Unicyclic Graph with Maximal Estrada Indices

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Abstract

Let $U_n^+$ be the set of bipartite unicyclic graphs with $n$ vertices. In $U_n^+$, ordering the unicyclic graphs in terms of their maximal Estrada indices was considered. We deduce the first four and three unicyclic graphs in $U_n^+$ 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

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

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

$$ \phi(G, \lambda) = \det[\lambda I - A(G)] $$ (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 $\lambda_i$ ($1 \leq i \leq n$) 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 $e^{\lambda_i}$, $EE(G)$ in (1) can be rewritten as

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

(3)

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

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

(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 \( U_n \), 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 \( U_n^+ \). For the graphs in \( U_n \), 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 \( U_n^+ \), 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 \( U_n^+ \) 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 \( G_{n+1}^l \) be the graph obtained from \( C_l \) by attaching
n − 1 pendent edges to \( u_1 \) of \( C_l \). Let \( G_n^{l,2} \) be the graph obtained from \( C_l \) by attaching \( n − 1 \) 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 \( l ≥ 3 \) and \( n ≥ l \), 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 neighbors of \( v \), respectively.

**Lemma 5.** [27,29] Let \( G \) be a connected graph and \( u, v \) be two vertices of \( G \). Suppose that \( v_1, v_2, \ldots, v_s \in N(v) \setminus N(u) \) (\( 1 ≤ s ≤ d(v) \)) and \( x = (x_1, x_2, \ldots, x_n) \) is the Perron vector of \( A(G) \), where \( x_i \) corresponds to the vertex \( v_i \) (\( 1 ≤ i ≤ n \)). Let \( G^* \) be the graph obtained from \( G \) by deleting the edges \( vv_i \) and adding the edges \( uv_i \) (\( 1 ≤ i ≤ s \)). If \( x_u ≥ x_v \), 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 \( n ≥ 3 \). 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

\[
x^k - y^k = (x - y)(x^{k-1} + x^{k-2}y + \cdots + y^{k-1})
\]

(5)

\[
(a - y)^k - (a - x)^k = (x - y) \left[ (a - y)^{k-1} + (a - y)^{k-2}(a - x) + \cdots + (a - x)^{k-1} \right].
\]

(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 \( t = \lfloor n - \eta(G) \rfloor / 2 \) 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 \( e^{\lambda_i} \), we have

\[
EE(G) = n + m + 2 \sum_{k=2}^{\infty} \frac{1}{(2k)!} \sum_{i=1}^{t} \lambda_i^{2k}.
\]

(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 \( \lambda_1^2(G_1) = x_i \) 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 \( \lambda_i^2 \) 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) $3 \leq t \leq n/2$.

Two subcases are considered as follows.

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

Obviously, $m > x_1 > y_1 \geq m/2$. 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

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

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

As $t = p$ and $p \geq 4$, 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 $y_1 > y_2 \geq \cdots \geq y_{p+1} > 0$ and $p \geq 4$, 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 $3 \leq t \leq n/2$.

Thus, by (7), we obtain $EE(G_1) > EE(G_2)$.

Lemma 8 is thus proved. □

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

Specially, we denote $C^4_n(n - 5, 0, 0, 1)$ by $C^4_n$ with $n \geq 6$ and $C^4_n(n_1, 0, n_3, 0)$ by $L^3_n$ with $n_1 = n - 4 - n_3$.

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

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

Specially, we denote $K^4_n(n - 5, 1)$ by $I^4_n$ with $n \geq 6$.

For example, $C^4_8$, $L^2_8$, $K^4_8(1, 3)$ and $I^4_8$ are shown in Fig. 1.

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

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

**Lemma 9.** $EE(L^0_n) > EE(C^4_n) > EE(I^4_n)$ for $n \geq 6$.

**Proof.** Straightforward derivation by Lemma 1 yields

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

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

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

From (9) and (10), we can see that $L^0_n$ and $C^4_n$ have two and three positive eigenvalues, respectively. Since $L^0_n = G^4_{n1}$, by Lemma 3(i), we have $\lambda_1(L^0_n) > \lambda_1(C^4_n)$ for $n \geq 6$. Since $L^0_n, C^4_n \in \mathcal{U}^+_n$, by Lemma 8, we get $EE(L^0_n) > EE(C^4_n)$ for $n \geq 6$. 

![Fig. 1: $C^4_8$, $L^2_8$, $K^4_8(1, 3)$, and $I^4_8$.](image-url)
We can check that
\[ g_1\left(\sqrt{0.38}\right) = 0.114872 - 0.0044n < 0 \quad (n \geq 27) \]
\[ g_1\left(\sqrt{0.382}\right) = 0.089743 + 0.000076n > 0 \quad (n \geq 6) \]
\[ g_1\left(\sqrt{2.6}\right) = -11.224 + 0.04n > 0 \quad (n \geq 281) \]
\[ g_1\left(\sqrt{2.62}\right) = -11.0753 - 0.0044n < 0 \quad (n \geq 7) \]
\[ g_1\left(\sqrt{n - 3 + 5/n}\right) = -11.224 + 0.04n > 0 \quad (n \geq 281) \]
\[ g_1\left(\sqrt{n - 3 + 8/n}\right) = -55 + \frac{512}{n^3} - \frac{576}{n^2} + \frac{240}{n} + 3n > 0 \quad (n \geq 14) . \]

According to the theorem of zero points, we have, for \( n \geq 281 \),
\[ n - 3 + \frac{5}{n} < \lambda_1^2(C_n^4) < n - 3 + \frac{8}{n}, \quad 2.6 < \lambda_2^2(C_n^4) < 2.626, \quad 0.38 < \lambda_3^2(C_n^4) < 0.382 . \] (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 \( n \geq 50 \), \( g_2\left(\sqrt{1.97}\right) > 0 \) for \( n \geq 6 \), \( g_2\left(\sqrt{1.97}\right) > 0 \) 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 \( n \geq 50 \),
\[ n - 3 + \frac{5}{n} < \lambda_1^2(I_n^4) < n - 3 + \frac{6}{n}, \quad 1.91 < \lambda_2^2(I_n^4) < 2, \quad 0.976 < \lambda_3^2(I_n^4) < 1 . \] (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 \( C_n^4 = G_n^4 \), 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 \( k \geq 2 \),
\[ x_1^k + x_2^k > y_1^k + (x_2 + x_1 - y_1)^k . \] (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 \( k \geq 2 \),
\[ (x_2 + x_1 - y_1)^k + x_3^k > y_2^k + y_3^k . \] (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 $n \geq 6$. □

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

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

$$EE(I_n^4) > n - 6 + e^{3\sqrt{n-3}} + e^{0.976} + e^{-7} + e^{-\sqrt{n-3}}.$$  

Straightforward derivation by Lemma 1 yields

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

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

$$\lambda_1(L_n^1) = \sqrt[4]{1/2(n + \sqrt{52 - 12n + n^2})}. \quad (18)$$

From (1) and (17), we obtain

$$EE(L_n^1) = n - 4 + e^{3/2(n + \sqrt{52 - 12n + n^2})} + e^{0.976} + e^{-7} + e^{-\sqrt{n-3}}.$$  

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

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. □
Lemma 12. 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 $n \geq 8$. 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 $\{r_1, \ldots, r_m\}$, $\{s_1, \ldots, s_m\}$, $\{t_1, \ldots, t_m\}$, and $\{v_1, \ldots, v_m\}$ the sets of pendant 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 $G^* = G - \{u_3 t_2, \ldots, u_3 t_m\} + \{u_1 t_2, \ldots, u_1 t_m\}$. 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 $G^* = G - \{u_4 v_3, \ldots, u_4 v_m\} + \{u_1 v_3, \ldots, u_1 v_m\}$. 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

$$G^* = \begin{cases} 
G - \{u_2 s_1\} + \{u_1 s_1\}, & \text{if } x_{u_1} \geq x_{u_2} \\
G - \{u_1 r_1, \ldots, u_1 r_n\} + \{u_2 r_1, \ldots, u_2 r_n\}, & \text{if } x_{u_1} < x_{u_2}.
\end{cases}$$

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 $G^* = G - \{u_3t_1, \ldots, u_3t_n\} + \{u_1t_1, \ldots, u_1t_n\}$. 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

$$G^* = G - \{u_4v_1, \ldots, u_4v_n\} + \{u_1v_1, \ldots, u_1v_n\}.$$ 

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 $\lambda_1(L_n^1) > \lambda_1(G^*) > \lambda_1(G)$. □

**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

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

and

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

Hence

$$\lambda_1(K_n^4(1, n - 5)) = \sqrt{\frac{1}{2} (n + \sqrt{72 - 16n + n^2})}$$

and

$$\lambda_1(K_n^4(n - 6, 2)) = \sqrt{\frac{1}{2} (-2 + n + \sqrt{60 - 12n + n^2})}.$$ 

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

$$G^* = \begin{cases} 
K_n^4(b, c) - \{u_1z_1, \ldots, u_1z_b\} + \{z_1z_2, \ldots, z_1z_b\}, & \text{if } x_{z_1} \geq x_{u_1} \\
K_n^4(b, c) - \{z_1w_3, \ldots, z_1w_c\} + \{u_1w_3, \ldots, u_1w_c\}, & \text{if } x_{z_1} < x_{u_1}.
\end{cases}$$
Then, in either case, $G^* \cong K^4_n(1, n - 5)$ or $G^* \cong K^4_n(n - 6, 2)$. By the results of Case (i) and Lemma 5, we have $\lambda_1(L^*_n) > \lambda_1(G^*) > \lambda_1(K^4_n(b, c)). \square$

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

**Lemma 14.** As $2 \leq b \leq n - 5$ and $n \geq 8$, $\lambda_1(K^4_n(b, c)) > \lambda_1(H^4_n(1; b - 1, c))$.

**Proof.** By the definition of $H^4_n(1; b - 1, c)$, for $u_1$ of $H^4_n(1; b - 1, c)$, 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 $H^4_n(1; b - 1, c)$. Let

$$G^* = \begin{cases} H^4_n(1; b - 1, c) - \{u_2w\} + \{u_1w\} & \text{if } x_{u_1} \geq x_{u_2} \\ H^4_n(1; b - 1, c) - \{u_1z_1, \ldots, u_1z_{b-1}\} + \{u_2z_1, \ldots, u_2z_{b-1}\} & \text{if } x_{u_1} < x_{u_2} \end{cases}$$

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

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

**Lemma 15.** As $n \geq 8$, we have

(i) $\lambda_1(L^*_n) > \lambda_1(Q^4_n)$, and

(ii) $\lambda_1(L^*_n) > \lambda_1(H^4_n(1; n - 6, 1))$.

**Proof.** By Lemma 1, we have

$$\phi(Q^4_n, \lambda) = \lambda^{n-8}(\lambda^2 - 1)(16 - 2n) - (16 - 3n)\lambda^2$$

$$+ (1 - n)\lambda^4 + \lambda^6 | \triangleq \lambda^{n-8}(\lambda^2 - 1)g_3(\lambda)$$

$$\phi(H^4_n(1; n - 6, 1), \lambda) = \lambda^{n-8}[(n - 7) - (4n - 25)\lambda^2$$

$$+ (4n - 18)\lambda^4 - n\lambda^6 + \lambda^8].$$

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

-950-
From (18), we can easily verify that, for $n \geq 8$, $\lambda_1(L^1_n) > \sqrt{n - 3 + 4/n}$. Thus, $\lambda_1(L^1_n) > \lambda_1(Q^4_n)$ for $n \geq 17$ and $\lambda_1(L^1_n) > \lambda_1(H^4_n(1; n - 6, 1))$ for $n \geq 29$. Calculation yields $\lambda_1(L^1_n) > \lambda_1(Q^4_n)$ for $16 \geq n \geq 8$ and $\lambda_1(L^1_n) > \lambda_1(H^4_n(1; n - 6, 1))$ for $28 \geq n \geq 8$. \hfill \square

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

**Proof.** Let $G \in \mathcal{U}^+_n \setminus \{L^0_n, C^4_n, L^1_n, I^4_n\}$, $l = 4$, $n \geq 8$, 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 $\text{deg}(u_i) - 2$ subtrees. Namely, $T_i$ can be viewed as the tree obtained by identifying a pendent vertex of each of the $\text{deg}(u_i) - 2$ 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 $G^* \cong C^4_{n_1, n_2, n_3, n_4}$. If $G^* \neq L^0_n, C^4_n, L^1_n$, then by Lemma 12, we obtain $\lambda_1(L^1_n) > \lambda_1(G)$. Otherwise, $G^* \cong L^0_n, C^4_n, L^1_n$. Next we consider three cases according to the types of $G^*$.

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

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 $G \neq L^0_n, I^4_n$. Applying the EGT to $G$ repeatedly, we obtain $\lambda_1(Q^4_n) \geq \lambda_1(G)$, with equality holding if and only if $G \cong Q^4_n$. Furthermore, by Lemma 15(i), we get $\lambda_1(L^1_n) > \lambda_1(G)$.

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 $\lambda_1(K^4_n(b, c)) \geq \lambda_1(G)$, with equality holding if and only if $G \cong K^4_n(b, c)$, where $b = n - 4 - c$. Obviously, $1 \leq b \leq n - 6$. Thus, by Lemma 13, we obtain $\lambda_1(L^1_n) > \lambda_1(G)$.

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

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. □

**Lemma 17.** Let $G \in U_n^+$ 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, $\lambda_1(G_n^{6,1}) = \sqrt{2}(-1 + n + \sqrt{57 - 14n + n^2})$. 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 $G \in U_n^+$ 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. □

By Lemmas 8–10, 16, and 17, we get the first four and three unicyclic graphs with the maximal ELs in $U_n^+$ for $n \geq 23$ and $22 \geq n \geq 8$, respectively.

**Theorem 1.** Let $G \in U_n^+$ with $l \geq 4$ and $n \geq 8$. We have

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

(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 $EE(L_0^i) > EE(C_4^i) > EE(I_4^i) > EE(L_1^i)$. As $22 \geq n \geq 8$, calculation yields $EE(C_4^i) > EE(L_1^i)$. Furthermore, by Lemmas 9 and 10, we get $EE(L_0^i) > EE(C_4^i) > EE(L_1^i) > EE(I_4^i)$ for $22 \geq n \geq 8$.

Let $G \in U_n^+ \setminus \{L_0^i, C_4^i, I_4^i, L_1^i\}$ with $l \geq 4$ and $n \geq 8$. By Lemmas 16 and 17, we obtain $\lambda_1(L_1^i) > \lambda_1(G)$. Since $L_1^i$ has exactly two positive eigenvalues and the other graphs in $U_n^+$ have at least two positive eigenvalues [28], by Lemma 8, we have $EE(L_1^i) > EE(G)$.

Theorem 1 is thus proved. □

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References


