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More on Laplacian Estrada indices of trees

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Dedicated to the Memory of Professor Sen-Yen Shaw

Abstract

The Laplacian Estrada index of a graph G is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$, where $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of G. We determine the unique tree with maximum Laplacian Estrada index among the set of trees with given bipartition. We also determine the unique trees with the third, the fourth, the fifth and the sixth maximum Laplacian Estrada indices.

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $\mathbf{A}(G)$ be the adjacency matrix of G. Let $n = |V(G)|$. The eigenvalues of G, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the eigenvalues of $\mathbf{A}(G)$ [3]. The Estrada index of a graph G is defined as [7]

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

It found various applications in a large variety of problems. It was proved that Estrada index is especially useful to characterize the folding degree of a protein chain, account for the contribution of amino acids to folding [7, 8, 9]. Later, Estrada index was extended to measure the centrality of complex networks [10, 11], extended atomic branching [12], and the carbon-atom skeleton [16]. More mathematical properties of the Estrada index can be found in [1, 6, 13, 14, 15, 17, 20, 21].

Let $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ be the Laplacian matrix of G, where $\mathbf{D}$(G) is the diagonal matrix of vertex degrees of the graph G. Denote by $\mu_1, \mu_2, \ldots, \mu_n$ the Laplacian eigenvalues of G [19]. In full analogy with the expression of Estrada index, the Laplacian Estrada index of a graph G is defined as [14]

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

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Ilić and Zhou [18] proved that the path and the star are respectively the unique trees with minimum and maximum Laplacian Estrada indices, which showed that the use of Laplacian Estrada index as a measure of branching in alkanes. In [18], the tree with the second maximum Laplacian Estrada index was also determined. More mathematical properties of the Laplacian Estrada index can be found in [1, 5, 14, 22, 23].

A bipartite graph G is a graph whose vertices can be partition into two disjoint sets $V_1(G)$ and $V_2(G)$ such that every edge connects a vertex in $V_1(G)$ to one in $V_2(G)$. If $|V_1(G)| = p$ and $|V_2(G)| = q$ with $p \geq q \geq 1$, then we say G has a (p, q)-bipartition. It is well-known that every tree is a bipartite graph.

In this paper, we determine the unique tree with maximum Laplacian Estrada index among the set of trees with given bipartition. We also determine the unique trees with the third, the fourth, the fifth and the sixth maximum Laplacian Estrada indices.

2 Preliminaries

Denote by $M_k(G)$ the k-th spectral moment of the graph G, i.e., $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$. It is well-known that $M_k(G)$ is equal to the number of closed walks of length k in G [3]. Then

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \tag{1}$$

Let G_1 and G_2 be two graphs. If $M_k(G_1) \leq M_k(G_2)$ for all positive integers k, then we write $G_1 \preceq G_2$. If $G_1 \preceq G_2$ and there is at least one positive integer k_0 such that $M_{k_0}(G_1) < M_{k_0}(G_2)$, then we write $G_1 \prec G_2$. By expression (1) for Estrada index, $G_1 \preceq G_2$ implies that $EE(G_1) \leq EE(G_2)$, and $G_1 \prec G_2$ implies that $EE(G_1) < EE(G_2)$.

Let $M_k(G; u)$ be the number of closed walks of length k in G starting at u.

Let $u \in V(G_1)$ and $v \in V(G_2)$. If $M_k(G_1; u) \leq M_k(G_2; v)$ for all positive integers k, then we write $(G_1; u) \preceq (G_2; v)$. If $(G_1; u) \preceq (G_2; v)$ and there is at least one positive integer k_0 such that $M_{k_0}(G_1; u) < M_{k_0}(G_2; v)$, then we write $(G_1; u) \prec (G_2; v)$.

First we give some lemmas will be used in our proof.

Lemma 1. ([6]) *Let H_1, H_2 be two non-trivial connected graphs with $u, v \in V(H_1)$, $w \in V(H_2)$. Let G_u be the graph obtained from H_1 and H_2 by identifying u with w, and G_v be the graph obtained from H_1 and H_2 by identifying v with w. If $(H_1; u) \prec (H_1; v)$, then $G_u \prec G_v$.*

Let $\mathcal{L}(G)$ be the line graph of a graph G. Zhou and Gutman [22] gave the following relationship between the Laplacian Estrada index of a bipartite graph and the Estrada index of its line graph.

Lemma 2. ([22]) *Let G be a bipartite graph with n vertices and m edges. Then*

$$LEE(G) = n - m + e^2 \cdot EE(\mathcal{L}(G)).$$

Let $d_G(v)$ be the degree of v in G. Let $d_G(u, v)$ be the distance from u to v in G.

For $v \in V(G)$, $G - v$ denotes the graph obtained from G by deleting the vertex v.

For two distinct vertices u, v of a graph G, let $A_k(G; u, [v])$ be the set of (u, u)-walks of length k containing v in G, let $M_k(G; u, [v]) = |A_k(G; u, [v])|$, let $r_k(G; u, v)$ be the number of walks of length $k \geq 1$ from u to v in G, and $r_0(G; u, v) = 1$.

3 The maximum Laplacian Estrada index of trees with given bipartition

Let G_1 and G_2 be two connected bipartite graphs shown in Fig. 1, where P, M, Q are connected subgraphs of G_1, and $d_{G_1}(u), d_{G_1}(v), d_{G_1}(w) \geq 2$. In G_2, all the neighbors of v in Q of G_1 are switched to be the neighbors of u in G_2.

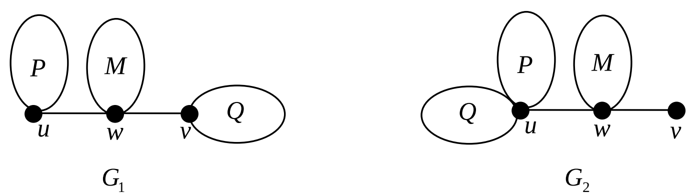

Figure 1: The graphs G_1 and G_2 in Lemma 3.

Let G be a graph with $y_1y_2 \in E(G)$. Denote by $x_{y_1y_2}(G)$ the vertex in $\mathcal{L}(G)$ corresponding to $y_1y_2 \in E(G)$.

Lemma 3. *Let G_1 and G_2 be two connected bipartite graphs shown in Fig.* 1*. If $d_{G_1}(u), d_{G_1}(v) \geq 2$, then $LEE(G_1) < LEE(G_2)$.*

Proof. By Lemma 2, we need only to show that $EE(\mathcal{L}(G_1)) < EE(\mathcal{L}(G_2))$.

Let H be the graph obtained from G_1 by deleting the vertices in Q different from v. Let P^* be the graph obtained from G_1 by deleting the vertices in M and Q different from w, and M^* be the graph obtained from G_1 by deleting the vertices in P and Q different from u, v. Then $\mathcal{L}(H)$ can be obtained from $\mathcal{L}(P^*)$ and $\mathcal{L}(M^*)$ by identifying $x_{uw}(P^*) \in V(\mathcal{L}(P^*))$ with $x_{uw}(M^*) \in V(\mathcal{L}(M^*))$. Let k be any positive integer.

First we will show that $(\mathcal{L}(H) - x_{uw}(H); x_{wv}(H)) \prec (\mathcal{L}(H) - x_{wv}(H); x_{uw}(H))$. Clearly,

$$M_k(\mathcal{L}(H) - x_{uw}(H); x_{wv}(H)) = M_k(\mathcal{L}(M^*) - x_{uw}(M^*); x_{wv}(M^*)).$$

Note that $\mathcal{L}(M^*) - x_{uw}(M^*) \cong \mathcal{L}(M^*) - x_{wv}(M^*)$, and thus

$$M_k(\mathcal{L}(M^*) - x_{uw}(M^*); x_{wv}(M^*)) = M_k(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*)).$$

It follows that

$$M_k(\mathcal{L}(H) - x_{uw}(H); x_{wv}(H)) = M_k(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*)).$$

This implies that we need only to show that

$$(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*)) \prec (\mathcal{L}(H) - x_{wv}(H); x_{uw}(H)),$$

which follows by noting that $d_G(u) \geq 2$ (i.e., $\mathcal{L}(P^*)$ is not trivial).

Now we will show that

$$M_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)]) \leq M_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)]).$$

We construct a mapping f from $A_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)])$ to $A_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)])$. For $W \in A_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)])$, we may decompose W into $W = W_1W_2$, where W_1 is the shortest $(x_{wv}(H), x_{uw}(H))$-section of W, and W_2 is the remaining $(x_{uw}(H), x_{wv}(H))$-section of W. It is easily seen that the neighbors of $x_{wv}(H)$ in $\mathcal{L}(H)$ different from $x_{uw}(H)$ are also the neighbors of $x_{uw}(H)$ in $\mathcal{L}(H)$. Denote by $w_1, w_2, \ldots, w_t$ the common neighbors of $x_{wv}(H)$ and $x_{uw}(H)$ in $\mathcal{L}(H)$, where $d_{\mathcal{L}(H)}(x_{wv}(H)) = t+1$. By the choice of W_1, we know that W_1 consists of an $(x_{wv}(M^*), x_{wv}(M^*))$-walk in $\mathcal{L}(M^*) - x_{uw}(M^*)$ whose length may be zero and a single edge $x_{wv}(M^*)x_{uw}(M^*)$, or an $(x_{wv}(M^*), w_i)$-walk in $\mathcal{L}(M^*) - x_{uw}(M^*)$ and a single edge $w_i x_{uw}(M^*)$ for $1 \leq i \leq t$. Then

$$\begin{aligned} & M_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)]) = |A_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)])| \\ = & \sum_{\substack{z \in \{x_{wv}(M^*), w_1, w_2 \ldots, w_t\} \\ k_1+k_2=k, k_1, k_2 \geq 1}} r_{k_1-1}(\mathcal{L}(M^*) - x_{uw}(M^*); x_{wv}(M^*), z) \\ & \cdot r_{k_2}(\mathcal{L}(H); x_{uw}(H), x_{wv}(H)). \end{aligned}$$

Similarly,

$$\begin{aligned} & M_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)]) = |A_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)])| \\ = & \sum_{\substack{z \in \{x_{uw}(H), w_1, w_2 \ldots, w_t\} \\ k_1+k_2=k, k_1, k_2 \geq 1}} r_{k_1-1}(\mathcal{L}(H) - x_{wv}(H); x_{uw}(H), z) \\ & \cdot r_{k_2}(\mathcal{L}(H); x_{wv}(H), x_{uw}(H)) \\ \geq & \sum_{\substack{z \in \{x_{uw}(M^*), w_1, w_2 \ldots, w_t\} \\ k_1+k_2=k, k_1, k_2 \geq 1}} r_{k_1-1}(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*), z) \\ & \cdot r_{k_2}(\mathcal{L}(H); x_{wv}(H), x_{uw}(H)). \end{aligned}$$

For any positive integer s and $z \in \{w_1, w_2 \ldots, w_t\}$,

$$r_s(\mathcal{L}(M^*) - x_{uw}(M^*); x_{wv}(M^*), z) = r_s(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*), z)$$

and

$$r_s(\mathcal{L}(M^*) - x_{uw}(M^*); x_{wv}(M^*), x_{wv}(M^*)) = r_s(\mathcal{L}(M^*) - x_{wv}(M^*); x_{uw}(M^*), x_{uw}(M^*))$$

since $\mathcal{L}(M^*) - x_{uw}(M^*) \cong \mathcal{L}(M^*) - x_{wv}(M^*)$, and it is well-known that [3]

$$r_s(\mathcal{L}(H); x_{uw}(H), x_{wv}(H)) = r_s(\mathcal{L}(H); x_{wv}(H), x_{uw}(H)).$$

It follows that $M_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)]) \leq M_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)])$.

Note that

$$M_k(\mathcal{L}(H); x_{wv}(H)) = M_k(\mathcal{L}(H) - x_{uw}(H); x_{wv}(H)) + M_k(\mathcal{L}(H); x_{wv}(H), [x_{uw}(H)]),$$

$$M_k(\mathcal{L}(H); x_{uw}(H)) = M_k(\mathcal{L}(H) - x_{wv}(H); x_{uw}(H)) + M_k(\mathcal{L}(H); x_{uw}(H), [x_{wv}(H)]).$$

Then we have $(\mathcal{L}(H); x_{wv}(H)) \prec (\mathcal{L}(H); x_{uw}(H))$.

Let H_1 be the graph obtained from G_1 by deleting the vertices in P and M different from w. It is easily seen that $\mathcal{L}(G_1)$ can be obtained from $\mathcal{L}(H)$ and $\mathcal{L}(H_1)$ by identifying $x_{wv}(H) \in V(\mathcal{L}(H))$ with $x_{wv}(H_1) \in V(\mathcal{L}(H_1))$. Let G^* be the graph obtained from $\mathcal{L}(H)$ and $\mathcal{L}(H_1)$ by identifying $x_{uw}(H) \in V(\mathcal{L}(H))$ with $x_{wv}(H_1) \in V(\mathcal{L}(H_1))$. It follows from Lemma 1 that $\mathcal{L}(G_1) \prec G^*$.

Note that G^* is a proper subgraph of $\mathcal{L}(G_2)$ since $d_{G_1}(u), d_{G_1}(v) \geq 2$ (i.e., P, Q are not trivial), and thus $G^* \prec \mathcal{L}(G_2)$, implying that $\mathcal{L}(G_1) \prec \mathcal{L}(G_2)$. □

Let $S_n(a, b)$ be the n-vertex tree obtained by adding one edge between the two centers of two stars S_a and S_b, where $a \geq b \geq 1$, $a + b = n$.

Theorem 1. *Let G be an n-vertex tree with a (p, q)-bipartition, where $p + q = n$, $p \geq q \geq 1$. Then $LEE(G) \leq LEE(S_n(p, q))$ with equality if and only if $G \cong S_n(p, q)$.*

Proof. Let G be a tree with maximum Laplacian Estrada index with a (p, q)-bipartition. Let $P = v_1 v_2 \ldots v_t$ be a diametrical path of G.

Suppose that the diameter of G is at least four. Then applying Lemma 3 to $G_1 = G$ by setting $u = v_2$ and $v = v_4$, we may get a tree G' such that $LEE(G) < LEE(G')$. Clearly, we may partition the vertices of G and G' in the same way, i.e., G' has also a (p, q)-bipartition, which is a contradiction to the choice of G. Then the diameter of G is at most three, i.e., $G \cong S_n(p, q)$. □

4 The first six maximum Laplacian Estrada indices of trees

Lemma 4. ([18]) *Let u be a vertex of a tree Q with at least two vertices. For integer $a \geq 1$, let G_1 be the tree obtained by attaching a star S_{a+1} at its center v to u of Q, and G_2 be the tree obtained by attaching $a + 1$ pendent vertices to u of Q, see Fig. 2. Then $LEE(G_1) < LEE(G_2)$.*

Lemma 5. ([18]) *If $G \cong S_n(a, b)$ with $a + b = n$, $a \geq b \geq 5$, then*

$$LEE(G) < LEE(S_n(n-4, 4)) < LEE(S_n(n-3, 3)) < LEE(S_n(n-2, 2)).$$

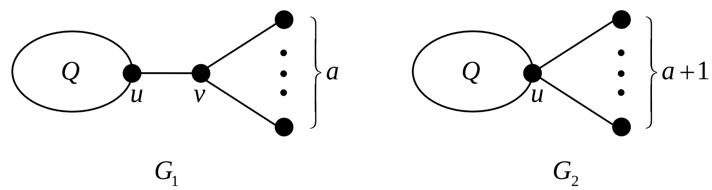

Figure 2: The trees G_1 and G_2 in Lemma 4.

Recall that a caterpillar is a tree in which removal of all pendent vertices gives a path.

Let $P_n(n_1, n_2, n_3)$ be the n-vertex caterpillar obtained from the path on five vertices, say $v_0v_1v_2v_3v_4$, by attaching n_i pendent vertices to v_i for $i = 1, 2, 3$, where $n_1 + n_2 + n_3 = n - 5$, $n_1 \geq n_3$, $n_1, n_2, n_3 \geq 0$.

Applying Lemmas 4 and 5, Ilić and Zhou [18] showed that $S_n(n-1, 1)$ and $S_n(n-2, 2)$ are respectively the unique trees with maximum and the second maximum Laplacian Estrada indices, and the third maximum Laplacian Estrada index for trees on $n \geq 6$ vertices is uniquely achieved by $S_n(n-3, 3)$ or a caterpillar of diameter four. Ilić and Zhou [18] also used computer to test the trees on $n \leq 22$ vertices, and found that $S_n(n-3, 3)$ and $P_n(0, n-5, 0)$ are respectively the unique trees with the third and the fourth maximum Laplacian Estrada indices.

Deng and Zhang [5] showed that $LEE(S_n(n-3, 3)) > LEE(P_n(0, n-5, 0))$ for $n \geq 6$. Now we give another proof for this inequality. Applying Lemma 3 to $G_1 = P_n(0, n-5, 0)$ by setting w to be the vertex with degree $n-3$ in $P_n(0, n-5, 0)$, we have $LEE(S_n(n-3, 3)) > LEE(P_n(0, n-5, 0))$.

In the following, we determine the unique trees with the third, the fourth, the fifth and the sixth maximum Laplacian Estrada indices.

Lemma 6. ([2]) *Let G be a graph on n vertices and vertex degrees $d_1 \geq d_2 \geq \cdots \geq d_n$. Suppose that $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the Laplacian eigenvalues of G. If G is not the vertex-disjoint union of the complete graph on s vertices and $n-s$ isolated vertices, then $\mu_s \geq d_s - s + 2$ for $1 \leq s \leq n$.*

Lemma 7. *For $n \geq 8$, $LEE(S_n(n-4, 4)) < LEE(P_n(n-5, 0, 0))$.*

Proof. The case for $n = 8$ can be checked by direct calculation. Suppose in the following that $n \geq 9$.

Let $\phi(G, x)$ be the characteristic polynomial of $\mathbf{L}(G)$. By direct calculation, $\phi(S_n(n-4, 4), x) = x(x-1)^{n-4} f(x)$, where $f(x) = x^3 - (n+2)x^2 + (5n-14)x - n$.

Let $x_1 \geq x_2 \geq x_3$ be the roots of $f(x) = 0$. It is easily checked that $f(1) = 3(n-5) > 0$, $f(5) = -n + 5 < 0$, $f(n - \frac{5}{2}) = \frac{1}{2}n^2 - 5n + \frac{55}{8} > 0$, implying that $x_1 < n - \frac{5}{2}$, $x_2 < 5$, $x_3 < 1$. Then $LEE(S_n(n-4, 4)) < e^{n-\frac{5}{2}} + e^5 + e^1 + e^0 + (n-4)e^1$.

Let $\mu_1 \geq \mu_2$ be the first two largest Laplacian eigenvalues of $P_n(n-5, 0, 0)$. By Lemma 6, $\mu_1 \geq n-2$, $\mu_2 \geq 2$. Then $LEE(P_n(n-5, 0, 0)) > e^{n-2} + e^2 + e^0 + (n-5)e^1$.

Note that

$$\begin{aligned} & (e^{n-2}+e^{2}+e^{0}+(n-5)e^{1})-(e^{n-\frac{5}{2}}+e^{5}+e^{1}+e^{0}+(n-4)e^{1}) \\ = \; & e^{n-2}-e^{n-\frac{5}{2}}+e^{2}-e^{5}-2e^{1} \\ > \; & e^{8-2}-e^{8-\frac{5}{2}}+e^{2}-e^{5}-2e^{1}>0, \end{aligned}$$

and thus $LEE(S_n(n-4,4)) < LEE(P_n(n-5,0,0))$. □

Lemma 8. *For $n \geq 6$, $LEE(P_n(n-5,0,0)) < LEE(P_n(0,n-5,0))$.*

Proof. By Lemma 2, we need only to show that

$$EE(\mathcal{L}(P_n(n-5,0,0))) < EE(\mathcal{L}(P_n(0,n-5,0))).$$

Let H be the graph obtained by attaching a pendent vertex to a vertex of the complete graph K_{n-3}. Denote by u the unique pendent vertex in H, v the unique neighbor of u, and w a neighbor of v different from u in H. Let k be any positive integer.

We will show that $(H;u) \prec (H;w)$. We construct a mapping f from $A_k(H;u)$ to $A_k(H;w)$. For $W \in A_k(H;u)$, let $f(W)$ be the walk obtained from W by replacing its first and last vertex u by w. Obviously, $f(W) \in A_k(H;w)$ and f is an injection. Since $n \geq 6$, we have $M_2(H;w) = d_H(w) = n-4 > M_2(H;u) = d_H(u) = 1$. It follows that f is an injection but not a surjection for $k=2$, implying that $(H;u) \prec (H;w)$.

It is easily seen that $\mathcal{L}(P_n(n-5,0,0))$ ($\mathcal{L}(P_n(0,n-5,0))$, respectively) can be obtained by identifying $u \in V(H)$ ($w \in V(H)$, respectively) with an end vertex of a single edge. Then the result follows from Lemma 1. □

Lemma 9. *For $n = n_1+n_2+n_3 \geq 8$, $LEE(P_n(n_1,n_2,n_3)) < LEE(S_n(n-4,4))$ if $(n_1,n_2,n_3) \neq (n-5,0,0),(0,n-5,0)$.*

Proof. By Lemma 4,

$$\begin{aligned} & LEE(P_n(n_1,n_2,n_3)) \\ < \; & \min\{LEE(S_n(n_1+n_2+3,n_3+2)), LEE(S_n(n_1+2,n_2+n_3+3))\} \end{aligned}$$

if $n_1+2 \geq n_2+n_3+3$, and

$$\begin{aligned} & LEE(P_n(n_1,n_2,n_3)) \\ < \; & \min\{LEE(S_n(n_1+n_2+3,n_3+2)), LEE(S_n(n_2+n_3+3,n_1+2))\} \end{aligned}$$

if $n_1+2 < n_2+n_3+3$.

Clearly, $n_1+n_2+3 > n_3+2$ as $n_1 \geq n_3$. If $n_3+2 \geq 4$, i.e., $n_3 \geq 2$, then by Lemma 5, $LEE(S_n(n_1+n_2+3,n_3+2)) \leq LEE(S_n(n-4,4))$, implying that $LEE(P_n(n_1,n_2,n_3)) < LEE(S_n(n-4,4))$.

If $n_1+2 \geq 4$ and $n_2+n_3+3 \geq 4$, i.e., $n_1 \geq 2$ and $n_2+n_3 \geq 1$, then by Lemma 5, $LEE(S_n(n_1+2, n_2+n_3+3)) \leq LEE(S_n(n-4,4))$ if $n_1+2 \geq n_2+n_3+3$, and $LEE(S_n(n_2+n_3+3, n_1+2)) \leq LEE(S_n(n-4,4))$ if $n_1+2 < n_2+n_3+3$, implying that $LEE(P_n(n_1,n_2,n_3)) < LEE(S_n(n-4,4))$.

We are left to consider the cases $n_3 \leq 1$, and $n_1 \leq 1$ or $n_2+n_3 \leq 0$. Obviously, the case $n_2+n_3 \leq 0$ does not hold since $(n_1,n_2,n_3) \neq (n-5,0,0)$. We need only to consider the cases $n_3 \leq 1$ and $n_1 \leq 1$.

It is easily seen that $P_n(n_1,n_2,n_3)$ has an (n_1+n_3+3, n_2+2)-bipartition if $n_1+n_3+3 \geq n_2+2$, and an (n_2+2, n_1+n_3+3)-bipartition if $n_1+n_3+3 < n_2+2$. Note that the case $n_1, n_3 = 0$ does not hold as $(n_1,n_2,n_3) \neq (0, n-5, 0)$, and thus $n_1+n_3+3 \geq 4$. If $n_2+2 \geq 4$, i.e., $n_2 \geq 2$, then by Theorem 1 and Lemma 5, $LEE(P_n(n_1,n_2,n_3)) < LEE(S_n(n-4,4))$.

Thus the remaining cases are $n_1,n_2,n_3 \leq 1$, recall that $n \geq 8$, implying that it only can be $n_1 = n_2 = n_3 = 1$. By direct calculation, $LEE(P_8(1,1,1)) < LEE(S_8(4,4))$. Then the result follows. □

Theorem 2. *The Laplacian Estrada indices of n-vertex trees with $n \geq 8$ may be ordered by the following inequalities, where G is an n-vertex tree different from any other tree in the inequalities:*

$$\begin{aligned} LEE(G) &< LEE(S_n(n-4,4)) < LEE(P_n(n-5,0,0)) \\ &< LEE(P_n(0,n-5,0)) < LEE(S_n(n-3,3)) \\ &< LEE(S_n(n-2,2)) < LEE(S_n(n-1,1)). \end{aligned}$$

Proof. Recall that $S_n(n-1,1)$ and $S_n(n-2,2)$ are respectively the unique trees with maximum and the second maximum Laplacian Estrada indices [18]. Let G be an n-vertex tree different from $S_n(n-1,1)$ and $S_n(n-2,2)$. Obviously, the diameter of G is at least three.

Suppose that the diameter of G is three. Then $G \cong S_n(a,b)$ for some integers a,b with $a+b=n$, $a \geq b \geq 3$. If $b \geq 5$, then by Lemma 5, $LEE(G) < LEE(S_n(n-4,4)) < LEE(S_n(n-3,3))$.

If G is a caterpillar of diameter four (i.e., $G \cong P_n(n_1,n_2,n_3)$) different from $P_n(n-5,0,0), P_n(0,n-5,0)$, then by Lemma 9, $LEE(G) < LEE(S_n(n-4,4))$.

Suppose that G is a non-caterpillar of diameter four. Suppose that G has a (p,q)-bipartition, where $p \geq q \geq 3$. If $q \geq 4$, then by Theorem 1 and Lemma 5, $LEE(G) < LEE(S_n(n-4,4))$. Suppose that $q = 3$. Let $P = u_0u_1u_2u_3u_4$ be a diametrical path of G. Then G is a tree obtained by attaching x_1 pendent vertices to u_1, a star $S_{x_2}(x_2-1,1)$ at its center to u_2, and x_3 pendent vertices to u_3, where $x_1 \geq x_3 \geq 0$, $x_2 \geq 2$. If $x_1 \geq 1$, then by Lemmas 4 and 9, $LEE(G) < LEE(P_n(x_1,x_2,x_3)) < LEE(S_n(n-4,4))$. Suppose that $x_1 = 0$. Then $x_3 = 0$. If $n = 8$, then by Lemmas 3 and 9, $LEE(G) < LEE(P_8(1,1,1)) < LEE(S_8(4,4))$. If $n \geq 9$, then by Lemmas 4 and 5, $LEE(G) < LEE(S_n(n-4,4))$.

If the diameter of G is at least five, then by Lemma 4

$$LEE(G) < LEE(P_n(n_1,n_2,n_3))$$

for some non-negative integers n_1, n_2, n_3 with $(n_1, n_2, n_3) \neq (n-5, 0, 0)$, $(0, n-5, 0)$, and thus by Lemma 9, $LEE(G) < LEE(S_n(n-4, 4))$.

We have shown that $LEE(G) < LEE(S_n(n-4, 4))$ if $G \ncong S_n(n-3, 3)$, $S_n(n-4, 4)$, $P_n(n-5, 0, 0)$, $P_n(0, n-5, 0)$. By Lemmas 7, 8 and 3,

$$\begin{aligned} & LEE(S_n(n-4,4)) < LEE(P_n(n-5,0,0)) \\ < \quad & LEE(P_n(0,n-5,0)) < LEE(S_n(n-3,3)). \end{aligned}$$

Then the result follows. □

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