) A_α -index among all connected graphs with given diameter (resp. clique number). Li and Zhou [20] determined the unique n -vertex

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block graph with prescribed independence number having the maximum A_α -index. In the same paper, they also characterized the unique n -vertex graph with given number of cut edges having the largest A_α -index, and it is surprising to see that in both cases, the extremal graphs always coincide. For more advances on the A_α -spectra, we refer the reader to [6, 12, 15, 16, 17, 18, 19, 21, 30, 32].

For a subset $S \subseteq V_G$, we call S a *dissociation set* if the induced subgraph $G[S]$ does not contain P_3 as a subgraph, which is equivalent to say that the degree of each vertex in $G[S]$ is at most one. A *maximum dissociation set* of G is a dissociation set with the maximum cardinality. The *dissociation number* of G , written as $\tau(G)$, is the cardinality of a maximum dissociation set of G . The problem of determining $\tau(G)$ is a classical problem, which may date back to the work of Yannakakis [34] in 1981. In the same paper, he also proved that this problem is NP-complete for bipartite graphs. Boliac, Cameron and Lozin [4] strengthened the result of Yannakakis by reducing the problem, in polynomial time, from general bipartite graphs to some particular classes such as bipartite graphs with maximum degree 3 or C_4 -free bipartite graphs. In the same paper, they also proved that finding the dissociation number is polynomially solvable for bipartite graphs containing no induced subgraph isomorphic to a tree obtained from P_4 by attaching a path of length three to one quasi-pendant vertex of P_4 . For more advances about this problem one may consult [1, 2, 3, 5, 25, 26].

Quite recently, characterizing the graphs having maximum number of maximum dissociation sets becomes an attractive problem. Tu, Zhang and Shi [29] determined all the trees having the maximum number of maximum dissociation sets among trees with given order. Tu, Zhang and Du [28] characterized all the trees having the maximum number of maximum dissociation sets among trees with given dissociation number. Li and Sun [14] identified all the trees (resp. forests) having the largest and the second largest number of maximum dissociation sets among trees (resp. forests) with given order and dissociation number. Tu, Li and Du [27] presented the upper bounds on the number of maximal (resp. maximum) dissociation sets in a general graph of order n and in a triangle-free graph of order n , and they also characterized the corresponding extremal graphs.

Naturally, one may be interested in relating the spectra of a graph and its dissociation number. Very recently, Huang, Li and Zhou [11] characterized all the graphs among all connected graphs (resp. bipartite graphs, trees) with given order and dissociation number having the maximum A_0 -spectral radius. Das and Mohanty [7] identified the unique block graph with given order and dissociation number having the largest A_0 -spectral radius.

In this paper we consider the relation between the A_α -spectra of a graph and its dissociation number, which extends the main results of [11]. We firstly characterize the n -vertex connected graph (resp. bipartite graph, tree) with dissociation number τ having the largest A_α -index. Secondly, we describe the structure of all the n -vertex graphs with dissociation number τ having the minimum A_α -index, where $\tau \geq \lceil \frac{2}{3}n \rceil$. Finally, we identify all the connected n -vertex graphs with dissociation number $\tau \in \{2, \lceil \frac{2}{3}n \rceil, n-1, n-2\}$ having the minimum A_α -index.

1.2. Basic notations and main results

In this subsection, we give some basic notations and then describe our main results. Throughout this paper, we consider only simple and finite graphs. For spectral graph theoretic notation and terminology not defined here, we refer to Godsil and Royle [9] and West [31].

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G . We call $n = |V_G|$ and $m = |E_G|$ the *order* and the *size* of G , respectively. We say that two vertices u and v are *adjacent* (or *neighbors*) if they are joined by an edge and we write $u \sim v$. As usual, let P_n, C_n, K_n and $K_{t,n-t}$ denote the path, cycle, complete graph and complete bipartite graph on n vertices, respectively. Denote by $K_{1,n-1}$ the star graph, which is also denoted by S_n as usual.

For a vertex $v \in V_G$, let $N_G(v)$ be the set of all neighbors of v in G . Then $d_G(v) = |N_G(v)|$ is the *degree* of v

in G . For simplicity, when there is no danger of confusion, we may omit the subscripts G for our notation. The vertex with degree $n - 1$ in a star S_n is called the *centre* of S_n . A *pendant vertex* (or a *leaf*) is a vertex of G whose degree is one. We denote by $\mathcal{P}_G$ the set of all pendant vertices of G . We call a vertex *quasi-pendant vertex* of G if it is adjacent to a pendant vertex of G . We denote by $\mathcal{Q}_G$ the set of all quasi-pendant vertices of G and let $\mathcal{Q}'_G$ consist of all quasi-pendant vertices of degree 2 of G . A *pendant path* of length r is a path with vertex set $V = \{v_0, v_1, \dots, v_r\}$ such that $d(v_0) \geq 2$, $d(v_1) = \dots = d(v_{r-1}) = 2$ and $d(v_r) = 1$. In particular, if $r = 1$, then it is a *pendant edge*. A *matching* M is a set of edges, no two of which have a vertex in common. In particular, M is a *perfect matching* if each vertex of G is incident with an edge from M . A subset I of V_G is called an *independent set* if any two vertices of I are not adjacent.

For two graphs G and H , we define $G \cup H$ their disjoint union. In addition, we use kG to denote the disjoint union of k copies of G . The *join* $G \vee H$ is the graph obtained by joining every vertex of G with every vertex of H with an edge. If $U \subseteq V_G$, then we write $G[U]$ to denote the induced subgraph of G with vertex set U and two vertices being adjacent if and only if they are adjacent in G . The *complement* of a graph G is a graph $\overline{G}$ with the same vertex set as G , in which any two distinct vertices are adjacent if and only if they are non-adjacent in G .

In order to formulate our main results, let $\mathcal{G}_n^\tau$ (resp. $\mathcal{B}_n^\tau, \mathcal{T}_n^\tau$) denote the set of connected graphs (resp. bipartite graphs, trees) with order n and dissociation number τ .

Our first main result characterizes the n -vertex connected graph with dissociation number τ having the largest A_α -index. Note that adding an edge to connect two nonadjacent vertices in a connected graph will strictly increase its A_α -index (see, for example, [22]). Consequently, the following theorem obviously holds.

Theorem 1.1. *Let G be in $\mathcal{G}_n^\tau$ having the maximum A_α -index and let $\alpha \in [0, 1)$. Then $G \cong K_{n-\tau} \vee (\frac{\tau}{2}K_2)$ if τ is even, and $G \cong K_{n-\tau} \vee (\frac{\tau-1}{2}K_2 \cup K_1)$ if τ is odd.*

Our second main result establishes a sharp upper bound on the A_α -index of bipartite graphs with given order and dissociation number. The corresponding extremal graph is also characterized.

Theorem 1.2. *Let G be a graph in $\mathcal{B}_n^\tau$. Assume that $\alpha \in [0, 1)$, then*

$$\lambda_\alpha(G) \leq \frac{1}{2} \left(\alpha n + \sqrt{\alpha^2 n^2 + 4\tau(n-\tau)(1-2\alpha)} \right)$$

with equality if and only if $G \cong K_{\tau, n-\tau}$.

Let $S_{n,\tau}^\dagger$ be a tree obtained from the star $S_{n-\tau}$ by attaching exactly two pendant edges to each leaf of $S_{n-\tau}$ and attaching $3\tau - 2n + 2$ pendant edges to the centre of $S_{n-\tau}$ (see Figure 1). The next result determines the n -vertex tree with dissociation number τ having the largest A_α -index, which reads as

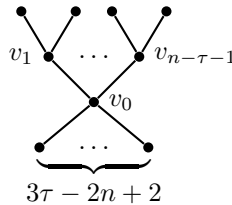


Figure 1: Tree $S_{n,\tau}^\dagger$ together with some labeled vertices.

Theorem 1.3. *Let T be a tree in $\mathcal{T}_n^\tau$ ($n \geq 3$) having the maximum A_α -index with $0 \leq \alpha < 1$. Then*

$$\lambda_\alpha(T) \leq \theta(\alpha, n, \tau)$$

with equality if and only if $T \cong S_{n,\tau}^\dagger$, where $\theta(\alpha, n, \tau)$ is the largest zero of

$$\begin{aligned} P_\alpha(x) = & x^4 + \alpha(n - 2\tau - 6)x^3 + (8\alpha^2\tau - 4\alpha^2n + 4\alpha\tau - 2\alpha n - 2\tau + n + 9\alpha^2 + 6\alpha - 3)x^2 \\ & + \alpha(16\alpha n - \alpha^2n - 8n - 28\alpha\tau + 14\tau - 20\alpha + 10)x + 2\alpha^3n - 17\alpha^2n + 16\alpha n - 4n \\ & + 24\alpha^2\tau - 24\alpha\tau + 6\tau - 2\alpha^3 + 17\alpha^2 - 16\alpha + 4. \end{aligned} \quad (1.2)$$

The next result characterizes the structure of all the n -vertex connected graphs with dissociation number τ ($\tau \geq \lceil \frac{2}{3}n \rceil$) having the minimum A_α -index.

Theorem 1.4. *Let $G^\dagger$ be a graph in $\mathcal{G}_n^\tau$ with $\tau \geq \lceil \frac{2}{3}n \rceil$ having the minimum A_α -index with $0 \leq \alpha < 1$. Then $G^\dagger$ is a tree.*

Denote by S_{k_1,k_2} the tree obtained from S_{k_1+1} by attaching k_2 pendant paths of length two to the centre of S_{k_1+1} . Let T_{r_1,p_1}^1 be the tree obtained from P_4 by attaching r_1 and p_1 pendant paths of length two to the two leaves of P_4 , respectively. Then let T_{r_2,p_2}^2 be the tree obtained from T_{r_2,p_2}^1 by attaching one pendant edge to the vertex of degree $r_2 + 1$ in T_{r_2,p_2}^1 . The trees S_{k_1,k_2} , T_{r_1,p_1}^1 and T_{r_2,p_2}^2 are depicted in Figure 2.

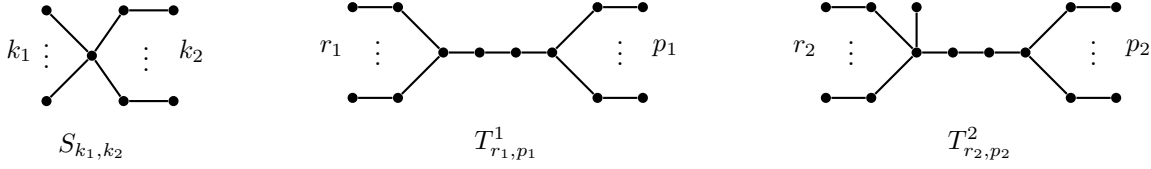


Figure 2: Trees S_{k_1,k_2} , T_{r_1,p_1}^1 and T_{r_2,p_2}^2

Our last main result determines all the connected n -vertex graphs with dissociation number $\tau \in \{2, \lceil \frac{2}{3}n \rceil, n-1, n-2\}$ having the minimum A_α -index.

Theorem 1.5. *Let G^* be a graph in $\mathcal{G}_n^\tau$ having the minimum A_α -index with $0 \leq \alpha < 1$.*

- (i) *If $\tau = 2$, then $G^* \cong K_n - M$, where M is a maximum matching of K_n .*
- (ii) *If $\tau = \lceil \frac{2}{3}n \rceil$, then $G^* \cong P_n$.*
- (iii) *If $n \geq 4$ and $\tau = n-1$, then $G^* \cong S_{0, \frac{n-1}{2}}$ if n is odd and $G^* \cong S_{1, \frac{n-2}{2}}$ if n is even.*
- (iv) *If $n \geq 6$ and $\tau = n-2$, then $G^* \cong T_{\lceil \frac{n-4}{4} \rceil, \lfloor \frac{n-4}{4} \rfloor}^1$ if n is even and $G^* \cong T_{\lfloor \frac{n-5}{4} \rfloor, \lceil \frac{n-5}{4} \rceil}^2$ if n is odd.*

The remainder of this paper is organized as follows. In Section 2, we give some essential definitions and some necessary preliminaries. In Section 3, we give the proofs of Theorems 1.2 and 1.3. In Section 4, we give the proofs for Theorems 1.4 and 1.5. Some concluding remarks are given in the last section.

2. Preliminaries

In this section, we give some necessary results, which will be used to prove our main results.

Lemma 2.1 ([22]). *If G is a connected graph and H is a proper subgraph of G , then $\lambda_\alpha(H) < \lambda_\alpha(G)$ for $\alpha \in [0, 1]$.*

Lemma 2.2 ([23]). *If T is a tree of order n and $\alpha \in [0, 1]$, then $\lambda_\alpha(T) \leq \frac{1}{2} \left(\alpha n + \sqrt{\alpha^2 n^2 + 4(n-1)(1-2\alpha)} \right)$ with equality if and only if $T \cong S_n$.*

Lemma 2.3 ([23]). *If G is a connected graph of order n and $\alpha \in [0, 1]$, then $\lambda_\alpha(G) \geq \lambda_\alpha(P_n)$ with equality if and only if $G \cong P_n$.*

For $V_1 \subseteq V_G$ and $E_1 \subseteq E_G$, we write $G - V_1$ and $G - E_1$ for the graphs obtained from G by deleting the vertices in V_1 and their incident edges and the edges in E_1 , respectively. For convenience, we may use $G - v$ and $G - uv$ to denote $G - \{v\}$ and $G - \{uv\}$, respectively. Similarly, $G + uv$ is obtained from G by adding the edge $uv \notin E_G$.

By the well-known Perron-Frobenius theorem, if G is connected, we know that the multiplicity of $\lambda_\alpha(G)$ is one and there exists a unit positive eigenvector, say $\mathbf{x} = (x_1, \dots, x_n)^T$, corresponding to it, where x_i is the component of $\mathbf{x}$ at $v_i \in V_G$ [22]. As usual we call $\mathbf{x}$ the *Perron vector* of $A_\alpha(G)$.

Lemma 2.4 ([33]). *Let G be a connected graph with $u, v \in V_G$ and let $\alpha \in [0, 1)$. Assume that $\mathbf{x}$ is the Perron vector of $A_\alpha(G)$ such that $x_u \geq x_v$. If $\{v_1, v_2, \dots, v_s\} \in N_G(v) \setminus N_G(u)$ ($1 \leq s \leq d_v$) and $G' = G - \{vv_1, \dots, vv_s\} + \{uv_1, \dots, uv_s\}$, then $\lambda_\alpha(G') > \lambda_\alpha(G)$.*

Lemma 2.5 ([10]). *Let G be a connected graph with $|E_G| \geq 1$ and $u \in V_G$. Denote by $G_{s,t}$ the graph obtained from G by attaching two pendant paths of length s and t to u , respectively. If $s \geq t \geq 1$ and $0 \leq \alpha < 1$, then $\lambda_\alpha(G_{s,t}) > \lambda_\alpha(G_{s+1,t-1})$.*

Let $P = v_1 v_2 \dots v_k$ with $k \geq 2$ be a path in a connected graph. Then we call P an *internal path*, if $\min\{d(v_1), d(v_k)\} \geq 3$ and $d(v_2) = \dots = d(v_{k-1}) = 2$. The *subdivision operation* for an edge $uv \in E_G$ is adding a new vertex w and substituting uv by a path uwv , and we denote the resultant graph by G_w .

Lemma 2.6 ([13]). *Let G be a connected graph with $\alpha \in [0, 1)$ and uv be an edge on an internal path of G . Let G_w be the graph obtained from G by the subdivision operation for the edge uv . Then $\lambda_\alpha(G_w) < \lambda_\alpha(G)$.*

Let R be a real matrix, whose rows and columns are indexed by $V = \{1, 2, \dots, n\}$. Assume that $\pi = \{V_1, V_2, \dots, V_t\}$ is a partition of V . Then R can be partitioned based on π as

$$R = \begin{pmatrix} R_{11} & \cdots & R_{1t} \\ \vdots & \ddots & \vdots \\ R_{t1} & \cdots & R_{tt} \end{pmatrix},$$

where R_{ij} denotes the submatrix of R , indexed by the rows and columns of V_i and V_j , respectively. Let r_{ij} be the average row sum of R_{ij} for $1 \leq i, j \leq t$. Usually, the $t \times t$ matrix $R^\pi = (r_{ij})$ is called the *quotient matrix* of R . Moreover, if the row sum of R_{ij} is constant for $1 \leq i, j \leq t$, then we call π an *equitable partition*.

Lemma 2.7 ([35]). *Let R be a real matrix with an equitable partition π , and let R^π be the corresponding quotient matrix. Then each eigenvalue of R^π is an eigenvalue of R . Furthermore, if R is nonnegative, then the spectral radii of R and R^π are equal.*

Recall that $\mathcal{P}_G$ denotes the set of all pendant vertices of G and $\mathcal{Q}'_G$ denotes the set of all quasi-pendant vertices of degree 2 of G . The following lemma reveals that there exists a maximum dissociation set of G containing all vertices in $\mathcal{P}_G \cup \mathcal{Q}'_G$, which plays an essential role in the proofs of our main results.

Lemma 2.8 ([11]). *Let G be a graph with order $n \geq 5$. Then there exists a maximum dissociation set S such that $\mathcal{P}_G \cup \mathcal{Q}'_G \subseteq S$.*

A maximum dissociation set is said to be *good* if it contains all vertices in $\mathcal{P}_G \cup \mathcal{Q}'_G$. According to Lemma 2.8, we know that such a set always exists.

3. Proofs of Theorems 1.2 and 1.3

In this section, we give the proofs for Theorems 1.2 and 1.3. The former identifies the unique n -vertex bipartite graph with dissociation number τ having the largest A_α -index, and the later characterizes the tree with given order n and dissociation number τ having the maximum A_α -index.

Proof of Theorem 1.2. Choose $G = (X, Y) \in \mathcal{B}_n^\tau$ such that its A_α -index is as large as possible. We first assume that G is connected. Without loss of generality, we assume that $|X| \geq |Y|$. Let S be a maximum dissociation set of G . Since X is a dissociation set of G , we have $\tau = |S| \geq |X|$. Clearly, our result is true for $n \leq 2$. So in what follows, we consider $n \geq 3$.

If $\tau = |X|$, by Lemma 2.1, we obtain that $G \cong K_{\tau, n-\tau}$. In the following, we may assume that $\tau > |X|$. Therefore, $S \cap Y \neq \emptyset$. Let $X_1 = X \cap S$, $Y_2 = Y \cap S$ and $X_2 = X \setminus X_1$, $Y_1 = Y \setminus Y_2$. For convenience, assume $|X_1| = a$, $|Y_1| = b$, $|X_2| = c$, and $|Y_2| = d$. Since $|X_1| + |Y_2| = |S| > |X| \geq |Y|$, we have $d > c$, $a > b$. According to the choice of G and by Lemma 2.1, one sees that both $G[(X_1, Y_1)]$ and $G[(X_2, Y)]$ are complete, and $G[(X_1, Y_2)]$ contains independent edges as many as possible. We proceed by considering the following three cases according to the values of a and d .

Case 1. $a = d$. In this case, $E_{G[X_1 \cup Y_2]}$ is a perfect matching of $G[X_1 \cup Y_2]$. It is easy to see that $\pi_1 := X_1 \cup X_2 \cup Y_1 \cup Y_2$ is an equitable partition of V_G , and the corresponding quotient matrix can be written as follows:

$$(A_\alpha)^{\pi_1} := \begin{pmatrix} \alpha(b+1) & 0 & (1-\alpha)b & 1-\alpha \\ 0 & \alpha(a+b) & (1-\alpha)b & (1-\alpha)a \\ (1-\alpha)a & (1-\alpha)c & \alpha(a+c) & 0 \\ 1-\alpha & (1-\alpha)c & 0 & \alpha(c+1) \end{pmatrix}.$$

Let $P_\alpha^1(x) := \det(xI_4 - (A_\alpha)^{\pi_1})$ be the characteristic polynomial of $(A_\alpha)^{\pi_1}$. Note that $(A_\alpha)^{\pi_1}$ is nonnegative and irreducible. Together with Lemma 2.7 and the Perron-Frobenius theorem, we know that $\lambda_\alpha(G)$ coincides with the largest root of $P_\alpha^1(x) = 0$.

Since $n \geq 3$ and G is connected, we have $a = d > \max\{b, c\} \geq 1$. Recall that $|X| \geq |Y|$ and $a = d$, we can deduce that $c \geq b$. Let $G' \cong K_{2a, b+c}$. It is easy to see that $G' \in \mathcal{B}_n^\tau$. By a simple calculation, we have

$$\lambda_\alpha(G') = \frac{1}{2} \left(\alpha(2a + b + c) + \sqrt{\alpha^2(2a + b + c)^2 + 8a(b + c)(1 - 2\alpha)} \right).$$

Utilizing calculations by Matlab, we obtain that $\min P_\alpha^1(x) \approx 2.598$ for $x \geq \lambda_\alpha(G')$ (see the Appendix), i.e. $P_\alpha^1(x) > 0$ when $x \geq \lambda_\alpha(G')$. Recall that $\lambda_\alpha(G)$ is the largest zero of $P_\alpha^1(x)$. That is to say, $\lambda_\alpha(G) < \lambda_\alpha(G')$, which contradicts the choice of G .

Case 2. $a < d$. In this case, there exists a set $Y'_2 \subseteq Y_2$ such that $|Y'_2| = a$ and $E_{G[X_1 \cup Y'_2]}$ is a perfect matching of $G[X_1 \cup Y'_2]$. Let $Y''_2 = Y_2 \setminus Y'_2$, then $Y''_2 \neq \emptyset$. Thus it is easy to see that $\pi_2 := X_1 \cup X_2 \cup Y_1 \cup Y'_2 \cup Y''_2$ is an equitable partition of V_G , and the corresponding quotient matrix can be written as follows:

$$(A_\alpha)^{\pi_2} := \begin{pmatrix} \alpha(b+1) & 0 & (1-\alpha)b & 1-\alpha & 0 \\ 0 & \alpha(b+d) & (1-\alpha)b & (1-\alpha)a & (1-\alpha)(d-a) \\ (1-\alpha)a & (1-\alpha)c & \alpha(a+c) & 0 & 0 \\ 1-\alpha & (1-\alpha)c & 0 & \alpha(c+1) & 0 \\ 0 & (1-\alpha)c & 0 & 0 & \alpha c \end{pmatrix}.$$

Let $P_\alpha^2(x) := \det(xI_5 - (A_\alpha)^{\pi_2})$ be the characteristic polynomial of $(A_\alpha)^{\pi_2}$. Note that $(A_\alpha)^{\pi_2}$ is nonnegative and irreducible. Together with Lemma 2.7 and the Perron-Frobenius theorem, we know that $\lambda_\alpha(G)$ coincides with the largest root of $P_\alpha^2(x) = 0$.

It is easy to see that $c \geq 1$ (since otherwise $|X| = |X_1| = a < d = |Y_2| \leq |Y|$, which contradicts $|X| \geq |Y|$). Thus we have $d \geq c + 1 \geq 2$. Let $G'' \cong K_{a+d, b+c}$. It is easy to see that $G'' \in \mathcal{B}_n^\tau$. By a simple calculation, we have

$$\lambda_\alpha(G'') = \frac{1}{2} \left(\alpha(a + b + c + d) + \sqrt{\alpha^2(a + b + c + d)^2 + 4(a + d)(b + c)(1 - 2\alpha)} \right).$$

With the same idea as the Appendix of calculations using Matlab, we obtain that $\min P_\alpha^2(x) = 1$ for $x \geq \lambda_\alpha(G'')$, that is to say, $P_\alpha^2(G) > 0$ when $x \geq \lambda_\alpha(G'')$. Recall that $\lambda_\alpha(G)$ is the largest zero of $P_\alpha^2(x)$. That is to say, $\lambda_\alpha(G) < \lambda_\alpha(G'')$, which contradicts the choice of G .

Case 3. $a > d$. We can also derive a contradiction in a similar way as Case 2, whose procedure is omitted here.

By Cases 1-3, we obtain $G \cong K_{\tau, n-\tau}$. A simple calculation gives us

$$\lambda_\alpha(G) = \frac{1}{2} \left(\alpha n + \sqrt{\alpha^2 n^2 + 4\tau(n - \tau)(1 - 2\alpha)} \right).$$

In what follows, we show G is connected. Otherwise suppose that G is disconnected. Let $G = \bigcup_{i=1}^s G_i$, where G_i is a connected bipartite graph in $\mathcal{B}_{n_i}^{\tau_i}$ and $s \geq 2$. Thus we have

$$\sum_{i=1}^s (n_i - \tau_i) = \sum_{i=1}^s n_i - \sum_{i=1}^s \tau_i = n - \tau.$$

Therefore, $n_i < n, \tau_i < \tau$ and $n_i - \tau_i < n - \tau$. Consequently, by Lemma 2.1,

$$\lambda_\alpha(G) = \max \{ \lambda_\alpha(G_i) \mid 1 \leq i \leq s \} \leq \max \{ \lambda_\alpha(K_{\tau_i, n_i - \tau_i}) \mid 1 \leq i \leq s \} < \lambda_\alpha(K_{\tau, n - \tau}),$$

a contradiction to the choice of G .

This completes the proof. $\square$

Let $\mathcal{T}_{n, \tau}^1$ be a set of all the n -vertex trees obtained from $S_{n-\tau+1}$ by attaching exactly one pendant edge to the centre of $S_{n-\tau+1}$, and attaching at least two pendent edges to each leaf of $S_{n-\tau+1}$ such that the total number of leaves of the resultant tree is $\tau - 1$, where $\tau \notin \{\frac{2}{3}n, \frac{2n+1}{3}\}$. Let $\mathcal{T}_{n, \tau}^2$ be a set of all the n -vertex trees obtained from $S_{n-\tau+1}$ by attaching at least two pendent edges to every leaf of $S_{n-\tau+1}$ such that the total number of leaves of the resultant tree is $\tau - 1$, where $\tau \neq \frac{2}{3}n$. Let $\mathcal{T}_{n, \tau}^3$ be a set of all the n -vertex trees obtained from $S_{n-\tau}$ by attaching at least two pendant edges to each vertex of $S_{n-\tau}$ such that the total number of leaves of the resultant tree is τ . In Figure 3, one sees a tree in $\mathcal{T}_{n, \tau}^1, \mathcal{T}_{n, \tau}^2$ and $\mathcal{T}_{n, \tau}^3$, respectively. Let $\mathcal{S}_{n, \tau} = \mathcal{T}_{n, \tau}^1 \cup \mathcal{T}_{n, \tau}^2 \cup \mathcal{T}_{n, \tau}^3$. In view of Lemma 2.8, we have $\mathcal{S}_{n, \tau} \subseteq \mathcal{T}_n^\tau$. Sun and Li [14] showed that $\tau(F) \geq \lceil \frac{2}{3}n \rceil$ for each forest F with order n . Therefore, for every tree T in $\mathcal{S}_{n, \tau}$, $\tau(T) \geq \lceil \frac{2}{3}n \rceil$, then $3\tau - 2n + 2 \geq 2$, which implies that $S_{n, \tau}^\dagger \in \mathcal{T}_{n, \tau}^3$.

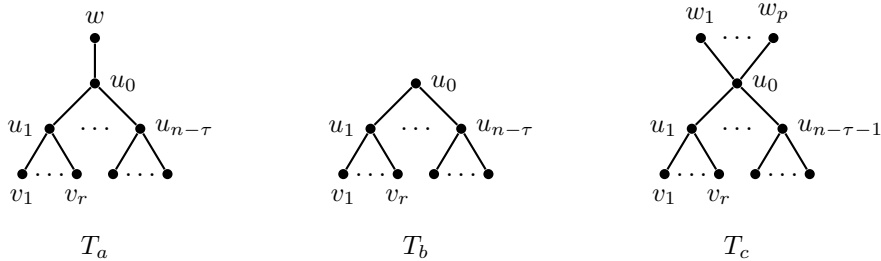


Figure 3: Trees $T_a \in \mathcal{T}_{n, \tau}^1$, $T_b \in \mathcal{T}_{n, \tau}^2$ and $T_c \in \mathcal{T}_{n, \tau}^3$ together with some labeled vertices.

In order to prove Theorem 1.3, we need the following lemma.

Lemma 3.1. For $0 \leq \alpha < 1$, the A_α -index of $S_{n,\tau}^\dagger$ is equal to the largest root of $P_\alpha(x) = 0$, where $P_\alpha(x)$ is defined in (1.2).

Proof. Recall that $S_{n,\tau}^\dagger$ is a tree obtained from the star $S_{n-\tau}$ by attaching exactly two pendant edges to each leaf of $S_{n-\tau}$ and attaching $3\tau - 2n + 2$ pendant edges to the centre of $S_{n-\tau}$ (see Figure 1). Let v_0 be the centre of $S_{n-\tau}$, V_1 be the set of $2(n - \tau - 1)$ pendant vertices adjacent to the leaves of $S_{n-\tau}$, and let V_2 be the set of $3\tau - 2n + 2$ pendant vertices adjacent to v_0 . Hence $\pi := \{v_0\} \cup (V_{S_{n-\tau}} \setminus \{v_0\}) \cup V_1 \cup V_2$ is an equitable partition of $V_{S_{n,\tau}^\dagger}$. Then the corresponding quotient matrix can be written as follows:

$$(A_\alpha)^\pi := \begin{pmatrix} \alpha(2\tau - n + 1) & (1 - \alpha)(n - \tau - 1) & 0 & (1 - \alpha)(3\tau - 2n + 2) \\ 1 - \alpha & 3\alpha & 2(1 - \alpha) & 0 \\ 0 & 1 - \alpha & \alpha & 0 \\ 1 - \alpha & 0 & 0 & \alpha \end{pmatrix}.$$

The characteristic polynomial of $(A_\alpha)^\pi$ is $P_\alpha(x)$, where $P_\alpha(x)$ is defined in (1.2). Note that $(A_\alpha)^\pi$ is nonnegative and irreducible. Together with Lemma 2.7 and the Perron-Frobenius theorem, our result holds immediately. $\square$

Proof of Theorem 1.3. Choose T among $\mathcal{T}_n^\tau$ such that its A_α -index is as large as possible. Let $\mathbf{x}$ be the Perron vector of $A_\alpha(T)$. In view of Lemma 2.2, we obtain that $T \cong S_n \cong S_{n,n-1}^\dagger$ if $\tau = n - 1$ or $3 \leq n \leq 4$. So, in what follows, we assume that $\tau \leq n - 2$ and $n \geq 5$. We are to characterize the structure of T through the following three claims.

Claim 1. $\mathcal{Q}'_T = \emptyset$.

Proof of Claim 1. Suppose that $\mathcal{Q}'_T \neq \emptyset$. Let $v \in \mathcal{Q}'_T$ and $N_T(v) = \{u, w\}$, where u is a leaf. Denote by $T_1 = T - vu + uw$. Then by Lemma 2.5, we have $\lambda_\alpha(T_1) > \lambda_\alpha(T)$. However, by Lemma 2.8, $T_1 \in \mathcal{T}_n^\tau$, a contradiction to the choice of T . Thus $\mathcal{Q}'_T = \emptyset$. This completes the proof of Claim 1. $\square$

Claim 2. $T \in \mathcal{S}_{n,\tau}$.

Proof of Claim 2. Let $T' = T - \mathcal{P}_T$. By Claim 1, one sees that $T \in \mathcal{S}_{n,\tau}$ is equivalent to $|\mathcal{Q}_{T'}| = 1$. Suppose that $|\mathcal{Q}_{T'}| \geq 2$. Choose two vertices $u, v \in \mathcal{Q}_{T'}$ such that the distance between u and v in T' is as large as possible. Let u' and v' be the neighbors of u and v lying on the path connecting u and v , respectively. Then we have $(N_T(u) \setminus \{u'\}) \cup (N_T(v) \setminus \{v'\}) \subseteq \mathcal{P}_T \cup \mathcal{Q}_T$, $(N_T(u) \setminus \{u'\}) \cap \mathcal{Q}_T \neq \emptyset$ and $(N_T(v) \setminus \{v'\}) \cap \mathcal{Q}_T \neq \emptyset$.

Assume that $(N_T(u) \setminus \{u'\}) \cap \mathcal{Q}_T = \{u_1, u_2, \dots, u_s\}$ and $(N_T(v) \setminus \{v'\}) \cap \mathcal{Q}_T = \{v_1, v_2, \dots, v_t\}$. Thus we have $s, t \geq 1$. By Claim 1, we know that there exist at least two leaves adjacent to each vertex in $\{u_1, \dots, u_s, v_1, \dots, v_t\}$. Let S be a good dissociation set of T . Then $u_i \notin S$ and $v_j \notin S$ for $1 \leq i \leq s$, $1 \leq j \leq t$. Let

$$T_2 = \begin{cases} T - \{vv_j \mid 1 \leq j \leq t\} + \{uv_j \mid 1 \leq j \leq t\}, & \text{if } x_u > x_v, \\ T - \{uu_i \mid 1 \leq i \leq s\} + \{vu_i \mid 1 \leq i \leq s\}, & \text{if } x_u \leq x_v. \end{cases}$$

In view of Lemmas 2.4 and 2.8, we have $\lambda_\alpha(T_2) > \lambda_\alpha(T)$ and $T_2 \in \mathcal{T}_n^\tau$, a contradiction. Thus we have $|\mathcal{Q}_{T'}| = 1$, i.e. $T \in \mathcal{S}_{n,\tau}$. $\square$

Claim 3. $T \in \mathcal{T}_{n,\tau}^3$.

Proof of Claim 3. Suppose that $T \notin \mathcal{T}_{n,\tau}^3$. Then by Claim 2, we know that $T \in \mathcal{T}_{n,\tau}^1 \cup \mathcal{T}_{n,\tau}^2$. For the star $S_{n-\tau+1}$, assume that u_0 is the centre of $S_{n-\tau+1}$, and $u_1, \dots, u_{n-\tau}$ are leaves of $S_{n-\tau+1}$ (see Figure 3). We proceed by considering the following two cases.

Case 1. $T \in \mathcal{T}_{n,\tau}^1$. Assume that $N(u_1) \setminus \{u_0\} = \{v_1, \dots, v_r\}$ and w is just the leaf adjacent to u_0 in T . Let

$$T_3 = \begin{cases} T - \{u_1v_i \mid 1 \leq i \leq r\} + \{u_0v_i \mid 1 \leq i \leq r\}, & \text{if } x_{u_0} > x_{u_1}, \\ T - u_0w + u_1w, & \text{if } x_{u_0} \leq x_{u_1}. \end{cases}$$

By Lemma 2.8, we obtain $T_3 \in \mathcal{T}_{n,\tau}^2 \cup \mathcal{T}_{n,\tau}^3$. However, in view of Lemma 2.4, $\lambda_\alpha(T_3) > \lambda_\alpha(T)$, which contradicts the choice of T .

Case 2. $T \in \mathcal{T}_{n,\tau}^2$. Similarly, assume that $N(u_1) \setminus \{u_0\} = \{v_1, \dots, v_r\}$. Let

$$T_4 = \begin{cases} T - \{u_1v_i \mid 1 \leq i \leq r\} + \{u_0v_i \mid 1 \leq i \leq r\}, & \text{if } x_{u_0} > x_{u_1}, \\ T - \{u_0u_j \mid 2 \leq j \leq n - \tau\} + \{u_1u_j \mid 2 \leq j \leq n - \tau\}, & \text{if } x_{u_0} \leq x_{u_1}. \end{cases}$$

By Lemma 2.8, we get that $T_4 \in \mathcal{T}_{n,\tau}^3$. And once again, by Lemma 2.4, $\lambda_\alpha(T_4) > \lambda_\alpha(T)$, a contradiction. $\square$

We come back to show Theorem 1.3.

By Claim 3, we have $T \in \mathcal{T}_{n,\tau}^3$. Similarly, for the star $S_{n-\tau}$, assume that $V_{S_{n-\tau}} = \{u_0, u_1, \dots, u_{n-\tau-1}\}$, where u_0 is the unique non-pendant vertex. Suppose that $T \not\cong S_{n,\tau}^\dagger$. Then there exists a vertex u_i , where $i \in \{1, 2, \dots, n - \tau - 1\}$, such that $d(u_i) \geq 4$. Without loss of generality, assume that $d(u_1) \geq 4$. Let $N(u_0) \cap \mathcal{P}_T = \{w_1, \dots, w_p\}$ and $N(u_1) \setminus \{u_0\} = \{v_1, \dots, v_r\}$. Then $p \geq 2$ and $r \geq 3$.

If $\tau = n - 2$, then T is a tree obtained from S_{p+1} and S_{r+1} by adding an edge to connect the centres of theirs. Since $T \not\cong S_{n,\tau}^\dagger$, we have $p \geq 3$. Let

$$T_5 = \begin{cases} T - \{u_1v_i \mid 3 \leq i \leq r\} + \{u_0v_i \mid 3 \leq i \leq r\}, & \text{if } x_{u_0} > x_{u_1}, \\ T - \{u_0w_j \mid 3 \leq j \leq p\} + \{u_1w_j \mid 3 \leq j \leq p\}, & \text{if } x_{u_0} \leq x_{u_1}. \end{cases}$$

Then $T_5 \cong S_{n,n-2}^\dagger$. By Lemma 2.4, we have $\lambda_\alpha(T_5) > \lambda_\alpha(T)$, a contradiction.

If $\tau \leq n - 3$, then let

$$T_6 = \begin{cases} T - \{u_1v_i \mid 3 \leq i \leq r\} + \{u_0v_i \mid 3 \leq i \leq r\}, & \text{if } x_{u_0} > x_{u_1}, \\ T - \{u_0u_k \mid 2 \leq k \leq n - \tau - 1\} + \{u_1u_k \mid 2 \leq k \leq n - \tau - 1\}, & \text{if } x_{u_0} \leq x_{u_1} \text{ and } p = 2, \\ T - \{u_0u_k \mid 2 \leq k \leq n - \tau - 1\} - \{u_0w_j \mid 3 \leq j \leq p\} \\ \quad + \{u_1u_k \mid 2 \leq k \leq n - \tau - 1\} + \{u_1w_j \mid 3 \leq j \leq p\}, & \text{if } x_{u_0} \leq x_{u_1} \text{ and } p \geq 3. \end{cases}$$

By Lemma 2.8, $\tau(T_6) = \tau(T)$. In view of Lemma 2.4, one has $\lambda_\alpha(T_6) > \lambda_\alpha(T)$, a contradiction. Therefore, $T \cong S_{n,\tau}^\dagger$. By Lemma 3.1, our result holds immediately.

This completes the proof. $\square$

4. Proofs of Theorems 1.4 and 1.5

In this section, we present the proofs for Theorems 1.4 and 1.5. The former shows that a connected graph with given order n and dissociation number τ ($\tau \geq \lceil \frac{2}{3}n \rceil$) having the minimum A_α -index is a tree, and the latter characterizes all the connected graphs with order n and dissociation number $\tau \in \{2, \lceil \frac{2}{3}n \rceil, n - 1, n - 2\}$ having the minimum A_α -index.

Let Y_1 (resp. Y_2) be a tree obtained from P_{n-2} (resp. P_{n-6}) by attaching exactly two pendant edges (resp. two pendant paths of length three) to one leaf of P_{n-2} (resp. P_{n-6}). Let Y_3 be a tree obtained from P_{n-4} by attaching one pendant edge and one pendant path of length three to one leaf of P_{n-4} . Recall that G_w is a graph constructed from G by a subdivision operation for an edge of G . The *triple subdivision operation* for an edge $uv \in E_G$ is adding three new vertices x, y, z and substituting uv by a path $uxyzv$, and we denote the resultant

graph by G_{xyz} . We call $\dot{G}$ a *subdivision transformation graph* of G if $\dot{G}$ is obtained from G by a (triple) subdivision operation for an edge on an internal path of G , and deleting one or three other vertices of G such that $|V_{\dot{G}}| = |V_G|$. A subdivision transformation graph $\dot{G}$ is said to be *optimal* if $\dot{G}$ is connected and $\tau(\dot{G}) \in \{\tau(G) - 1, \tau(G)\}$.

In order to show Theorem 1.4, we need the following key lemma. It presents the relationship between $\tau(G_w)$ (resp. $\tau(G_{xyz})$) and $\tau(G)$.

Lemma 4.1 ([11]). *Let G be a connected graph with $uv \in E_G$ and let G_w and G_{xyz} be the graph obtained from G by the subdivision operation and triple subdivision operation for uv , respectively. Then*

- (i) $\tau(G_w) \in \{\tau(G), \tau(G) + 1\}$;
- (ii) $\tau(G_{xyz}) = \tau(G) + 2$.

Let T be a tree, we call $v \in V_T$ a *branching vertex* if $d_T(v) \geq 3$. The next lemma was obtained previously in [11]. We include its proof here.

Lemma 4.2 ([11]). *Let T be a tree with at least two branching vertices. Then there exists an optimal subdivision transformation graph of T .*

Proof. We use T_x and T_{xyz} to denote the trees obtained from T by the subdivision operation and triple subdivision operation for an edge on an internal path of T , respectively. Choose a diameter path $P_d = u_1 u_2 u_3 u_4 \cdots u_d$ of T such that $d_T(u_2)$ is as large as possible. Then $N_T(u_2) \setminus \{u_3\} \subseteq \mathcal{P}_T$ and $N_T(u_3) \setminus \{u_4\} \subseteq \mathcal{P}_T \cup \mathcal{Q}_T$.

If $d_T(u_2) = d_T(u_3) = 2$, then by Lemma 2.8, we obtain

$$\tau(T_{xyz} - u_1 - u_2 - u_3) = \tau(T_{xyz}) - 2. \quad (4.1)$$

By Lemma 4.1, we have $\tau(T_{xyz}) = \tau(T) + 2$. Combining this with (4.1) yields $\tau(T_{xyz} - u_1 - u_2 - u_3) = \tau(T)$. Therefore, $T_{xyz} - u_1 - u_2 - u_3$ is an optimal subdivision transformation graph of T .

If $d_T(u_2) = 2$ and $d_T(u_3) \geq 3$, then according to the choice of P_d , we know that $N_T(u_3) \setminus \{u_4\} \subseteq \mathcal{P}_T \cup \mathcal{Q}'_T$. Hence, in view of Lemmas 2.8 and 4.1, we obtain that $T_x - u_1$ is a tree with $\tau(T_x - u_1) = \tau(T_x) - 1 \in \{\tau(T), \tau(T) - 1\}$. This implies that $T_x - u_1$ is an optimal subdivision transformation graph of T .

If $d_T(u_2) = 3$, then by Lemmas 2.8 and 4.1, we have $T_{xyz} - u_1 - u_2 - v$ is a tree with $\tau(T_{xyz} - u_1 - u_2 - v) = \tau(T_{xyz}) - 2 = \tau(T)$, where v is the only pendant vertex adjacent to u_2 other than u_1 . This indicates that $T_{xyz} - u_1 - u_2 - v$ is an optimal subdivision transformation graph of T .

If $d_T(u_2) \geq 4$, then in view of Lemmas 2.8 and 4.1, we have $T_x - u_1$ is a tree with $\tau(T_x - u_1) = \tau(T_x) - 1 \in \{\tau(T), \tau(T) - 1\}$. Hence $T_x - u_1$ is an optimal subdivision transformation graph of T .

This completes the proof. $\square$

Now we are ready to show Theorem 1.4.

Proof of Theorem 1.4. If $\tau(G^\dagger) = \lceil \frac{2}{3}n \rceil$, then by Lemma 2.3, we have $G^\dagger \cong P_n$ since $\tau(P_n) = \lceil \frac{2}{3}n \rceil$, and our result holds obviously. So, in what follows, we assume that $\tau(G^\dagger) > \lceil \frac{2}{3}n \rceil$.

Suppose to the contrary that $G^\dagger$ is not a tree. If $G^\dagger$ is a subgraph of $(nK_2) \vee K_1$, then $\tau(G^\dagger) = n - 1$ and there exists a cycle $v_0 v_1 v_2 v_0$ such that $d(v_1) = d(v_2) = 2$. Let $G_1^\dagger = G^\dagger - v_1 v_2$. By Lemmas 2.1 and 2.8, we have $\lambda_\alpha(G_1^\dagger) < \lambda_\alpha(G^\dagger)$ and $G_1^\dagger \in \mathcal{G}_n^{n-1}$, which contradicts the choice of $G^\dagger$. This means that there exists a spanning tree, say $T^\dagger$, of $G^\dagger$ such that $T^\dagger \not\cong S_{k_1, k_2}$ (see Figure 2) for all $k_1 + 2k_2 = n - 1$.

It is clear that $\tau(T^\dagger) \geq \tau(G^\dagger)$. By Lemma 2.1, we have

$$\lambda_\alpha(T^\dagger) < \lambda_\alpha(G^\dagger). \quad (4.2)$$

If $\tau(T^\dagger) = \tau(G^\dagger)$, then we can derive a contradiction by the choice of $G^\dagger$. Hence,

$$\tau(T^\dagger) > \tau(G^\dagger) \geq \left\lceil \frac{2}{3}n \right\rceil + 1. \quad (4.3)$$

Since $\tau(T^\dagger) > \left\lceil \frac{2}{3}n \right\rceil = \tau(P_n)$, we have $T^\dagger \not\cong P_n$, which implies that there exists at least one branching vertex in $T^\dagger$.

If $T^\dagger$ has at least two branching vertices, then by Lemma 4.2, there exists an optimal subdivision transformation graph, say $\dot{T}_1$, of $T^\dagger$. Denote by $\dot{T}_0 = T^\dagger$. In view of Lemma 2.6 and (4.2), we obtain $\lambda_\alpha(\dot{T}_1) < \lambda_\alpha(\dot{T}_0) < \lambda_\alpha(G^\dagger)$. We can repeat the above transformation to get an n -vertex tree sequence

$$\dot{T}_0, \dot{T}_1, \dots, \dot{T}_i, \dots, \dot{T}_s$$

such that $\dot{T}_s$ is a tree having exactly one branching vertex with $\tau(\dot{T}_s) = \left\lceil \frac{2}{3}n \right\rceil$ and $\tau(\dot{T}_i) \in \{\tau(\dot{T}_{i-1}) - 1, \tau(\dot{T}_{i-1})\}$ and $\lambda_\alpha(\dot{T}_i) < \lambda_\alpha(\dot{T}_{i-1})$ for $1 \leq i \leq s$. According to the proof of Lemma 4.2, we know that such $\dot{T}_s$ must exist, for example, Y_1, Y_2, Y_3 . By (4.3), $\tau(\dot{T}_0) \geq \left\lceil \frac{2}{3}n \right\rceil + 2 = \tau(\dot{T}_s) + 2$, which implies that $s \geq 2$. Since $\tau(\dot{T}_0) > \tau(G^\dagger) > \left\lceil \frac{2}{3}n \right\rceil = \tau(\dot{T}_s)$, there exists $j \in \{1, 2, \dots, s-1\}$ such that $\tau(\dot{T}_j) = \tau(G^\dagger)$. However, $\lambda_\alpha(\dot{T}_j) < \lambda_\alpha(\dot{T}_0) < \lambda_\alpha(G^\dagger)$, which contradicts the choice of $G^\dagger$.

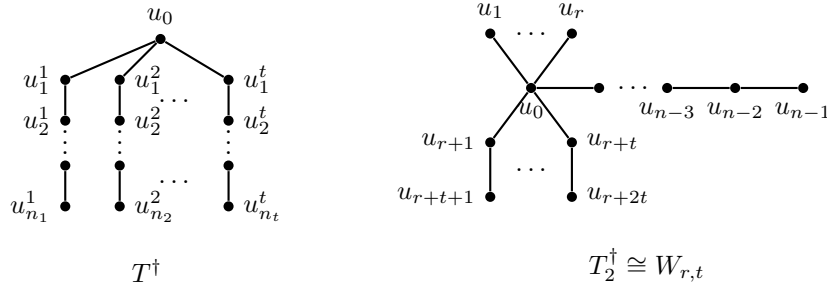


Figure 4: Trees $T^\dagger$ and $T_2^\dagger$.

In what follows, we assume that $T^\dagger$ has exact one branching vertex. Let u_0 be the branching vertex of $T^\dagger$. Then $T^\dagger$ can be obtained from t paths $P_{n_1+1}, P_{n_2+1}, \dots, P_{n_t+1}$ by sharing a common vertex u_0 , where $t \geq 3$. Let $u_0, u_1^i, \dots, u_{n_i}^i$ denote the vertices of P_{n_i+1} for $1 \leq i \leq t$ (see Figure 4). Without loss of generality, we can assume that $n_1 \geq n_2 \geq \dots \geq n_t \geq 1$. Since $T^\dagger \not\cong S_{k_1, k_2}$ for all $k_1 + 2k_2 = n - 1$, we have $n_1 \geq 3$. Let

$$T_1^\dagger = \begin{cases} T^\dagger, & \text{if } n_2 \in \{1, 2\}, \\ T^\dagger - u_0 u_1^2 + u_{n_1}^1 u_1^2, & \text{if } n_2 \equiv 0 \pmod{3}, \\ T^\dagger - u_1^2 u_2^2 + u_{n_1}^1 u_2^2, & \text{if } n_2 \equiv 1 \pmod{3} \text{ and } n_2 \geq 4, \\ T^\dagger - u_2^2 u_3^2 + u_{n_1}^1 u_3^2, & \text{if } n_2 \equiv 2 \pmod{3} \text{ and } n_2 \geq 5. \end{cases}$$

In view of Lemmas 2.5 and 2.8, we get that $\tau(T_1^\dagger) = \tau(T^\dagger)$ and $\lambda_\alpha(T_1^\dagger) \leq \lambda_\alpha(T^\dagger)$. Repeating the above procedure for $T_1^\dagger$, we finally obtain an n -vertex tree $T_2^\dagger \cong W_{r,t}$, such that

$$\lambda_\alpha(T_2^\dagger) \leq \lambda_\alpha(T^\dagger), \quad \tau(T_2^\dagger) = \tau(T^\dagger), \quad (4.4)$$

where $W_{r,t}$ is an n -vertex tree obtained from a star S_{r+1} by attaching t pendant paths of length 2 and one pendant path of length $n - r - 2t - 1$ to the centre of S_{r+1} (see Figure 4).

If $(r, t) = (3, 0)$ or $r + t \leq 2$, then we can obtain

$$\tau(T_2^\dagger) = \begin{cases} \left\lceil \frac{2}{3}n \right\rceil, & \text{if } (r, t) \in \{(0, 0), (0, 1), (1, 0), (2, 0)\}, \\ \left\lceil \frac{2n-1}{3} \right\rceil + 1, & \text{if } (r, t) = (0, 2), \\ \left\lceil \frac{2n-2}{3} \right\rceil + 1, & \text{if } (r, t) \in \{(1, 1), (3, 0)\}. \end{cases}$$

By (4.3) and (4.4), we have $\tau(T_2^\dagger) = \tau(T^\dagger) \geq \lceil \frac{2}{3}n \rceil + 2$, a contradiction.

If $t = 0$ and $r \geq 4$, then by Lemmas 2.5 and 2.8, we have

$$\lambda_\alpha(W_{r-2,t+1}) < \lambda_\alpha(W_{r,t}), \quad \tau(W_{r-2,t+1}) = \tau(W_{r,t}). \quad (4.5)$$

In view of (4.5), we assume that $t \geq 1$ and $r + t \geq 3$ in what follows. The labels of the vertices of $T_2^\dagger$ are shown in Figure 4. Let

$$T_3^\dagger = \begin{cases} T_2^\dagger - \{u_0 u_{r+j} \mid 1 \leq j \leq t-2\} + \{u_{n-3} u_{r+j} \mid 1 \leq j \leq t-2\}, & \text{if } r = 0, t \geq 3, \\ T_2^\dagger - \{u_0 u_{r+j} \mid 1 \leq j \leq t-1\} + \{u_{n-3} u_{r+j} \mid 1 \leq j \leq t-1\}, & \text{if } r = 1, t \geq 2, \\ T_2^\dagger - \{u_0 u_i \mid 1 \leq i \leq r-1\} + \{u_{n-3} u_i \mid 1 \leq i \leq r-1\}, & \text{if } r \geq 2, t = 1, \\ T_2^\dagger - \{u_0 u_{r+j} \mid 1 \leq j \leq t-1\} - \{u_0 u_i \mid 1 \leq i \leq r-1\} \\ \quad + \{u_{n-3} u_{r+j} \mid 1 \leq j \leq t-1\} + \{u_{n-3} u_i \mid 1 \leq i \leq r-1\}, & \text{if } r, t \geq 2. \end{cases}$$

In view of Lemma 2.8, we have

$$\tau(T_3^\dagger) = \tau(T_2^\dagger). \quad (4.6)$$

Let $\mathbf{y} = (y_0, y_1, \dots, y_{n-1})^T$ be the Perron vector of $T_3^\dagger$, where y_i corresponds to u_i ($0 \leq i \leq n-1$). If $y_0 < y_{n-3}$, let

$$T_4^\dagger = \begin{cases} T_3^\dagger - u_0 u_{r+t-1} + u_{n-3} u_{r+t-1}, & \text{if } r = 0, \\ T_3^\dagger - u_0 u_r + u_{n-3} u_r, & \text{if } r > 0. \end{cases}$$

It is obvious that $T_4^\dagger \cong T_2^\dagger$. By Lemma 2.4, we have $\lambda_\alpha(T_3^\dagger) < \lambda_\alpha(T_4^\dagger) = \lambda_\alpha(T_2^\dagger)$. If $y_0 \geq y_{n-3}$, then we can undo the step from $T_2^\dagger$ to $T_3^\dagger$. By Lemma 2.4, we have $\lambda_\alpha(T_3^\dagger) < \lambda_\alpha(T_2^\dagger)$. Consequently, both cases yield $\lambda_\alpha(T_3^\dagger) < \lambda_\alpha(T_2^\dagger)$. Together with (4.2), (4.3), (4.4) and (4.6), we have

$$\lambda_\alpha(T_3^\dagger) < \lambda_\alpha(G^\dagger), \quad \tau(T_3^\dagger) > \tau(G^\dagger) \geq \lceil \frac{2}{3}n \rceil + 1. \quad (4.7)$$

Note that $T_3^\dagger$ has two branching vertices. We obtain, similarly as in the case “ $T^\dagger$ has at least two branching vertices,” that there exists an n -vertex tree sequence

$$\ddot{T}_0, \ddot{T}_1, \dots, \ddot{T}_i, \dots, \ddot{T}_p$$

such that $\ddot{T}_0 \cong T_3^\dagger$, $\ddot{T}_p$ is a tree having exactly one branching vertex with $\tau(\ddot{T}_s) = \lceil \frac{2}{3}n \rceil$ and $\tau(\ddot{T}_i) \in \{\tau(\ddot{T}_{i-1}) - 1, \tau(\ddot{T}_{i-1})\}$, $\lambda_\alpha(\ddot{T}_i) < \lambda_\alpha(\ddot{T}_{i-1})$ for $1 \leq i \leq p$. Note that $p \geq 2$. By (4.7), we have $\tau(\ddot{T}_0) > \tau(G^\dagger) > \tau(\ddot{T}_p)$. This implies that there exists $j \in \{1, 2, \dots, p-1\}$ such that $\tau(\ddot{T}_j) = \tau(G^\dagger)$. However, we know that $\lambda_\alpha(\ddot{T}_j) < \lambda_\alpha(\ddot{T}_0) < \lambda_\alpha(G^\dagger)$, which contradicts the choice of $G^\dagger$.

This completes the proof. $\square$

For an n -vertex graph G , denote by $P_\alpha(G, x) = \det(xI_n - A_\alpha(G))$ the characteristic polynomial of $A_\alpha(G)$, where I_n is the identity matrix of order n . The following result is obvious.

Lemma 4.3. *Let G_1 and G_2 be two connected graphs. If $P_\alpha(G_2, x) > P_\alpha(G_1, x)$ for $x \geq \lambda_\alpha(G_1)$, then $\lambda_\alpha(G_2) < \lambda_\alpha(G_1)$.*

Recall that T_{r_1, p_1}^1 is a tree obtained from P_4 by attaching r_1 and p_1 pendant paths of length two to the two leaves of P_4 , respectively, whereas T_{r_2, p_2}^2 is a tree obtained from T_{r_2, p_2}^1 by attaching one pendant edge to the vertex of degree $r_2 + 1$ in T_{r_2, p_2}^1 (see Figure 2). In order to show Theorem 1.5, we need the following lemma.

Lemma 4.4. *If $r_1 \geq p_1 \geq 1$, then $\lambda_\alpha(T_{r_1, p_1}^1) < \lambda_\alpha(T_{r_1+1, p_1-1}^1)$.*

Proof. For simplicity, let $G^* := T_{r_1, p_1}^1$ and $G' := T_{r_1+1, p_1-1}^1$. If $p_1 = 1$, then the result follows immediately from Lemma 2.5. So in what follows, we may assume that $r_1 \geq p_1 \geq 2$. We can easily obtain an equitable partition of V_{G^*} (resp. $V_{G'}$), with four parts each of which contains only one vertex, two parts each of which contains r_1 (resp. $r_1 + 1$) vertices and two parts each of which contains p_1 (resp. $p_1 - 1$) vertices. Therefore, the corresponding quotient matrices can be written as follows:

$$(A_\alpha)^{\pi_3} := \begin{pmatrix} \alpha & 1-\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & (1-\alpha)r_1 & \alpha(r_1+1) & 1-\alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-\alpha & \alpha(p_1+1) & (1-\alpha)p_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha \\ 0 & 0 & 0 & 0 & 0 & 0 & 1-\alpha & \alpha \end{pmatrix},$$

$$(A_\alpha)^{\pi_4} := \begin{pmatrix} \alpha & 1-\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\ 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & (1-\alpha)(r_1+1) & \alpha(r_1+2) & 1-\alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-\alpha & \alpha p_1 & (1-\alpha)(p_1-1) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-\alpha & 2\alpha & 1-\alpha \\ 0 & 0 & 0 & 0 & 0 & 0 & 1-\alpha & \alpha \end{pmatrix}.$$

Let $P_\alpha^3(x) := \det(xI_8 - (A_\alpha)^{\pi_3})$ (resp. $P_\alpha^4(x) := \det(xI_8 - (A_\alpha)^{\pi_4})$) be the characteristic polynomial of $(A_\alpha)^{\pi_3}$ (resp. $(A_\alpha)^{\pi_4}$). Note that $(A_\alpha)^{\pi_3}$ (resp. $(A_\alpha)^{\pi_4}$) is nonnegative and irreducible. Together with Lemma 2.7 and the Perron-Frobenius theorem, we know that $\lambda_\alpha(G^*)$ (resp. $\lambda_\alpha(G')$) coincides with the largest zero of $P_\alpha^3(x)$ (resp. $P_\alpha^4(x)$).

Note that G' contains S_{r_1+3} as its proper subgraph, then by Lemma 2.1, we have

$$\lambda_\alpha(G') > \lambda_\alpha(S_{r_1+3}), \quad (4.8)$$

and a simple calculation gives us

$$\lambda_\alpha(S_{r_1+3}) = \frac{1}{2} \left(\alpha(r_1+3) + \sqrt{\alpha^2(r_1+3)^2 + 4(r_1+2)(1-2\alpha)} \right).$$

With the same idea as the Appendix of calculations using Matlab, we obtain that $\min(P_\alpha^3(x) - P_\alpha^4(x)) \approx 0.6527$ for $x \geq \lambda_\alpha(S_{r_1+3})$, that is to say, $P_\alpha^3(x) - P_\alpha^4(x) > 0$ when $x \geq \lambda_\alpha(S_{r_1+3})$. Combining this with (4.8) yields $P_\alpha^3(x) - P_\alpha^4(x) > 0$ when $x \geq \lambda_\alpha(G')$. Then by Lemma 4.3, we have $\lambda_\alpha(G^*) < \lambda_\alpha(G')$, as desired. $\square$

Let T_{r_3, p_3}^3 (resp. T_{r_4, p_4}^4) be the tree obtained from S_4 (resp. P_2) by attaching r_3 (resp. r_4) and p_3 (resp. p_4) pendant paths of length two to two leaves of S_4 (resp. P_2), respectively. Let T_{r_5, p_5}^5 be the tree obtained from P_3 by attaching one pendant edge and r_5 pendant paths of length two to one leaf of P_3 and attaching p_5 pendant paths of length two to the other leaf of P_3 . Let T_{r_6, p_6}^6 be the tree obtained from $S_{1,2}$ by attaching r_6 and p_6 pendant paths of length two to the two quasi-pendant vertices with degree 2 of $S_{1,2}$, respectively. Let T_{r_7, p_7}^7 (resp. T_{r_8, p_8}^8) be the tree obtained from P_4 (resp. P_6) by attaching r_7 (resp. r_8) and p_7 (resp. p_8) pendant paths of length two to two quasi-pendant vertices of P_4 (resp. P_6), respectively. T_{r_i, p_i}^i for $i \in \{3, \dots, 8\}$ are depicted in Figure 5.

Now we are ready to give the proof for Theorem 1.5.

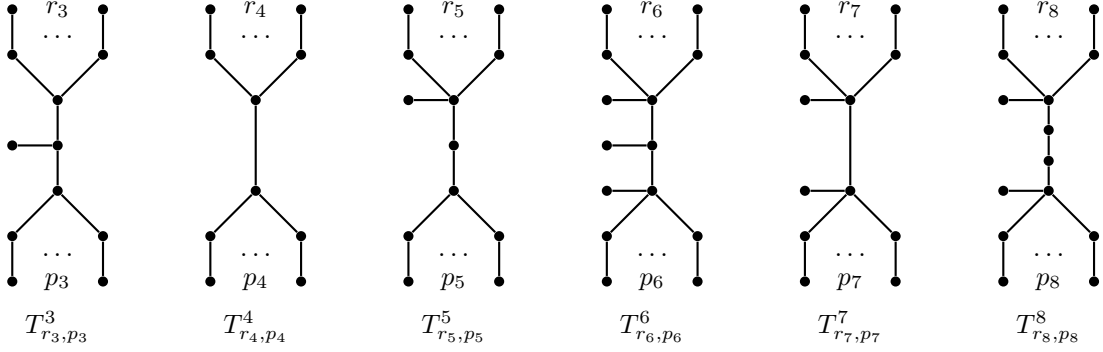


Figure 5: Trees T_{r_i, p_i}^i for $3 \leq i \leq 8$.

Proof of Theorem 1.5. (i) Let G^* be a graph in $\mathcal{G}_n^2$ having the minimum A_α -index. Then we know that G^* does not contain $K_1 \cup K_2$ and $3K_1$ as its induced subgraph. Let $\overline{G^*}$ be the complement of G^* . Then we have $d_{\overline{G^*}}(v) \leq 1$ for each vertex $v \in V_{G^*}$ (since otherwise there exist two vertices, say u, w , of V_{G^*} satisfying $uv, vw \notin E_{G^*}$, and thus $G^*[u, v, w] \cong K_1 \cup K_2$ or $G^*[u, v, w] \cong 3K_1$). This implies that $E_{\overline{G^*}}$ is a matching of K_n . Combining this with Lemma 2.1 gives us that $G^* \cong K_n - M$, where M is a maximum matching of K_n .

(ii) Since $\tau(P_n) = \lceil \frac{2}{3}n \rceil$, the result follows immediately from Lemma 2.3.

(iii) Let G^* be a graph in $\mathcal{G}_n^{n-1}$ having the minimum A_α -index with $n \geq 4$. Since $n - 1 \geq \lceil \frac{2}{3}n \rceil$, we have $G^* \in \mathcal{T}_n^{n-1}$ (based on Theorem 1.4). Let $S = S' \cup S''$ be a maximum dissociation set of G^* such that S' is an independent set and $E_{G^*[S'']}$ is a matching of G^* . Assume that $V_{G^*} = \{u_1, u_2, \dots, u_n\}$ and $S = V_{G^*} \setminus \{u_1\}$. Then $G^* \cong S_{k_1, k_2}$, where S_{k_1, k_2} is depicted in Figure 2, and $|S'| = k_1$.

Claim 4. $k_1 \leq 1$.

Proof of Claim 4. Suppose that $k_1 \geq 2$, i.e., there exist two vertices u_s, u_t in S' , where $s, t \in \{2, \dots, n\}$. Then let $G_1^* = G^* - u_1 u_s + u_t u_s$. In view of Lemma 2.8, we know that $G_1^* \in \mathcal{T}_n^{n-1}$. However, by Lemma 2.5, we have $\lambda_\alpha(G_1^*) < \lambda_\alpha(G^*)$, which contradicts the choice of G^* . Therefore, $k_1 \leq 1$, as desired. $\square$

According to Claim 4, we obtain $G^* \cong S_{0, \frac{n-1}{2}}$ if n is odd and $G^* \cong S_{1, \frac{n-2}{2}}$ if n is even.

(iv) Let G^* be a graph in $\mathcal{G}_n^{n-2}$ having the minimum A_α -index with $n \geq 6$. Since $n - 2 \geq \lceil \frac{2}{3}n \rceil$, we have $G^* \in \mathcal{T}_n^{n-2}$ by Theorem 1.4. Let $S = S' \cup S''$ be a maximum dissociation set of G^* such that S' is an independent set and $E_{G^*[S'']}$ is a matching of G^* . Assume that $V_{G^*} = \{u_1, u_2, \dots, u_n\}$ and $S = V_{G^*} \setminus \{u_1, u_2\}$, then we have $\min\{|N(u_1) \setminus \{u_2\}|, |N(u_2) \setminus \{u_1\}|\} \geq 1$.

Note that G^* is a tree. Then we know that $|N(u_1) \cap N(u_2)| \leq 1$, and thus there exist at least $|S'| - 1$ leaves in S' . By a similar discussion as that in (iii), we obtain $|S'| \leq 3$. We first assume that n is even. Since $n = |S| + 2 = |S'| + |S''| + 2$ and $|S''|$ is even, we have $|S'|$ is even, i.e., $|S'| \in \{0, 2\}$. We split the proof in the following two cases.

Case 1 $|N(u_1) \cap N(u_2)| = 1$. In this case, we proceed by considering the size of S' .

Subcase 1.1 $|S'| = 0$. In this subcase, we have $G^* \cong T_{r_3, p_3}^3$ with $(r_3, p_3) \neq (0, 0)$ and $r_3 + p_3 = \frac{n-4}{2}$. If $\max\{r_3, p_3\} \leq 1$, then by Lemma 2.5, we have $\lambda_\alpha(T_{r_3, p_3}^1) < \lambda_\alpha(T_{r_3, p_3}^3)$. If $\max\{r_3, p_3\} \geq 2$, without loss of generality, we assume that $r_3 \geq 2$. Let T'_{i_1, j_1} be the tree obtained from T_{i_1, j_1}^1 by attaching a pendant edge to a

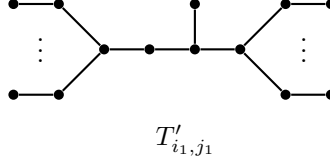


Figure 6: Tree T'_{i_1, j_1}

2-degree vertex on its internal path of length 3 (see Figure 6). Then by Lemma 2.6, we obtain

$$\lambda_\alpha(T'_{r_3, p_3}) < \lambda_\alpha(T_{r_3, p_3}^3). \quad (4.9)$$

It is easy to see that T_{r_3, p_3}^1 is a proper subgraph of T'_{r_3, p_3} , thus we have $\lambda_\alpha(T_{r_3, p_3}^1) < \lambda_\alpha(T'_{r_3, p_3})$ by Lemma 2.1. Together this with (4.9), we have $\lambda_\alpha(T_{r_3, p_3}^1) < \lambda_\alpha(T_{r_3, p_3}^3)$. Note that $T_{r_3, p_3}^1 \in \mathcal{T}_n^{n-2}$. Both cases yield a contradiction to the choice of G^* .

Subcase 1.2 $|S'| = 2$ and $N(u_1) \cap N(u_2) \subseteq S'$. In this subcase, we have $G^* \cong T_{r_5, p_5}^5$ with $r_5 \geq 0, p_5 \geq 1$ and $r_5 + p_5 = \frac{n-4}{2}$. If $r_5 = 0$, then $G^* \cong T_{0, p_5}^1$. If $r_5 \geq 1, p_5 = 1$, then by Lemma 2.5, we have $\lambda_\alpha(T_{r_5, 1}^1) < \lambda_\alpha(G^*)$, a contradiction. If $r_5 \geq 1, p_5 \geq 2$, then by Lemma 2.6, we obtain

$$\lambda_\alpha(T_{r_5, p_5}^2) < \lambda_\alpha(T_{r_5, p_5}^5). \quad (4.10)$$

Note that T_{r_5, p_5}^1 is a proper subgraph of T_{r_5, p_5}^2 . Therefore, by Lemma 2.1, $\lambda_\alpha(T_{r_5, p_5}^1) < \lambda_\alpha(T_{r_5, p_5}^2)$. Combining this with (4.10) yields $\lambda_\alpha(T_{r_5, p_5}^1) < \lambda_\alpha(T_{r_5, p_5}^5)$. Thus we derive a contradiction to the choice of G^* .

Subcase 1.3 $|S'| = 2$ and $N(u_1) \cap N(u_2) \subseteq S''$. In this subcase, we have $G^* \cong T_{r_6, p_6}^6$ with $(r_6, p_6) \neq (0, 0)$ and $r_6 + p_6 = \frac{n-6}{2}$. Similarly, by Lemmas 2.1 and 2.6, we obtain $\lambda_\alpha(T_{r_6, p_6}^8) < \lambda_\alpha(T_{r_6, p_6}^6)$. Note that $T_{r_6, p_6}^8 \in \mathcal{T}_n^{n-1}$, a contradiction again.

Case 2 $|N(u_1) \cap N(u_2)| = 0$. In this case, we proceed by considering the following four subcases.

Subcase 2.1 $|S'| = 0$ and $u_1 \sim u_2$. In this subcase, we have $G^* \cong T_{r_4, p_4}^4$ with $\min\{r_4, p_4\} \geq 1$ and $r_4 + p_4 = \frac{n-2}{2}$. If $r_4 = p_4 = 1$, then $G^* \cong T_{1, 0}^1$. If $r_4 = 1$ and $p_4 \geq 2$, then $G^* \cong T_{0, p_4}^1$. If $r_4 \geq 2$ and $p_4 = 1$, then $G^* \cong T_{r_4, 0}^1$. If $r_4, p_4 \geq 2$, then by Lemmas 2.1 and 2.6, we obtain

$$\min\{\lambda_\alpha(T_{r_4-1, p_4}^1), \lambda_\alpha(T_{r_4, p_4-1}^1)\} < \lambda_\alpha(T_{r_4, p_4}^1) < \lambda_\alpha(G^*). \quad (4.11)$$

It is easy to see that both T_{r_4-1, p_4}^1 and T_{r_4, p_4-1}^1 are in $\mathcal{T}_n^{n-2}$. Combining this with (4.11) gives us a contradiction to the choice of G^* .

Subcase 2.2 $|S'| = 0$ and $u_1 \approx u_2$. In this subcase, we have $G^* \cong T_{r_1, p_1}^1$ with $r_1 + p_1 = \frac{n-4}{2}$.

Subcase 2.3 $|S'| = 2$ and $u_1 \sim u_2$. In this subcase, we have $G^* \cong T_{r_7, p_7}^7$ with $\min\{r_7, p_7\} \geq 1$ and $r_7 + p_7 = \frac{n-4}{2}$. Similarly, by Lemmas 2.1 and 2.6, we get $\lambda_\alpha(T_{r_7, p_7}^1) < \lambda_\alpha(T_{r_7, p_7}^8) < \lambda_\alpha(G^*)$, and thus we get a contradiction.

Subcase 2.4 $|S'| = 2$ and $u_1 \approx u_2$. In this subcase, we have $G^* \cong T_{r_8, p_8}^8$ with $r_8 + p_8 = \frac{n-6}{2}$. If $(r_8, p_8) = (0, 0)$, then $G^* \cong T_{1, 0}^1$, and the result holds. So, In what follows, we assume that $(r_8, p_8) \neq (0, 0)$. If $r_8 \geq 1$ and $p_8 = 0$, then by Lemma 2.5, we obtain that $\lambda_\alpha(T_{r_8, 1}^1) < \lambda_\alpha(G^*)$. If $r_8 = 0$ and $p_8 \geq 1$, then by Lemma 2.5 again, $\lambda_\alpha(T_{1, p_8}^1) < \lambda_\alpha(G^*)$. Both cases give us a contradiction. Therefore, in what follows we may assume that $r_8, p_8 \geq 1$. By a similar proof of Lemma 4.4, applying Matlab to compare the spectral radii of the corresponding quotient matrices, we get $\min\{\lambda_\alpha(T_{r_8, p_8+1}^1), \lambda_\alpha(T_{r_8+1, p_8}^1)\} < \lambda_\alpha(G^*)$, which leads to a contradiction since $\{T_{r_8, p_8+1}^1, T_{r_8+1, p_8}^1\} \subseteq \mathcal{T}_n^{n-2}$.

By Cases 1 and 2, we obtain that $G^* \cong T_{r_1, p_1}^1$ with $r_1 + p_1 = \frac{n-4}{2}$. Without loss of generality, we may assume that $r_1 \geq p_1$. If $(r_1, p_1) = (1, 0)$, then $G^* \cong T_{1,0}^1$, and thus the result holds. If $p_1 = 0$ and $r_1 \geq 2$, then by Lemma 2.5, we have $\lambda_\alpha(T_{r_1-1,1}^1) < \lambda_\alpha(T_{r_1,0}^1)$, a contradiction. If $p_1 \geq 1$, then in view of Lemma 4.4, we obtain $G^* \cong T_{\lfloor \frac{n-4}{4} \rfloor, \lfloor \frac{n-4}{4} \rfloor}^1$, the result holds. If n is odd, we can also get $G^* \cong T_{\lfloor \frac{n-5}{4} \rfloor, \lceil \frac{n-5}{4} \rceil}^2$ in a similar way, whose procedure is omitted here. $\square$

5. Concluding remarks

In this paper, we mainly head in characterizing the extremal graphs having the maximum A_α -index over all graphs in $\mathcal{G}_n^\tau$, $\mathcal{B}_n^\tau$ and $\mathcal{T}_n^\tau$, respectively, and determining the structure of graphs having the minimum A_α -index among all graphs in $\mathcal{G}_n^\tau$ with some restrictions on τ . Theorem 1.1 (resp. Theorem 1.2, Theorem 1.3) characterizes all the connected graphs (resp. bipartite graphs, trees) having the maximum A_α -index among all connected graphs (resp. bipartite graphs, trees) with given order and dissociation number. Theorem 1.4 shows that the graph over $\mathcal{G}_n^\tau$ having the minimum A_α -index is a tree provided that $\tau \geq \lceil \frac{2}{3}n \rceil$; whereas Theorem 1.5 determines the graphs with fixed order n and dissociation number $\tau \in \{2, \lceil \frac{2}{3}n \rceil, n-1, n-2\}$ having the minimum A_α -index.

In view of (1.1), if we put $\alpha = 0$, respectively, in Theorems 1.1–1.5, then we may deduce the main results obtained for the adjacency spectral radius of graphs with given order and dissociation number (see [11] for details), whereas if we put $\alpha = \frac{1}{2}$, respectively, in Theorems 1.1–1.5, we may also deduce the corresponding results for the signless Laplacian spectral radius, say $q(G)$, of graphs with given order and dissociation number. Then the next corollaries follow immediately.

Corollary 5.1. *Let G be in $\mathcal{G}_n^\tau$ having the maximum signless Laplacian spectral radius. Then $G \cong K_{n-\tau} \vee (\frac{\tau}{2}K_2)$ if τ is even, and $G \cong K_{n-\tau} \vee (\frac{\tau-1}{2}K_2 \cup K_1)$ if τ is odd.*

Corollary 5.2. *Let G be a graph in $\mathcal{B}_n^\tau$. Then $q(G) \leq n$ with equality if and only if $G \cong K_{\tau, n-\tau}$.*

Corollary 5.3. *Let T be a tree in $\mathcal{T}_n^\tau$ ($n \geq 3$) having the maximum signless Laplacian spectral radius. Then $q(T) \leq \theta(n, \tau)$ with equality if and only if $T \cong S_{n, \tau}^\dagger$, where $\theta(n, \tau)$ is the largest root of $x^3 + (n-2\tau-6)x^2 + (8\tau-4n+9)x - n = 0$.*

Corollary 5.4. *Let $G^\dagger$ be a graph in $\mathcal{G}_n^\tau$ with $\tau \geq \lceil \frac{2}{3}n \rceil$ having the minimum signless Laplacian spectral radius. Then $G^\dagger$ is a tree.*

Corollary 5.5. *Let G^* be a graph in $\mathcal{G}_n^\tau$ having the minimum signless Laplacian spectral radius.*

- (i) *If $\tau = 2$, then $G^* \cong K_n - M$, where M is a maximum matching of K_n .*
- (ii) *If $\tau = \lceil \frac{2}{3}n \rceil$, then $G^* \cong P_n$.*
- (iii) *If $n \geq 4$ and $\tau = n-1$, then $G^* \cong S_{0, \frac{n-1}{2}}$ if n is odd and $G^* \cong S_{1, \frac{n-2}{2}}$ if n is even.*
- (iv) *If $n \geq 6$ and $\tau = n-2$, then $G^* \cong T_{\lfloor \frac{n-4}{4} \rfloor, \lfloor \frac{n-4}{4} \rfloor}^1$ if n is even and $G^* \cong T_{\lfloor \frac{n-5}{4} \rfloor, \lceil \frac{n-5}{4} \rceil}^2$ if n is odd.*

Declaration of competing interest

There is no competing interest.

Appendix.

```

clear
clc
syms a b c alpha x
AA=[alpha*(b+1) 0 (1-alpha)*b 1-alpha
    0 alpha*(a+b) (1-alpha)*b (1-alpha)*a
    (1-alpha)*a (1-alpha)*c alpha*(a+c) 0
    1-alpha (1-alpha)*c 0 alpha*(c+1)];
I=eye(4);
y=simplify(det(x*I-AA))
fun=matlabFunction(y);
objfun=@(x) fun(x(1),x(2),x(3),x(4),x(5));
x0=[0 0 0 0 0];
A=[-1 0 0 1 0;0 0 1 -1 0];
b=[-1 0];
Aeq=[];
beq=[];
lb=[2 0 0 1 0];
ub=[inf 1 inf inf inf];
[x,fval]=fmincon(objfun,x0,A,b,Aeq,beq,lb,ub,@confun)
function [c,ceq]=confun(x)
c=0.5.*(x(2).*(2.*x(1)+x(3)+x(4))+sqrt(x(2).^2.*(2.*x(1)+x(3)+x(4)).^2
+8.*x(1).*(x(3)+x(4)).*(1-2.*x(2))))-x(5);
ceq=0;
end

```

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