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The Majorization Theorems of Single-Cone Trees and Single-Cone Unicyclic Graphs

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Abstract

A single-cone tree (unicyclic graph) is the join of a complete graph K_1 and a tree (unicyclic graph). Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d_1', d_2', \ldots, d_n')$ are two non-increasing degree sequences. We say π is majorizated by π', denoted by $\pi \lhd \pi'$, if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d_i'$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d_i'$ for all $j = 1, 2, \ldots, n-1$. We use J_π to denote the class of single-cone trees (unicyclic graphs) with degree sequence π. Suppose that π and π' are two different non-increasing degree sequences of single-cone trees (unicyclic graphs). Let ρ and ρ' be the largest spectral radius of the graphs in J_π and $J_{\pi'}$, respectively, μ and μ' be the largest signless Laplacian spectral radius of the graphs in J_π and $J_{\pi'}$, respectively. In this paper, we prove that if $\pi \lhd \pi'$, then $\rho < \rho'$ and $\mu < \mu'$.

Keywords (Signless Laplacian) Spectral radius · Degree sequence · Majorization · Single-cone tree · Single-cone unicyclic graph

Mathematics Subject Classification 05C35 · 05C50

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1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = \{e_1, e_2, \ldots, e_m\}$, i.e., $|V| = n$ and $|E| = m$. If $m = n + c - 1$, then G is called a c-cyclic graph. Particularly, if $c = 0, 1, 2, 3$, then G is called a tree, a unicyclic graph, a bicyclic graph, a tricyclic graph, respectively. For $v \in V(G)$, $N(v)$ denotes the neighborhood of v in G and $d(v) = |N(v)|$ denotes the degree of vertex v. If $d_i = d_G(v_i)$ for $1 \leq i \leq n$, then we call the sequence $\pi = (d_1, d_2, \ldots, d_n)$ the degree sequence of G. Throughout this paper, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. A non-increasing sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called graphic if there exists a graph G having π as its degree sequence. We use C_π to denote the class of connected graphs with degree sequence π.

For a graph G, $A(G)$ is its adjacency matrix and $D(G)$ is the diagonal matrix of its degrees. The matrix $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix of G. The largest eigenvalue of $A(G)$ (resp., $Q(G)$) is called the spectral radius (resp., signless Laplacian spectral radius) of G and denoted by $\rho(G)$ (resp., $\mu(G)$). If G is connected, then $A(G)$ (resp., $Q(G)$) is irreducible and by the Perron–Frobenius theorem, $\rho(G)$ (resp., $\mu(G)$) has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho(G)$ (resp., $\mu(G)$). In this paper, we use $f = \big(f(v_1), f(v_2), \ldots, f(v_n)\big)^T$ to indicate the unique positive unit eigenvector corresponding to $\rho(G)$ (resp., $\mu(G)$), and call f the *Perron vector* of $A(G)$ (resp., $Q(G)$). Furthermore, if $\rho(G)$ (resp., $\mu(G)$) is greatest in C_π, then G is called an *extremal greatest graph* of C_π for $\rho(G)$ (resp., $\mu(G)$).

Suppose $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two non-increasing degree sequences. We say π is majorizated by π', denoted by $\pi \lhd \pi'$, if and only if $\pi \neq \pi'$, $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, \ldots, n-1$.

In 2008, Bıyıkoğlu and Leydold connected the majorization of degree sequences with ordering graphs by their spectral radius, and they obtained the majorization theorem of trees as follows.

Theorem 1.1 [1] Let π and π' be two different non-increasing degree sequences of trees with $\pi \lhd \pi'$. Suppose T and T' are the trees with the greatest spectral radius in C_π and $C_{\pi'}$, respectively. Then, $\rho(T) < \rho(T')$.

Almost at the same time, Zhang [15] proved the majorization theorem for the Laplacian spectral radius of trees. In the sequel, similar problems have been studied extensively. Liu et al. [9] and Zhang [16] proved the majorization theorems for the spectral radius and signless Laplacian spectral radius of unicyclic graphs, respectively. Jiang et al. [6] and Huang et al. [5] proved the majorization theorems for the spectral radius and signless Laplacian spectral radius of bicyclic graphs, respectively, and Jiang et al. [6] provided a counterexample to show that the majorization theorem cannot hold for tricyclic graphs. Liu and Liu et al. [7,9,12,13] proved the majorization theorems for the spectral radius and signless Laplacian spectral radius of c-cyclic graphs with additional restrictions, respectively. Recently, Liu et al. [10] proved the majorization theorems for the spectral radius and signless Laplacian spectral radius of pseudographs. For more results, one may refer to [8,11].

Let G_1 and G_2 be graphs with disjoint vertex sets, and $G_1 \vee G_2$ denote the join of G_1 and G_2. If G is connected, then $K_1 \vee G$ is called a single-cone graph. In particular, if G is a tree (unicyclic graph) of order $n-1$, then we call $K_1 \vee G$ a single-cone tree (unicyclic graph) of order n. For a non-increasing graphic sequence $\pi = (d_1, d_2, \ldots, d_n)$, let

$$J_\pi = \{G : G \text{ is a single-cone graph with degree sequence } \pi\}.$$

If $G \in J_\pi$ and $\rho(G) \geq \rho(G')$ (resp., $\mu(G) \geq \mu(G')$) for any other $G' \in J_\pi$, then we call G has the greatest spectral radius (resp., signless Laplacian spectral radius) in J_π.

In this paper, we give the majorization theorems for the spectral radius and signless Laplacian spectral radius of single-cone trees and single-cone unicyclic graphs, and the main results can be stated as follows:

Theorem 1.2 *Let π and π' be two different non-increasing degree sequences of single-cone trees with $\pi \lhd \pi'$. Suppose G and G' are the single-cone trees with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_π and $J_{\pi'}$, respectively. Then, $\rho(G) < \rho(G')$ (resp., $\mu(G) < \mu(G')$).*

Theorem 1.3 *Let π and π' be two different non-increasing degree sequences of single-cone unicyclic graphs with $\pi \lhd \pi'$. Suppose G and G' are the single-cone unicyclic graphs with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_π and $J_{\pi'}$, respectively. Then, $\rho(G) < \rho(G')$ (resp., $\mu(G) < \mu(G')$).*

The rest of the paper is organized as follows. In Sect. 2, we recall some basic notions and lemmas used further, and prove a new lemma. In Sect. 3, we give the proof of Theorem 1.2. In Sect. 4, we give the proof of Theorem 1.3.

2 Preliminaries

Given a unit n-vector $g = (g_1, g_2, \ldots, g_n)^T \in \mathbf{R}^n$, g can be considered as a function defined on $V(G)$, that is, each vertex v_i is mapped to $g_i = g(v_i)$. The Rayleigh quotients of the adjacency matrix $A(G)$ and signless Laplacian matrix $Q(G)$ are defined, respectively, as follows:

$$\mathcal{R}_{A(G)}(g) = \sum_{uv \in E} 2g(u)g(v) \quad \text{and} \quad \mathcal{R}_{Q(G)}(g) = \sum_{uv \in E} (g(u)+g(v))^2.$$

It follows from the Rayleigh–Ritz theorem that

Lemma 2.1 [3,4] Let S denote the set of unit vectors on V. Then,

$$\rho(G) = \max_{g \in S} \mathcal{R}_{A(G)}(g) = 2 \max_{g \in S} \sum_{uv \in E} g(u)g(v),$$

$$\mu(G) = \max_{g \in S} \mathcal{R}_{Q(G)}(g) = \max_{g \in S} \sum_{uv \in E} (g(u)+g(v))^2.$$

Moreover, if $\mathcal{R}_{A(G)}(g) = \rho(G)$ (resp., $\mathcal{R}_{Q(G)}(g) = \mu(G)$) for a positive vector $g \in S$, then g is an eigenvector corresponding to $\rho(G)$ (resp., $\mu(G)$).

Let $f = (f(v_1), f(v_2), \ldots, f(v_n))^T$ be the Perron vector of $A(G)$ (resp., $Q(G)$). Then, $\rho(G)f(v) = \sum_{uv\in E} f(u)$ (resp., $\mu(G)f(v) = d(v)f(v) + \sum_{uv\in E} f(u)$) for $v \in V(G)$. We will refer to such an equation as the eigenvalue equation of $\rho(G)$ (resp., $\mu(G)$). Let $G - u$ denote the graph that arises from G by deleting the vertex $u \in V(G)$ and all the edges incident with u, and $G - uv$ denote the graph that arises from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph that arises from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.

In order to complete the proof of the theorems, we also need the following definition and lemmas.

Lemma 2.2 [4,14] Let u, v be two vertices of the connected graph G. Suppose $v_1, v_2, \ldots, v_s \in N_G(v)\backslash N_G(u)$ $(1 \le s \le d_G(v))$, and f is the Perron vector of $A(G)$ (resp., $Q(G)$). Let $G^{'}$ be the graph obtained from G by deleting the edges vv_i and adding the edges uv_i $(1 \le i \le s)$. If $f(u) \ge f(v)$, then $\rho(G^{'}) > \rho(G)$ (resp., $\mu(G^{'}) > \mu(G)$).

Lemma 2.3 [1,15] Let G be a connected graph of order n such that $v_1v_3, v_2v_4 \in E(G)$, $v_1v_2, v_3v_4 \notin E(G)$. Let $G^{'} = G - v_1v_3 - v_2v_4 + v_1v_2 + v_3v_4$. Suppose f is the Perron vector of $A(G)$ (resp., $Q(G)$); if $f(v_1) \ge f(v_4)$ and $f(v_2) \ge f(v_3)$, then $\rho(G^{'}) \ge \rho(G)$ (resp., $\mu(G^{'}) \ge \mu(G)$), where the equalities hold if and only if $f(v_1) = f(v_4)$ and $f(v_2) = f(v_3)$.

Lemma 2.4 [8] Let G be a connected graph and f be the Perron vector of $A(G)$ (resp., $Q(G)$). Let G' be a connected graph obtained from G by deleting t (≥ 1) edges and adding another t new edges such that $G \ncong G'$. Suppose that there exists a vertex $v \in V(G)$ such that $N_G(v) \subset N_{G'}(v)$ or $N_{G'}(v) \subset N_G(v)$. If $\mathcal{R}_{A(G')}(f) \ge \mathcal{R}_{A(G)}(f)$ (resp., $\mathcal{R}_{Q(G')}(f) \ge \mathcal{R}_{Q(G)}(f)$), then $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$).

Lemma 2.5 [2,9] Let $\pi = (d_1, d_2, \ldots, d_n)$ be a sequence with $d_1 \ge d_2 \ge \cdots \ge d_n > 0$. Then, π is graphic if and only if

$$\sum_{i=1}^{n} d_i \text{ is even and } \sum_{i=1}^{k} d_i \le k(k-1) + \sum_{i=k+1}^{n} \min\{d_i, k\} \quad \text{for all} \quad k = 1, 2, \ldots, n-1.$$

Lemma 2.6 [12] Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d_1', d_2', \ldots, d_n')$ be two non-increasing degree sequences with $\pi \lhd \pi'$. Then, $d_n \ge d_n'$.

Lemma 2.7 [2,15] Let π and π' be two non-increasing graphic degree sequences. If $\pi \lhd \pi'$, then there exists a series non-increasing graphic degree sequences $\pi_1, \ldots, \pi_k$ such that $(\pi =)\ \pi_0 \lhd \pi_1 \lhd \cdots \lhd \pi_k \lhd \pi_{k+1} (= \pi')$, and π_i and π_{i+1} differ only at two positions, where the differences are 1 for $0 \le i \le k$.

Definition 2.8 [6,10] Let $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d_1', d_2', \ldots, d_n')$ be two different non-increasing degree sequences. We say π is star majorizated by π', denoted by $\pi \lhd^* \pi'$, if and only if $\pi \lhd \pi'$ and only two components of π and π' are different by 1, that is, $d_i = d_i'$ for $i \ne k, l$, $1 \le k < l \le n$ and $d_k' = d_k + 1$, $d_l' = d_l - 1$.

Lemma 2.9 *Suppose $\pi = (d_1, d_2, \ldots, d_n)$ is a non-increasing degree sequence. If G is* an extremal greatest single-cone graph *for $\rho(G)$ (resp., $\mu(G)$) in J_π with Perron vector f, then there exists an ordering of the vertices of G such that $d(v_i) = d_i$ for $1 \le i \le n$ and $f(v_1) \ge f(v_2) \ge \cdots \ge f(v_n)$.*

Proof Since G is a single-cone graph, there exists a vertex v_1 such that $d_G(v_1) = n-1$ and $G - v_1$ is a connected graph. Create an ordering of the vertices of G beginning with v_1 and appending other vertices after it. We use the notation $v_i \prec v_j$ to indicate that the vertex v_i precedes the vertex v_j in the ordering of vertices. Clearly, $v_1 \prec v_i$ for $i = 2, 3, \ldots, n$. The order of other vertices is defined as follows: if $d_G(v_i) > d_G(v_j)$, or $d_G(v_i) = d_G(v_j)$ and $f(v_i) \ge f(v_j)$, then $v_i \prec v_j$. It is easy to see that this ordering satisfies $d_G(v_1) \ge d_G(v_2) \ge \cdots \ge d_G(v_n)$. We will prove that $f(v_1) \ge f(v_2) \ge \cdots \ge f(v_n)$.

Firstly, we claim that $f(v_1) \ge f(v_i)$ for $2 \le i \le n$. Otherwise, we suppose that there exists some vertex v_i such that $f(v_1) < f(v_i)$. If $d_G(v_i) = n-1$, then $N_G(v_1)\backslash\{v_i\} = N_G(v_i)\backslash\{v_1\}$. By the eigenvalue equation of $\rho(G)$ (resp., $\mu(G)$), we have $f(v_1) = f(v_i)$, contradicting $f(v_1) < f(v_i)$. If $d_G(v_i) < n-1$, then $N_G(v_1)\backslash(N_G(v_i) \cup \{v_i\}) \ne \varnothing$. Let

$$G' = G - \sum_{u \in N_G(v_1)\backslash(N_G(v_i)\cup\{v_i\})} v_1 u + \sum_{u \in N_G(v_1)\backslash(N_G(v_i)\cup\{v_i\})} v_i u.$$

Then, $d_{G'}(v_i) = d_G(v_1)$, $d_{G'}(v_1) = d_G(v_i)$ and $d_{G'}(v) = d_G(v)$ for $v \in V(G)\backslash\{v_1, v_i\}$. Noting that $G - v_1$ is a connected graph and the neighbors of v_i in $G - v_1$ are adjacent to v_1 in $G' - v_i$, we have $G' - v_i$ which is a connected graph. This implies that $G' \in J_\pi$. By Lemma 2.2, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$), a contradiction because G is an extremal greatest single-cone graph for $\rho(G)$ (resp., $\mu(G)$) in J_π. Therefore, $f(v_1) \ge f(v_i)$ for $2 \le i \le n$.

Secondly, we show that $v_i \prec v_j$ implies $f(v_i) \ge f(v_j)$ for all $v_i, v_j \in V(G)\backslash\{v_1\}$. Otherwise, we suppose that there exist two vertices such that $v_i \prec v_j$ but $f(v_j) > f(v_i)$. Then, $d(v_i) \ge d(v_j)$. Noting that $v_i, v_j \in V(G)\backslash\{v_1\}$, there exists a shortest path P_{ij} from v_i to v_j in $G - v_1$. If $d_G(v_i) > d_G(v_j)$, let $k = d_G(v_i) - d_G(v_j)$, $v_l \in V(P_{ij})$ and $v_l v_i \in E(G)$. Then, there exist k vertices $u_1, \ldots, u_k \in N_G(v_i)\backslash(N_G(v_j) \cup \{v_l\})$. Let

$$G' = G - \sum_{s=1}^{k} v_i u_s + \sum_{s=1}^{k} v_j u_s.$$

Then, $G' \in J_\pi$. By Lemma 2.2, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$), a contradiction because G is an extremal greatest single-cone graph for $\rho(G)$ (resp., $\mu(G)$) in J_π. If $d_G(v_i) = d_G(v_j)$, noting that $v_i \prec v_j$, we have $f(v_i) \ge f(v_j)$, contradicting $f(v_j) > f(v_i)$.

Combining the above arguments, we have $f(v_1) \ge f(v_2) \ge \cdots \ge f(v_n)$. □

3 The proof of Theorem 1.2

The proof of Theorem 1.2 Since $\pi \lhd \pi'$, it follows from Lemma 2.7 and Definition 2.8 that there exists a series non-increasing graphic degree sequences $\pi_1, \ldots, \pi_k$ such that $(\pi =)\ \pi_0 \lhd^* \pi_1 \lhd^* \cdots \lhd^* \pi_k \lhd^* \pi_{k+1} (= \pi')$. Let $\pi_i = (d_1^{(i)}, d_2^{(i)}, \ldots, d_n^{(i)})$ for $0 \le i \le k$. Clearly, $d_1 = d_1^{(1)} = \cdots = d_1^{(k)} = d_1' = n-1$. By Lemma 2.6, we have $d_n \ge d_n^{(1)} \ge \cdots \ge d_n^{(k)} \ge d_n'$. Noting that π and π' are two different non-increasing degree sequences of single-cone trees, we have $d_n = d_n' = 2$. This implies that $d_n = d_n^{(1)} = \cdots = d_n^{(k)} = d_n' = 2$.

Since $\pi \lhd^* \pi_1$, without loss of generality, we suppose that $d_k + 1 = d_k^{(1)}$, $d_l - 1 = d_l^{(1)}$, $d_j = d_j^{(1)}$ for $j \notin \{k, l\}$, and $1 < k < l < n$. Let f be the Perron vector of $A(G)$ (resp., $Q(G)$). Then, Lemma 2.9 implies that there exists an ordering of the vertices of G such that $d(v_i) = d_i$ for $1 \le i \le n$ and $f(v_1) \ge f(v_2) \ge \cdots \ge f(v_n)$. Particularly, $f(v_k) \ge f(v_l)$.

Assume that $G - v_1$ is a tree and P_{kl} is a shortest path from v_k to v_l in $G - v_1$. Noting that $d_l = d_l^{(1)} + 1 > 2$, there must exist some $w \in N_{G-v_1}(v_l) \backslash N_{G-v_1}(v_k)$ such that $w \notin V(P_{kl})$. Let $G_1 = G - v_l w + v_k w$. Then, $G_1 - v_1$ is a tree, $d_{G_1}(v_k) = d_G(v_k) + 1$, $d_{G_1}(v_l) = d_G(v_l) - 1$, and $d_{G_1}(v) = d_G(v)$ for $v \in V(G) \backslash \{v_k, v_l\}$. This implies that G_1 is a single-cone tree and $G_1 \in J_{\pi_1}$. Noting that $f(v_k) \ge f(v_l)$, by Lemma 2.2, we have $\rho(G) < \rho(G_1)$ (resp., $\mu(G) < \mu(G_1)$). Let G_1^* be the single-cone tree with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_{π_1}. Then, $\rho(G) < \rho(G_1) \le \rho(G_1^*)$ (resp., $\mu(G) < \mu(G_1) \le \mu(G_1^*)$).

By a similar reasoning as the above, we can obtain that π_i is a non-increasing degree sequence of a single-cone tree for each $2 \le i \le k$. Let G_i^* be a single-cone tree with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_{π_i}. Then, we have $\rho(G) < \rho(G_1^*) < \cdots < \rho(G_k^*) < \rho(G')$ (resp., $\mu(G) < \mu(G_1^*) < \cdots < \mu(G_k^*) < \mu(G')$). □

4 The proof of Theorem 1.3

Lemma 4.1 *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a non-increasing degree sequence of a single-cone unicyclic graph, and G be an extremal greatest single-cone unicyclic graph for $\rho(G)$ (resp., $\mu(G)$) in J_π. Suppose $\pi' = (d_1', d_2', \ldots, d_n')$ ($d_n' \ge 2$) is a non-increasing graphic degree sequence such that $\pi \lhd^* \pi'$. Then, there exists a single-cone unicyclic graph $G' \in J_{\pi'}$ such that $\rho(G) < \rho(G')$ (resp., $\mu(G) < \mu(G')$).*

Proof Since $\pi \lhd^* \pi'$, without loss of generality, we suppose that $d_k + 1 = d_k'$, $d_l - 1 = d_l'$, and $d_i = d_i'$ for $i \ne k, l$. Since π is a non-increasing degree sequence of a single-cone unicyclic graph, then $d_1 = d_1' = n-1$, $d_i \ge 2$ for $1 \le i \le n$, and $1 < k < l \le n$. Assume that $G - v_1$ is a unicyclic graph. Let P_{kl} be a shortest path from v_k to v_l in $G - v_1$, $u \in N_{G-v_1}(v_l) \cap V(P_{kl})$ and f be the Perron vector of $A(G)$ (resp., $Q(G)$). By Lemma 2.9, there exists an ordering of the vertices of G such that $d(v_i) = d_i$ for $1 \le i \le n$ and $f(v_1) \ge f(v_2) \ge \cdots \ge f(v_n)$. Particularly, $f(v_k) \ge f(v_l)$.

Case 1 $N_{G-v_1}(v_l)\backslash(N_{G-v_1}(v_k)\cup\{u\}) \neq \emptyset$. Assume $w \in N_{G-v_1}(v_l)\backslash(N_{G-v_1}(v_k) \cup \{u\})$. Let $G' = G - v_l w + v_k w$. Then, $G' - v_1$ is a unicyclic graph, $d_{G'}(v_k) = d_G(v_k) + 1$, $d_{G'}(v_l) = d_G(v_l) - 1$, and $d_{G'}(v) = d_G(v)$ for $v \in V(G)\backslash\{v_k, v_l\}$. This implies that G' is a single-cone unicyclic graph and $G' \in J_{\pi'}$. Noting that $f(v_k) \geq f(v_l)$, by Lemma 2.2, we have $\rho(G) < \rho(G')$ (resp., $\mu(G) < \mu(G')$).

Case 2 $N_{G-v_1}(v_l)\backslash(N_{G-v_1}(v_k) \cup \{u\}) = \emptyset$. Noting that G is a single-cone unicyclic graph, we have $d_l \leq 3$, and so $d'_l \leq 2$. Since $d'_l \geq d'_n \geq 2$, it follows that $d'_l = 2$, $d_l = 3$, $d_i = d'_i = 2$ for $l + 1 \leq i \leq n$. Let $w \in N_{G-v_1}(v_l)\backslash\{u\}$. Then, $w \in N_{G-v_1}(v_k)$. This implies that $|V(P_{kl})| \leq 3$.

Subcase 2.1 $|V(P_{kl})| = 2$. In this case, $C_3 = v_k w v_l v_k$ is the unique cycle of $G - v_1$. We claim that $l \geq 5$. Otherwise, we suppose $l \leq 4$. Noting that π' is a non-increasing degree sequence and $d'_l = 2$, we have $d'_i = 2$ for $4 \leq i \leq n$. By $\pi \lhd \pi'$, we have $\sum_{i=1}^{n} d'_i = \sum_{i=1}^{n} d_i = 2(2n - 2)$. It follows that

$$\sum_{i=1}^{3} d'_i = \sum_{i=1}^{n} d'_i - \sum_{i=4}^{n} d'_i = 2n + 2 > 2n = 3(3-1) + \sum_{i=4}^{n} \min\{d'_i, 3\},$$

a contradiction to Lemma 2.5. Therefore, $l \geq 5$. This implies that there must exist vertices a, b such that $a \notin \{v_1, v_k, v_l, w\}$, $d_G(a) \geq 3$, $d_G(b) = 2$, and $ab \in E(G)$.

If $av_k \notin E(G)$, noting that $d_G(v_l) = 3$ and $d_G(b) = 2$, we have $f(v_l) \geq f(b)$, $av_l \notin E(G)$, and $bv_k \notin E(G)$. We claim that $f(v_k) \geq f(a)$. Otherwise, we suppose $f(a) > f(v_k)$. Let $G^* = G - ab - v_l v_k + av_l + bv_k$. By Lemma 2.3, we have $\rho(G) < \rho(G^*)$ (resp., $\mu(G) < \mu(G^*)$). It is easy to see that $G^* \in J_\pi$, which is a contradiction because G has the greatest spectral radius (resp., signless Laplacian spectral radius) in J_π. Therefore, $f(v_k) \geq f(a)$. Noting that $d_i = d'_i = 2$ for $l + 1 \leq i \leq n$, we have $a \prec v_l$. It follows that $f(a) \geq f(v_l)$. Let $G' = G - v_k v_l - ab + v_k a + v_k b$. Then, $d_{G'}(v_k) = d_G(v_k) + 1$, $d_{G'}(v_l) = d_G(v_l) - 1$, and $d_{G'}(v) = d_G(v)$ for $v \in V(G)\backslash\{v_k, v_l\}$. It is not difficult to see that $G' - v_1$ is a unicyclic graph, $G' \in J_{\pi'}$,

$$\begin{aligned}\mathcal{R}_{A(G')}(f) - \mathcal{R}_{A(G)}(f) &= 2\sum_{xy\in E(G')} f(x)f(y) - 2\sum_{xy\in E(G)} f(x)f(y)\\ &= 2f(v_k)f(a) + 2f(v_k)f(b) - 2f(a)f(b) - 2f(v_k)f(v_l)\\ &= 2f(v_k)(f(a) - f(v_l)) + 2f(b)(f(v_k) - f(a)) \geq 0,\end{aligned}$$

and

$$\begin{aligned}\mathcal{R}_{Q(G')}(f) - \mathcal{R}_{Q(G)}(f) &= \sum_{xy\in E(G')} (f(x) + f(y))^2 - \sum_{xy\in E(G)} (f(x) + f(y))^2\\ &= f^2(v_k) - f^2(v_l) + 2f(v_k)(f(a) - f(v_l))\\ &\quad +2f(b)(f(v_k) - f(a)) \geq 0.\end{aligned}$$

By Lemma 2.1, we have $\rho(G') \geq \mathcal{R}_{A(G')}(f) \geq \mathcal{R}_{A(G)}(f) = \rho(G)$ (resp., $\mu(G') \geq \mathcal{R}_{Q(G')}(f) \geq \mathcal{R}_{Q(G)}(f) = \mu(G)$). Noting that $N_{G'}(v_l) \subset N_G(v_l)$, by Lemma 2.4, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$).

If $av_k \in E(G)$, we can show $f(v_k) \geq f(a)$ similarly. Let $G' = G - wv_l - ab + wa + v_kb$. Then, $d_{G'}(v_k) = d_G(v_k) + 1$, $d_{G'}(v_l) = d_G(v_l) - 1$, and $d_{G'}(v) = d_G(v)$ for $v \in V(G)\backslash\{v_k, v_l\}$. It is not difficult to see that $G' - v_1$ is a unicyclic graph, $G' \in J_{\pi'}$,

$$\begin{aligned}\mathcal{R}_{A(G')}(f) - \mathcal{R}_{A(G)}(f) &= 2\sum_{xy\in E(G')} f(x)f(y) - 2\sum_{xy\in E(G)} f(x)f(y)\\ &= 2f(w)f(a) + 2f(v_k)f(b) - 2f(a)f(b) - 2f(w)f(v_l)\\ &= 2f(w)(f(a) - f(v_l)) + 2f(b)(f(v_k) - f(a)) \geq 0,\end{aligned}$$

and

$$\begin{aligned}\mathcal{R}_{Q(G')}(f) - \mathcal{R}_{Q(G)}(f) &= \sum_{xy\in E(G')} (f(x)+f(y))^2 - \sum_{xy\in E(G)} (f(x)+f(y))^2\\ &= f^2(v_k) - f^2(v_l) + 2f(w)(f(a) - f(v_l))\\ &\quad + 2f(b)(f(v_k) - f(a)) \geq 0.\end{aligned}$$

By Lemma 2.1, we have $\rho(G') \geq \mathcal{R}_{A(G')}(f) \geq \mathcal{R}_{A(G)}(f) = \rho(G)$ (resp., $\mu(G') \geq \mathcal{R}_{Q(G')}(f) \geq \mathcal{R}_{Q(G)}(f) = \mu(G)$). Noting that $N_{G'}(v_l) \subset N_G(v_l)$, by Lemma 2.4, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$).

Subcase 2.2 $|V(P_{kl})| = 3$. In this case, $P_{kl} = v_kuv_l$ and $C_4 = v_kwv_luv_k$ is the unique cycle of $G - v_1$. This implies that $d_G(v_k) \geq 3$, $d_G(w) \geq 3$, $d_G(u) \geq 3$. By $d_i = d_i' = 2$ for $l+1 \leq i \leq n$, we have $w \prec v_l$ and $u \prec v_l$. It follows that $f(w) \geq f(v_l)$ and $f(u) \geq f(v_l)$.

If $f(v_k) \geq f(w)$, let $G' = G - wv_l - uv_l + v_kv_l + wu$. Then, $d_{G'}(v_k) = d_G(v_k)+1$, $d_{G'}(v_l) = d_G(v_l) - 1$, $d_{G'}(v) = d_G(v)$ for $v \in V(G)\backslash\{v_k, v_l\}$. This implies that $G' - v_1$ is a unicyclic graph, $G' \in J_{\pi'}$,

$$\begin{aligned}\mathcal{R}_{A(G')}(f) - \mathcal{R}_{A(G)}(f) &= 2\sum_{xy\in E(G')} f(x)f(y) - 2\sum_{xy\in E(G)} f(x)f(y)\\ &= 2f(v_k)f(v_l) + 2f(w)f(u) - 2f(w)f(v_l) - 2f(u)f(v_l)\\ &= 2f(v_l)(f(v_k) - f(w)) + 2f(u)(f(w) - f(v_l)) \geq 0,\end{aligned}$$

and

$$\begin{aligned}\mathcal{R}_{Q(G')}(f) - \mathcal{R}_{Q(G)}(f) &= \sum_{xy\in E(G')} (f(x)+f(y))^2 - \sum_{xy\in E(G)} (f(x)+f(y))^2\\ &= f^2(v_k) - f^2(v_l) + 2f(v_l)(f(v_k) - f(w))\\ &\quad + 2f(u)(f(w) - f(v_l)) \geq 0.\end{aligned}$$

By Lemma 2.1, we have $\rho(G') \geq \mathcal{R}_{A(G')}(f) \geq \mathcal{R}_{A(G)}(f) = \rho(G)$ (resp., $\mu(G') \geq \mathcal{R}_{Q(G')}(f) \geq \mathcal{R}_{Q(G)}(f) = \mu(G)$. Noting that $N_G(v_k) \subset N_{G'}(v_k)$, by Lemma 2.4, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$).

If $f(w) > f(v_k)$, let $G' = G - wv_l - uv_k + wu + v_k v_l$. It is easy to see that $G' - v_1$ is a unicyclic graph and $d_{G'}(v) = d_G(v)$ for $v \in V(G)$. This implies that $G' \in J_\pi$. By Lemma 2.3, we have $\rho(G') > \rho(G)$ (resp., $\mu(G') > \mu(G)$), a contradiction because G has the greatest spectral radius (resp., signless Laplacian spectral radius) in J_π. □

The proof of Theorem 1.3 Since $\pi \lhd \pi'$, it follows from Lemma 2.7 and Definition 2.8 that there exists a series non-increasing graphic degree sequences $\pi_1, \ldots, \pi_k$ such that $(\pi =)\ \pi_0 \lhd^* \pi_1 \lhd^* \cdots \lhd^* \pi_k \lhd^* \pi_{k+1} (= \pi')$. Let $\pi_i = (d_1^{(i)}, d_2^{(i)}, \ldots, d_n^{(i)})$ for $0 \leq i \leq k$. By Lemma 2.6, we have $d_n \geq d_n^{(1)} \geq \cdots \geq d_n^{(k)} \geq d'_n \geq 2$.

For π and π_1, Lemma 4.1 implies that there exists a single-cone unicyclic graph $G_1 \in J_{\pi_1}$ such that $\rho(G) < \rho(G_1)$ (resp., $\mu(G) < \mu(G_1)$). It follows that π_1 is a non-increasing degree sequence of a single-cone unicyclic graph. Let G_1^* be a single-cone unicyclic graph with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_{π_1}. Then, $\rho(G) < \rho(G_1) \leq \rho(G_1^*)$ (resp., $\mu(G) < \mu(G_1) \leq \mu(G_1^*)$).

By a similar reasoning as the above, we can obtain that π_j is a non-increasing degree sequence of a single-cone unicyclic graph for each $2 \leq j \leq k$. Let G_j^* be a single-cone unicyclic graph with the greatest spectral radius (resp., signless Laplacian spectral radius) in J_{π_j} for $2 \leq j \leq k$. By Lemma 4.1, we have $\rho(G) < \rho(G_1^*) < \cdots < \rho(G_k^*) < \rho(G')$ (resp., $\mu(G) < \mu(G_1^*) < \cdots < \mu(G_k^*) < \mu(G')$). □

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