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Unicyclic Graph with Maximal Estrada Indices

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Abstract

Let $\mathcal{U}_n^+$ be the set of bipartite unicyclic graphs with n vertices. In $\mathcal{U}_n^+$, ordering the unicyclic graphs in terms of their maximal Estrada indices was considered. We deduce the first four and three unicyclic graphs in $\mathcal{U}_n^+$ for $n \geq 23$ and $22 \geq n \geq 8$, respectively. For two bipartite graphs, we construct a relation between the Estrada index and the largest eigenvalue.

1 Introduction

Let $G = (V(G), E(G))$ be a simple, connected graph with n vertices, where $V(G)$ and $E(G)$ are the set of vertices and edges of G, respectively. The Estrada index (EI), put forward by Estrada [12, 14], is defined as

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

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of G, namely the n roots of $\phi(G, \lambda) = 0$. Here

$$\phi(G, \lambda) = \det[\lambda I - A(G)] \tag{2}$$

is the characteristic polynomial of G [6], where I is the unit matrix of order n and $A(G)$ the adjacency matrix of G. It is obvious that each λ_i $(1 \leq i \leq n)$ is real since

$A(G)$ is real and symmetric. Without loss of generality, we assume $\lambda_1 \geq \cdots \geq \lambda_n$. Next we also write $\lambda_i = \lambda_i(G)$ for $1 \leq i \leq n$.

The largest eigenvalue $\lambda_1(G)$ is called the spectral radius of G. If G is connected, then $A(G)$ is irreducible. According to the Perron–Frobenius theory of non-negative matrices, $\lambda_1(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\lambda_1(G)$. Such an eigenvector is referred to as the Perron vector of G [17].

The EI has already found numerous applications in the last decade, for example, measuring the degree of protein folding [12] and the centrality of complex networks (such as neural, social, metabolic, protein–protein interaction networks, and the World Wide Web) [13]. Some mathematical properties of the EI, including lower and upper bounds may be found in Refs. [1, 3, 5, 8, 15, 16]. The Laplacian– and signless Laplacian–spectral variants of the Estrada index were also studied [2, 25, 31]. For the characterization of graphs with the extremal EI, one can refer to Refs. [7, 9, 10, 20, 23, 24, 30]. More details on the theory of EI and an exhaustive bibliography can be found in the recent survey [19].

For $k \geq 0$, we denote $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ and refer to $M_k(G)$ as the k-th spectral moment of G. It is well-known that $M_k(G)$ is equal to the number of closed walks of length k in G [6]. From the Taylor expansion of e^{λ_i}, $EE(G)$ in (1) can be rewritten as

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!} \ . \tag{3}$$

In particular, if G is a bipartite graph, then $M_{2k+1}(G) = 0$ for $k \geq 0$. Hence, we have

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_{2k}(G)}{(2k)!} \ . \tag{4}$$

Let G_1 and G_2 be two bipartite graphs. If $M_{2k}(G_1) \geq M_{2k}(G_2)$ holds for any positive integer k, then $EE(G_1) \geq EE(G_2)$. Moreover, if the strict inequality $M_{2k}(G_1) > M_{2k}(G_2)$ holds for at least one integer k, then $EE(G_1) > EE(G_2)$. By constructing a mapping and using this relation, the characterization of trees with the extremal Estrada indices (EIs) has successfully been obtained. For the trees on n vertices, some results were recently reported [9,10,24,30]. Deng [9] obtained the trees with the minimal and the maximal EIs. Among the trees with exactly two vertices having the maximum degree, Li et al. [24] deduced the tree with the minimal EI. Among the trees with a given matching number and among the trees with a fixed diameter, Zhang et al. [30] determined the trees with the maximum EIs. Among the trees with a given number of pendent vertices, Du and Zhou [10] determined the tree with the maximum EI.

The set of unicyclic graphs on n vertices is denoted by $\mathcal{U}_n$, in which each graph has only one cycle C_l of length l with $3 \leq l \leq n$. The set of bipartite unicyclic graphs on n vertices is denoted by $\mathcal{U}_n^+$. For the graphs in $\mathcal{U}_n$, by constructing a mapping, Du and Zhou [11] determined the graph with the maximum EI and showed two candidates with the minimum EI. For the graphs in $\mathcal{U}_n^+$, Du and Zhou [11] found the graph with the maximum EI and the graph of a given bipartition with the maximum EI. In this paper, we will study the connected bipartite unicyclic graphs. We construct a relation between the EI and the largest eigenvalue of the graph. Thus, by this relation, the results of Du and Zhou [11] will be extended. We deduce the first four and three unicyclic graphs in $\mathcal{U}_n^+$ for $n \geq 23$ and $22 \geq n \geq 8$, respectively.

2 Preliminaries

To deduce the main results of the present paper, some definitions and necessary lemmas are simply quoted here.

Let $G - v$ and $G - uv$ be the graphs obtained from G by deleting the vertex $v \in V(G)$ and the edge $uv \in E(G)$, respectively. Similarly, $G + uv$ is a graph obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$.

Lemma 1. [6] *Let v be a vertex of degree 1 in G and u be the vertex adjacent to v. Then*

$$\phi(G, \lambda) = \lambda\, \phi(G - v, \lambda) - \phi(G - u - v, \lambda)\ .$$

Lemma 2. [22] *Let G_1 and G_2 be two graphs. If $\phi(G_2, \lambda) > \phi(G_1, \lambda)$ for $\lambda \geq \lambda_1(G_2)$, then $\lambda_1(G_1) > \lambda_1(G_2)$.*

Let C_l be a cycle with l vertices, and the vertices of C_l are labelled consecutively by $u_1, u_2, \ldots, u_l$, where $l \geq 3$. Let $G_n^{l;1}$ be the graph obtained from C_l by attaching

$n-l$ pendent edges to u_1 of C_l. Let $G_n^{l,2}$ be the graph obtained from C_l by attaching $n-l-1$ pendent edges and one pendent edge to u_1 and u_2 of C_l, respectively.

Lemma 3. [4, 21] *If the length of circle contained in G is l with $l \geq 3$ and $n \geq l$, then we have*

(i) for any $G \in \mathcal{U}_n - \{G_n^{l,1}\}$, $\lambda_1(G_n^{l,1}) > \lambda_1(G)$;

(ii) for any $G \in \mathcal{U}_n - \{G_n^{l,1}, G_n^{l,2}\}$, $\lambda_1(G_n^{l,2}) > \lambda_1(G)$;

(iii) $\lambda_1(G_n^{l,1}) > \lambda_1(G_n^{l+1,1})$.

Lemma 4. [26] *Let G be a connected graph, and let G' be a proper spanning subgraph of G. Then $\lambda_1(G) > \lambda_1(G')$.*

For $v \in V(G)$, let $d(v)$ and $N(v)$ denote the degree of v and the set of all eighbors of v, respectively.

Lemma 5. [27,29] *Let G be a connected graph and u, v be two vertices of G. Suppose that $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u)$ $(1 \leq s \leq d(v))$ and $x = (x_1, x_2, \ldots, x_n)$ is the Perron vector of $A(G)$, where x_i corresponds to the vertex v_i $(1 \leq i \leq n)$. Let G^* be the graph obtained from G by deleting the edges vv_i and adding the edges uv_i $(1 \leq i \leq s)$. If $x_u \geq x_v$, then $\lambda_1(G^*) > \lambda_1(G)$.*

Lemma 6. [18] *Let G be a connected graph and $e = uv$ be a non-pendent edge of G with $N(u) \cap N(v) = \emptyset$. Let G^* be the graph obtained from G by deleting the edge uv, identifying u with v, and adding a pendent edge to u $(= v)$. Then $\lambda_1(G^*) > \lambda_1(G)$.*

The transformation from G to G^* in Lemma 6 is hereinafter called the *edge–growing transformation* (EGT) of G on the edge e.

3 Main results

For simplicity, we refer to the connected graphs having n vertices and m edges as the (n, m)-graphs, where $n \geq 3$. For two bipartite (n, m)-graphs, from Lemma 7, we have Lemma 8, which shows a relationship between the EI and the largest eigenvalue. Lemma 8 will play a key role in the paper.

Lemma 7. *Let x, y, a and b be real numbers and k an integer not less than 2.*

(i) If $a > x > y \geq \frac{a}{2} > 0$, then $x^k + (a-x)^k > y^k + (a-y)^k$;

(ii) If $x > b > 0$, then $x^k > (x-b)^k + b^k$.

Proof. As $a > x > y \geq a/2 > 0$, obviously, it holds that

$$x^k - y^k = (x-y)(x^{k-1} + x^{k-2}y + \cdots + y^{k-1}) \tag{5}$$

$$\begin{aligned}(a-y)^k - (a-x)^k &= (x-y)\left[(a-y)^{k-1} + (a-y)^{k-2}(a-x) + \cdots \right.\\ &+ \left.(a-x)^{k-1}\right] .\end{aligned} \tag{6}$$

Since $x > y \geq a/2$, we have $x - y > 0$, $x > a - x$, and $y \geq a - y$. Thus, by (5) and (6), we get $x^k - y^k > (a-y)^k - (a-x)^k$. Hence, we have Lemma 7(i).

By methods similar to that for Lemma 7(i), we can get Lemma 7(ii). □

Lemma 8. *Let G_1 and G_2 be two connected bipartite (n,m)-graphs. If G_1 has exactly two positive eigenvalues and G_2 has at least two positive eigenvalues with $\lambda_1(G_1) > \lambda_1(G_2)$, then $EE(G_1) > EE(G_2)$.*

Proof. For an (n,m)-graph G, we have $\sum_{i=1}^n \lambda_i^2 = 2m$ [6]. Furthermore, if G is a connected bipartite (n,m)-graph, then it is well known that the eigenvalues of G are symmetric with respect to the origin [6]. Thus G has $t = [n - \eta(G)]/2$ positive eigenvalues and $\sum_{i=1}^t \lambda_i^2 = m$, where $\eta(G)$ is the multiplicity of zero eigenvalue of G. By (1) and the Taylor expansion of e^{λ_i}, we have

$$EE(G) = n + m + 2\sum_{k=2}^{\infty}\left(\frac{1}{(2k)!}\sum_{i=1}^{t}\lambda_i^{2k}\right) . \tag{7}$$

Let G_1 and G_2 be two connected bipartite (n,m)-graphs, where G_1 has exactly two positive eigenvalues, G_2 has at least two positive eigenvalues, and $\lambda_1(G_1) > \lambda_1(G_2)$. Let $\lambda_i^2(G_1) = x_i$ with $i = 1, 2$ and $\lambda_i^2(G_2) = y_i$ with $1 \leq i \leq t$ and $2 \leq t \leq \frac{n}{2}$. Obviously, $x_1 > y_1$, $x_1 > x_2 > 0$, $y_1 > y_2 \geq \cdots \geq y_t > 0$, and $\sum_{i=1}^2 x_i = \sum_{i=1}^t y_i = m$. The expressions for $EE(G_1)$ and $EE(G_2)$ can be obtained by replacing λ_i^2 in (7) with x_i and y_i, respectively.

Let $k \geq 2$. Next, we prove $x_1^k + x_2^k > y_1^k + \cdots + y_t^k$. Two cases are considered as follows.

Case (i) $t = 2$.

Since $y_1 > y_2$ and $\sum_{i=1}^{2} x_i = \sum_{i=1}^{2} y_i = m$, we get $m > x_1 > y_1 > m/2$. By Lemma 7(i), we have $x_1^k + x_2^k > y_1^k + y_2^k$. Thus, by (7), we have $EE(G_1) > EE(G_2)$.

Case (ii) $3 \le t \le n/2$.

Two subcases are considered as follows.

Subcase (ii.i) $y_1 \ge m/2$.

Obviously, $m > x_1 > y_1 \ge \frac{m}{2}$. By Lemma 7(i), we get $x_1^k + x_2^k = x_1^k + (m - x_1)^k > y_1^k + (m - y_1)^k$. Since $m - y_1 = y_2 + \cdots + y_t$, using Lemma 7(ii) repeatedly, we obtain $(m - y_1)^k > y_2^k + \cdots + y_t^k$. Thus, we get $x_1^k + x_2^k > y_1^k + y_2^k + \cdots + y_t^k$. Hence, by (7), we get $EE(G_1) > EE(G_2)$.

Subcase (ii.ii) $y_1 < m/2$.

For $y_1 < m/2$ and a fixed k, we prove $x_1^k + x_2^k > y_1^k + \cdots + y_t^k$ by induction on t.

As $t = 3$, we have

$$x_1^k + x_2^k > \left(\frac{m}{2}\right)^k + \left(\frac{m}{2}\right)^k > \left(\frac{m}{2}\right)^k + y_1^k + \left(\frac{m}{2} - y_1\right)^k > y_1^k + y_2^k + y_3^k \ . \qquad (8)$$

The first inequality in (8) follows from Lemma 7(i) since $\sum_{i=1}^{2} x_i = m$ and $x_1 > m/2$, the second one in (8) from Lemma 7(ii) since $m/2 > y_1 > 0$, and the third one in (8) from Lemma 7(i) since

$$\frac{m}{2} > y_1 > y_2 \ge \frac{y_2 + y_3}{2} \qquad \text{and} \qquad \frac{m}{2} + \left(\frac{m}{2} - y_1\right) = y_2 + y_3 \ .$$

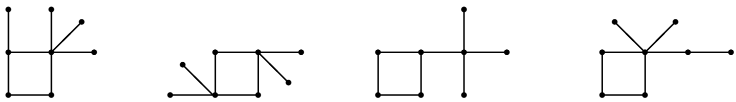
As $t = p$ and $p \ge 4$, we suppose $x_1^k + x_2^k > y_1^k + \cdots + y_p^k$, where $\sum_{i=1}^{2} x_i = \sum_{i=1}^{p} y_i = m$.

As $t = p + 1$, we have $\sum_{i=1}^{p+1} y_i = m$. Since $y_1 > y_2 \ge \cdots \ge y_{p+1} > 0$ and $p \ge 4$, we have $m/2 > y_p + y_{p+1}$. By the induction and Lemma 7(ii), we get

In conclusion, we obtain $x_1^k + x_2^k > y_1^k + \cdots + y_t^k$ for $y_1 < m/2$ and $3 \le t \le n/2$. Thus, by (7), we obtain $EE(G_1) > EE(G_2)$.

Lemma 8 is thus proved. $\square$

Remark: For those (n, m)-graphs which are not bipartite, Eq. (1) can not be changed into (7) and Lemma 8 is not applicable to obtain the graph with the maximum EI.



(a) C_8^4 (b) L_8^2 (c) $K_8^4(1,3)$ (d) I_8^4

Fig. 1: C_8^4, L_8^2, $K_8^4(1,3)$, and I_8^4.

Let $C_n^4(n_1, n_2, n_3, n_4)$ be the unicyclic graph obtained from C_4 by attaching n_i pendent edges to every u_i of C_4, where $0 \le n_i \le n-4$, $\sum_{i=1}^4 n_i = n-4$ and $1 \le i \le 4$.

Specially, we denote $C_n^4(n-5,0,0,1)$ by C_n^4 with $n \ge 6$ and $C_n^4(n_1, 0, n_3, 0)$ by $L_n^{n_3}$ with $n_1 = n-4-n_3$.

For example, L_{b+4}^0 is the graph obtained from C_4 by attaching b pendent edges to u_1 of C_4. In L_{b+4}^0, we denote by $\{z_1, z_2, \ldots, z_b\}$ the set of the b pendent vertices.

Let $K_n^4(b,c)$ be the unicyclic graph obtained by attaching c pendent edges to z_1 of L_{b+4}^0, where $c = n-4-b$ and $1 \le b \le n-5$. In $K_n^4(b,c)$, we denote by $\{w_1, w_2, \ldots, w_c\}$ the set of the c pendent vertices adjacent to z_1 .

Specially, we denote $K_n^4(n-5,1)$ by I_n^4 with $n \ge 6$.

For example, C_8^4, L_8^2, $K_8^4(1,3)$ and I_8^4 are shown in Fig. 1.

In this paper, for the ordering of the graphs in $\mathcal{U}_n^+$ in terms of their maximal EIs, we will show that L_n^0, C_n^4, I_n^4, and L_n^1 are the first four graphs for $n \ge 23$ while L_n^0, C_n^4, and L_n^1 are the first three ones for $22 \ge n \ge 8$.

We introduce Lemmas 9–17 from which the main results of this paper follows.

Lemma 9. *$EE(L_n^0) > EE(C_n^4) > EE(I_n^4)$ for $n \ge 6$.*

Proof. Straightforward derivation by Lemma 1 yields

$$\phi(L_n^0, \lambda) = \lambda^{n-4}\left[(2n-8) - n\lambda^2 + \lambda^4\right] \tag{9}$$

$$\phi(C_n^4, \lambda) = \lambda^{n-6}\left[-(n-5) + (3n-13)\lambda^2 - n\lambda^4 + \lambda^6\right] \triangleq \lambda^{n-6} g_1(\lambda) \tag{10}$$

$$\phi(I_n^4, \lambda) = \lambda^{n-6}\left[-(2n-12) + (3n-12)\lambda^2 - n\lambda^4 + \lambda^6\right] \triangleq \lambda^{n-6} g_2(\lambda) \; . \tag{11}$$

From (9) and (10), we can see that L_n^0 and C_n^4 have two and three positive eigenvalues, respectively. Since $L_n^0 = G_n^{4,1}$, by Lemma 3(i), we have $\lambda_1(L_n^0) > \lambda_1(C_n^4)$ for $n \ge 6$. Since $L_n^0, C_n^4 \in \mathcal{U}_n^+$, by Lemma 8, we get $EE(L_n^0) > EE(C_n^4)$ for $n \ge 6$.

We can check that

$$g_1\left(\sqrt{0.38}\right) = 0.114872 - 0.0044n < 0 \qquad (n \geq 27)$$

$$g_1\left(\sqrt{0.382}\right) = 0.089743 + 0.000076n > 0 \qquad (n \geq 6)$$

$$g_1\left(\sqrt{2.6}\right) = -11.224 + 0.04n > 0 \qquad (n \geq 281)$$

$$g_1\left(\sqrt{2.62}\right) = -11.0753 - 0.0044n < 0 \qquad (n \geq 7)$$

$$g_1\left(\sqrt{n-3+5/n}\right) = \frac{125 - 225n + 120n^2 - 28n^3}{n^3} < 0 \qquad (n \geq 7)$$

$$g_1\left(\sqrt{n-3+8/n}\right) = -55 + \frac{512}{n^3} - \frac{576}{n^2} + \frac{240}{n} + 3n > 0 \qquad (n \geq 14)\,.$$

According to the theorem of zero points, we have, for $n \geq 281$,

$$n - 3 + \frac{5}{n} < \lambda_1^2(C_n^4) < n - 3 + \frac{8}{n},\ 2.6 < \lambda_2^2(C_n^4) < 2.62,\ 0.38 < \lambda_3^2(C_n^4) < 0.382\,. \qquad (12)$$

The explicit expressions for $g_j(\cdot)$ with $j \geq 2$ can be obtained by a straightforward calculation and will be omitted hereinafter for the sake of conciseness. One can readily obtain the following expressions: $g_2\left(\sqrt{0.976}\right) < 0$ for $n \geq 50$, $g_2\left(\sqrt{1}\right) > 0$ for $n \geq 6$, $g_2\left(\sqrt{1.91}\right) > 0$ for $n \geq 49$, $g_2\left(\sqrt{2}\right) < 0$ for $n \geq 6$, $g_2\left(\sqrt{n-3+5/n}\right) < 0$ for $n \geq 6$, and $g_2\left(\sqrt{n-3+6/n}\right) > 0$ for $n \geq 28$. According to the theorem of zero points, we have, for $n \geq 50$,

$$n - 3 + \frac{5}{n} < \lambda_1^2(I_n^4) < n - 3 + \frac{6}{n},\quad 1.91 < \lambda_2^2(I_n^4) < 2,\quad 0.976 < \lambda_3^2(I_n^4) < 1. \qquad (13)$$

As $n \geq 281$, let $\lambda_i^2(C_n^4) = x_i$ and $\lambda_i^2(I_n^4) = y_i$, where $i = 1, 2, 3$. Since $C_n^4 = G_n^{4,2}$, by Lemma 3(ii), we have $x_1 > y_1$. By (12) and (13), we get $y_1 \geq \frac{x_1+x_2}{2}$. Hence, by Lemma 7(i), we have, for $k \geq 2$,

$$x_1^k + x_2^k > y_1^k + (x_2 + x_1 - y_1)^k\,. \qquad (14)$$

Since $x_1 > y_1$ and $x_2 > y_2$, we have $x_2 + x_1 - y_1 > y_2$. Since $x_2 + x_1 - y_1 + x_3 = y_2 + y_3$ and $y_2 > \frac{y_2+y_3}{2}$, by Lemma 7(i), we get, for $k \geq 2$,

$$(x_2 + x_1 - y_1)^k + x_3^k > y_2^k + y_3^k\,. \qquad (15)$$

It follows from (14) and (15) that $\sum_{i=1}^{3} x_i^k > \sum_{i=1}^{3} y_i^k$ for $n \geq 281$. By (7), we have $EE(C_n^4) > EE(I_n^4)$ for $n \geq 281$. Calculation yields $EE(C_n^4) > EE(I_n^4)$ for $280 \geq n \geq 6$. Therefore, $EE(C_n^4) > EE(I_n^4)$ for $n \geq 6$. $\square$

Lemma 10. *$EE(I_n^4) > EE(L_n^1)$ for $n \geq 23$ and $EE(L_n^1) > EE(I_n^4)$ for $22 \geq n \geq 6$.*

Proof. By (1), (11) and (13), we have, for $n \geq 50$,

$$EE(I_n^4) > n - 6 + \mathrm{e}^{\sqrt{n-3+5/n}} + \mathrm{e}^{\sqrt{1.91}} + \mathrm{e}^{\sqrt{0.976}} + \mathrm{e}^{-\sqrt{1}} + \mathrm{e}^{-\sqrt{2}} + \mathrm{e}^{-\sqrt{n-3+6/n}}. \quad (16)$$

Straightforward derivation by Lemma 1 yields

$$\phi(L_n^1, \lambda) = \lambda^{n-4}[(3n-13) - n\lambda^2 + \lambda^4] \,. \quad (17)$$

It follows from (17) that L_n^1 has two positive eigenvalues and

$$\lambda_1(L_n^1) = \sqrt{\frac{1}{2}(n + \sqrt{52 - 12n + n^2})} \,. \quad (18)$$

From (1) and (17), we obtain

$$EE(L_n^1) = n - 4 + \mathrm{e}^{\sqrt{1/2(n+\sqrt{52-12n+n^2})}} + \mathrm{e}^{\sqrt{1/2(n-\sqrt{52-12n+n^2})}}$$

$$+ \mathrm{e}^{-\sqrt{1/2(n-\sqrt{52-12n+n^2})}} + \mathrm{e}^{-\sqrt{1/2(n+\sqrt{52-12n+n^2})}}. \quad (19)$$

We can check that the right-hand side of (16) is greater than that of (19) as $n \geq 50$. Therefore, $EE(I_n^4) > EE(L_n^1)$ for $n \geq 50$. Calculation yields $EE(I_n^4) > EE(L_n^1)$ for $49 \geq n \geq 23$ while $EE(L_n^1) > EE(I_n^4)$ for $22 \geq n \geq 6$. $\square$

We introduce Lemmas 11–15 from which Lemma 16 follows.

Lemma 11. *As $n \geq 8$, $\lambda_1(L_n^1) > \lambda_1(C_n^4(n-6,0,0,2))$.*

Proof. Straightforward derivation by Lemma 1 yields

$$\phi(C_n^4(n-6,0,0,2), \lambda) = \lambda^{n-6}[-(2n-12) + (4n-20)\lambda^2 - n\lambda^4 + \lambda^6] \,. \quad (20)$$

For $n \geq 8$, the union of the star $K_{1,n-4}$ and three isolated vertices is a proper spanning subgraph of $C_n^4(n-6,0,0,2)$. Hence, by Lemma 4, we have $\lambda_1(C_n^4(n-6,0,0,2)) > \lambda_1(K_{1,n-4}) = \sqrt{n-4}$. As $n \geq 8$ and $\lambda \geq \lambda_1(C_n^4(n-6,0,0,2)$, by (17), we have

$$\phi(C_n^4(n-6,0,0,2), \lambda) - \phi(L_n^1, \lambda) = \lambda^{n-6}[-(2n-12) + (n-7)\lambda^2] > 0. \quad (21)$$

Thus, by Lemma 2, we have Lemma 11. $\square$

Lemma 12. *Let* $G \in \{C_n^4(n_1, n_2, n_3, n_4)\} \backslash \{L_n^0, C_n^4, L_n^1\}$ *and* $n \geq 8$. *We have* $\lambda_1(L_n^1) > \lambda_1(G)$.

Proof. Let $G \in \{C_n^4(n_1, n_2, n_3, n_4)\} \setminus \{L_n^0, C_n^4, L_n^1\}$ and $n \geq 8$. In G, we denote by $\{r_1, \dots, r_{n_1}\}$, $\{s_1, \dots, s_{n_2}\}$, $\{t_1, \dots, t_{n_3}\}$, and $\{v_1, \dots, v_{n_4}\}$ the sets of pendent vertices adjacent to u_1 , u_2, u_3, and u_4, respectively. Since $G \neq L_n^0$, at most two of n_1, n_2, n_3, n_4 are zero. Without loss of generality, we suppose $n_1 \neq 0$. We consider three cases as follows.

Case (i) Two of n_2, n_3, n_4 are zero.

Two subcases are considered.

Subcase (i.i) $n_2 = n_4 = 0$, $n_3 \neq 0$.

In this subcase, $G \cong C_n^4(n_1, 0, n_3, 0)$. Since $G \neq L_n^1$, $2 \leq n_1, n_3 \leq n-6$. We suppose $x_{u_1} \geq x_{u_3}$. Let $G^* = G - \{u_3t_2, \dots, u_3t_{n_3}\} + \{u_1t_2, \dots, u_1t_{n_3}\}$. Obviously, $G^* \cong L_n^1$. By Lemma 5, we have $\lambda_1(L_n^1) = \lambda_1(G^*) > \lambda_1(G)$.

Subcase (i.ii) $n_2 = n_3 = 0$, $n_4 \neq 0$.

In this subcase, $G \cong C_n^4(n_1, 0, 0, n_4)$. Since $G \neq C_n^4$, $2 \leq n_1, n_4 \leq n-6$. We suppose $x_{u_1} \geq x_{u_4}$. Let $G^* = G - \{u_4v_3, \dots, u_4v_{n_4}\} + \{u_1v_3, \dots, u_1v_{n_4}\}$. Obviously, $G^* \cong C_n^4(n-6, 0, 0, 2)$. By Lemmas 11 and 5, we have $\lambda_1(L_n^1) > \lambda_1(C_n^4(n-6, 0, 0, 2)) = \lambda_1(G^*) \geq \lambda_1(G)$.

Case (ii) One of n_2, n_3, n_4 is zero.

Without loss of generality, we may assume that $n_4 = 0$ and $n_2, n_3 \neq 0$. Thus, $G \cong C_n^4(n_1, n_2, n_3, 0)$, where $1 \leq n_1, n_2, n_3 \leq n-6$. Two subcases are considered.

Subcase (ii.i) $n_2 = 1$.

In this subcase, $G \cong C_n^4(n_1, 1, n_3, 0)$. We suppose $n_3 \geq n_1 \geq 1$. Let

$$G^* = \begin{cases} G - \{u_2s_1\} + \{u_1s_1\}, & \text{if } x_{u_1} \geq x_{u_2} \\ G - \{u_1r_1, \dots, u_1r_{n_1}\} + \{u_2r_1, \dots, u_2r_{n_1}\}, & \text{if } x_{u_1} < x_{u_2} . \end{cases}$$

Then, in either case, $G^* \cong C_n^4(n_1+1, 0, n_3, 0)$ or $G^* \cong C_n^4(0, n_1+1, n_3, 0)$. By Lemma 5, we have $\lambda_1(G^*) > \lambda_1(G)$. For $n \geq 8$, we have $2 \leq n_1+1, n_3 \leq n-6$ (If $n_3 = 1$, then it will contradict with $n_3 \geq n_1$). By the results of Subcase (i.i) and (i.ii), we have $\lambda_1(L_n^1) > \lambda_1(G^*)$. Thus, $\lambda_1(L_n^1) > \lambda_1(G)$.

Subcase (ii.ii) $2 \leq n_2 \leq n-6$.

Suppose that $x_{u_1} \geq x_{u_3}$. Let $G^* = G - \{u_3t_1, \ldots, u_3t_{n_3}\} + \{u_1t_1, \ldots, u_1t_{n_3}\}$. Obviously, $G^* \cong C_n^4(n_1+n_3, n_2, 0, 0)$. Since $2 \leq n_1+n_3, n_2 \leq n-6$, by the result of Subcase (i.ii) and Lemma 5, we have $\lambda_1(L_n^1) > \lambda_1(C_n^4(n_1+n_3, 0, 0, n_2)) = \lambda_1(G^*) > \lambda_1(G)$.

Case (iii) None of n_2, n_3, n_4 is zero.

Without loss of generality, we suppose that $x_{u_1} \geq x_{u_4}$. Let

$$G^* = G - \{u_4v_1, \ldots, u_4v_{n_4}\} + \{u_1v_1, \ldots, u_1v_{n_4}\} .$$

Obviously, $G^* \cong C_n^4(n_1+n_4, n_2, n_3, 0)$. By the result of Case (ii) and Lemma 5, we have $\lambda_1(L_n^1) > \lambda_1(G^*) > \lambda_1(G)$. $\square$

Lemma 13. *As* $1 \leq b \leq n-6$ *and* $n \geq 8$, $\lambda_1(L_n^1) > \lambda_1(K_n^4(b,c))$.

Proof. Let $n \geq 8$. We consider the following two cases.

Case (i) $b = 1$ and $b = n-6$.

Lemma 1 yields

$$\phi(K_n^4(1, n-5), \lambda) = \lambda^{n-4}\left[(4n-18) - n\lambda^2 + \lambda^4\right]$$

and

$$\phi(K_n^4(n-6, 2), \lambda) = \lambda^{n-6}\,(\lambda^2-2)[(2n-14) - (n-2)\lambda^2 + \lambda^4] .$$

Hence

$$\begin{aligned} \lambda_1(K_n^4(1, n-5)) &= \sqrt{\frac{1}{2}(n + \sqrt{72 - 16n + n^2})} \\ \lambda_1(K_n^4(n-6, 2)) &= \sqrt{\frac{1}{2}(-2 + n + \sqrt{60 - 12n + n^2})} . \end{aligned}$$

From (18), we can easily verify that $\lambda_1(L_n^1) > \lambda_1(K_n^4(1, n-5))$ and $\lambda_1(L_n^1) > \lambda_1(K_n^4(n-6, 2))$ for $n \geq 8$.

Case (ii) $2 \leq b \leq n-7$.

In this case, since $b + c = n-4$, we have $3 \leq c \leq n-6$. In $K_n^4(b,c)$, bearing in mind that $N(u_1) = \{u_2, u_4, z_1, \ldots, z_b\}$ and $N(z_1) = \{u_1, w_1, \ldots, w_c\}$, we let

$$G^* = \begin{cases} K_n^4(b,c) - \{u_1z_2, \ldots, u_1z_b\} + \{z_1z_2, \ldots, z_1z_b\}, & \text{if } x_{z_1} \geq x_{u_1} \\ K_n^4(b,c) - \{z_1w_3, \ldots, z_1w_c\} + \{u_1w_3, \ldots, u_1w_c\}, & \text{if } x_{z_1} < x_{u_1} . \end{cases}$$

Then, in either case, $G^* \cong K_n^4(1, n-5)$ or $G^* \cong K_n^4(n-6, 2)$. By the results of Case (i) and Lemma 5, we have $\lambda_1(L_n^1) > \lambda_1(G^*) > \lambda_1(K_n^4(b, c))$. $\square$

Let $H_n^4(1; b-1, c)$ be the unicyclic graph obtained from $K_{n-1}^4(b-1, c)$ by attaching one pendent edge to u_2 of C_4, where $c = n-4-b$ and $2 \le b \le n-5$. We have Lemma 14 as follows.

Lemma 14. *As* $2 \le b \le n-5$ *and* $n \ge 8$, $\lambda_1(K_n^4(b, c)) > \lambda_1(H_n^4(1; b-1, c))$.

Proof. By the definition of $H_n^4(1; b-1, c)$, for u_1 of $H_n^4(1; b-1, c)$, we have $N(u_1) = \{u_2, u_4, z_1, \ldots, z_{b-1}\}$. Let w be the vertex of degree 1 adjacent to u_2 in $H_n^4(1; b-1, c)$. Let

$$G^* = \begin{cases} H_n^4(1; b-1, c) - \{u_2 w\} + \{u_1 w\} & \text{if } x_{u_1} \ge x_{u_2} \\ H_n^4(1; b-1, c) - \{u_1 z_1, \ldots, u_1 z_{b-1}\} + \{u_2 z_1, \ldots, u_2 z_{b-1}\} & \text{if } x_{u_1} < x_{u_2}\ . \end{cases}$$

Then, in either case, $G^* \cong K_n^4(b, c)$. By Lemma 5, we have Lemma 14. $\square$

Let Q_n^4 be the unicyclic graph obtained from C_4 by attaching $n-8$ pendent edges and two paths of length two to u_1, where $n \ge 8$.

Lemma 15. *As* $n \ge 8$, *we have*
(i) $\lambda_1(L_n^1) > \lambda_1(Q_n^4)$, *and*
(ii) $\lambda_1(L_n^1) > \lambda_1(H_n^4(1; n-6, 1))$.

Proof. By Lemma 1, we have

$$\begin{aligned} \phi(Q_n^4, \lambda) &= \lambda^{n-8}\, (\lambda^2 - 1)[(16 - 2n) - (16 - 3n)\lambda^2 \\ &+ (1 - n)\lambda^4 + \lambda^6] \triangleq \lambda^{n-8}\, (\lambda^2 - 1) g_3(\lambda) \\ \phi(H_n^4(1; n-6, 1), \lambda) &= \lambda^{n-8}\, [(n - 7) - (4n - 25)\lambda^2 \\ &+ (4n - 18)\lambda^4 - n\lambda^6 + \lambda^8]\ . \end{aligned}$$

We can check $g_3(\sqrt{0.7}) < 0$ for $n \ge 15$, $g_3(\sqrt{1}) > 0$ for $n \ge 6$, $g_3(\sqrt{1.7}) > 0$ for $n \ge 17$, $g_3(\sqrt{2}) < 0$ for $n \ge 6$, $g_3(\sqrt{n-4}) < 0$ for $n \ge 6$, and $g_3(\sqrt{n-3}) > 0$ for $n \ge 11$. According to the theorem of zero points, we have $\sqrt{n-4} < \lambda_1(Q_n^4) < \sqrt{n-3}$ for $n \ge 17$. Similarly, we can check $\sqrt{n-4} < \lambda_1(H_n^4(1; n-6, 1)) < \sqrt{n-3.7}$ for $n \ge 29$.

From (18), we can easily verify that, for $n \geq 8$, $\lambda_1(L_n^1) > \sqrt{n-3+4/n}$. Thus, $\lambda_1(L_n^1) > \lambda_1(Q_n^4)$ for $n \geq 17$ and $\lambda_1(L_n^1) > \lambda_1(H_n^4(1; n-6, 1))$ for $n \geq 29$. Calculation yields $\lambda_1(L_n^1) > \lambda_1(Q_n^4)$ for $16 \geq n \geq 8$ and $\lambda_1(L_n^1) > \lambda_1(H_n^4(1; n-6, 1))$ for $28 \geq n \geq 8$. $\square$

Lemma 16. *Let $G \in \mathcal{U}_n^+ \setminus \{L_n^0, C_n^4, L_n^1, I_n^4\}$ with $l = 4$ and $n \geq 8$. We have $\lambda_1(L_n^1) > \lambda_1(G)$.*

Proof. Let $G \in \mathcal{U}_n^+ \setminus \{L_n^0, C_n^4, L_n^1, I_n^4\}$, $l = 4$, $n \geq 8$, and $1 \leq i \leq 4$. For $G \in \mathcal{U}_n^+$, we denote by T_i the tree attached to u_i of C_4. We say that u_i is attached by $\deg(u_i) - 2$ subtrees. Namely, T_i can be viewed as the tree obtained by identifying a pendent vertex of each of the $\deg(u_i) - 2$ subtrees with u_i. We assume that the vertices of T_i and of its subtrees include u_i. The number of the vertices of T_i is called the order of T_i and is denoted by $n_i + 1$, where $0 \leq n_i \leq n - 4$.

Applying the EGT to G repeatedly, we obtain $\lambda_1(G^*) \geq \lambda_1(G)$, where $G^* \cong C_n^4(n_1, n_2, n_3, n_4)$. If $G^* \neq L_n^0, C_n^4, L_n^1$, then by Lemma 12, we obtain $\lambda_1(L_n^1) > \lambda_1(G)$. Otherwise, $G^* \cong L_n^0, C_n^4, L_n^1$. Next we consider three cases according to the types of G^*.

Case (i). $G^* \cong L_n^0$.

For G, only one vertex u_1 on C_4 is attached by T_1.

If all the subtrees of T_1 are pendent edges or paths of length 2, then u_1 is attached by at least two paths of length 2 since $G \neq L_n^0, I_n^4$. Applying the EGT to G repeatedly, we obtain $\lambda_1(Q_n^4) \geq \lambda_1(G)$, with equality holding if and only if $G \cong Q_n^4$. Furthermore, by Lemma 15(i), we get $\lambda_1(L_n^1) > \lambda_1(G)$.

In other cases, at least one subtree of T_1 has order greater than 4. We suppose that the order of this subtree is $c + 2$. Obviously, $2 \leq c \leq n - 5$. Applying the EGT to G repeatedly, we obtain $\lambda_1(K_n^4(b, c)) \geq \lambda_1(G)$, with equality holding if and only if $G \cong K_n^4(b, c)$, where $b = n - 4 - c$. Obviously, $1 \leq b \leq n - 6$. Thus, by Lemma 13, we obtain $\lambda_1(L_n^1) > \lambda_1(G)$.

Case (ii). $G^* \cong C_n^4$.

For G, u_1 is attached by T_1 with $2 \leq n_1 \leq n - 5$ (since $n \geq 8$) and u_2 is attached by one pendent edge.

If all the subtrees of T_1 are pendent edges or paths of length 2, then u_1 is attached by at least one path of length 2 since $G \neq C_n^4$. Applying the EGT to G repeatedly, we get $\lambda_1(H_n^4(1; n-6, 1)) \geq \lambda_1(G)$, with equality holding if and only if $G \cong H_n^4(1; n-6, 1)$. Thus, by Lemma 15(ii), we obtain $\lambda_1(L_n^1) > \lambda_1(G)$.

In other cases, at least one subtree of T_1 has order greater than 4. We suppose that the order of this subtree is $c+2$. Obviously, $2 \leq c \leq n-6$. Applying the EGT to G repeatedly, we get $\lambda_1(H_n^4(1; b-1, c)) \geq \lambda_1(G)$, with equality holding if and only if $G \cong H_n^4(1; b-1, c)$, where $b = n-4-c$. Obviously, $2 \leq b \leq n-6$. Thus, by Lemmas 13 and 14, we get $\lambda_1(L_n^1) > \lambda_1(G)$.

Case (iii). $G^* \cong L_n^1$.

For G, u_1 is attached by T_1 with $2 \leq n_1 \leq n-5$ (since $n \geq 8$) and u_3 is attached by one pendent edge. Applying the EGT to G repeatedly, we get $\lambda_1(L_n^1) > \lambda_1(G)$ since $G \neq L_n^1$.

In conclusion, we obtain $\lambda_1(L_n^1) > \lambda_1(G)$ for $G^* \cong L_n^0, C_n^4, L_n^1$ as $n \geq 8$ in Cases (i)–(iii). Thus, Lemma 16 is proved. $\square$

Lemma 17. *Let $G \in \mathcal{U}_n^+$ and $l \geq 6$ and $n \geq 8$. We have $\lambda_1(L_n^1) > \lambda_1(G)$.*

Proof. Bearing in mind that $G_n^{6,1}$ is the graph obtained from C_6 by attaching $n-6$ pendent edges to u_1 of C_6, by Lemma 1, we get $\phi(G_n^{6,1}, \lambda) = \lambda^{n-6}(\lambda^2 - 1)[(3n-14) - (n-1)\lambda^2 + \lambda^4]$. Hence, $\lambda_1(G_n^{6,1}) = \sqrt{\frac{1}{2}(-1 + n + \sqrt{57 - 14n + n^2})}$. From (18), we can check $\lambda_1(L_n^1) > \lambda_1(G_n^{6,1})$ as $n \geq 8$. By Lemma 3(i) and (iii), for $G \in \mathcal{U}_n^+$ with $l \geq 6$ and $n \geq 8$, we have $\lambda_1(G_n^{6,1}) \geq \lambda_1(G)$, with equality holding if and only if $G \cong G_n^{6,1}$. Thus, we obtain Lemma 17. $\square$

By Lemmas 8–10, 16, and 17, we get the first four and three unicyclic graphs with the maximal EIs in $\mathcal{U}_n^+$ for $n \geq 23$ and $22 \geq n \geq 8$, respectively.

Theorem 1. *Let $G \in \mathcal{U}_n^+$ with $l \geq 4$ and $n \geq 8$. We have*

(i) $EE(L_n^0) > EE(C_n^4) > EE(I_n^4) > EE(L_n^1) > EE(G)$ for $n \geq 23$, where $G \neq L_n^0, C_n^4, I_n^4, L_n^1$.

(ii) $EE(L_n^0) > EE(C_n^4) > EE(L_n^1) > EE(G)$ for $22 \geq n \geq 8$, where $G \neq L_n^0, C_n^4, L_n^1$.

Proof. As $n \geq 23$, Lemmas 9 and 10 yield $EE(L_n^0) > EE(C_n^4) > EE(I_n^4) > EE(L_n^1)$. As $22 \geq n \geq 8$, calculation yields $EE(C_n^4) > EE(L_n^1)$. Furthermore, by Lemmas 9 and 10, we get $EE(L_n^0) > EE(C_n^4) > EE(L_n^1) > EE(I_n^4)$ for $22 \geq n \geq 8$.

Let $G \in \mathcal{U}_n^+ \setminus \{L_n^0, C_n^4, I_n^4, L_n^1\}$ with $l \geq 4$ and $n \geq 8$. By Lemmas 16 and 17, we obtain $\lambda_1(L_n^1) > \lambda_1(G)$. Since L_n^1 has exactly two positive eigenvalues and the other graphs in $\mathcal{U}_n^+$ have at least two positive eigenvalues [28], by Lemma 8, we have $EE(L_n^1) > EE(G)$.

Theorem 1 is thus proved. □

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