On the Laplacian Estrada Index of Unicyclic Graphs

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Abstract

Let $G$ be a simple graph with $n$ vertices. If $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of $G$, then the Laplacian Estrada index is defined as $\text{LEE}(G) = \sum_{i=1}^{n} e^{\mu_i}$. In this paper, the unicyclic graph on $n$ vertices with the maximal Laplacian Estrada index is determined.

1 Introduction

Given a simple graph $G$ with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, the adjacency matrix $A(G) = [a_{ij}]$ of $G$ is an $n \times n$ symmetric matrix of 0’s and 1’s with $a_{ij} = 1$ if and only if $v_i$ and $v_j$ are joined by an edge. Denote the degree of vertex $v_i$ by $d_G(v_i)$. Then the Laplacian matrix of $G$ is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix $\text{diag}(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$. Since $A(G), L(G)$ are real symmetric matrices, their eigenvalues $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ and $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$, respectively, are real numbers. The eigenvalues of $A(G)$ and $L(G)$ are called the adjacency eigenvalues and the Laplacian eigenvalues of $G$, respectively. In what follows we assume that $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$ and $\mu_1(G) \geq \mu_2(G) \geq \ldots \mu_{n-1}(G) \geq \mu_n(G) = 0$.

The Laplacian Estrada index of a graph $G$ is defined in [9] as $\text{LEE}(G) = \sum_{i=1}^{n} e^{\mu_i(G)}$.
(Independently of [9], another variant of the Laplacian Estrada index was put forward in [10], defined as $LEE^*(G) = \sum_{i=1}^{n} e^{\lambda_i(G) - 2m/n}$. Bounds and various properties of Laplacian Estrada index were found in [9–14]. For a bipartite graph $G$ with $n$ vertices and $m$ edges, it is shown [8] that

$$LEE(G) = n - m + e^2 \cdot EE(L(G)),$$

where $L(G)$ is the line graph of $G$, and $EE(L(G)) = \sum_{i=1}^{n} e^{\lambda_i(L(G))}$ is the Estrada index ([5–7]) of $L(G)$. Using the formal (1) and the results of Estrada index, Allić and Zhou [8] showed that the path $P_n$ has minimal, while the star $S_n$ has maximal Laplacian Estrada index among trees on $n$ vertices. Obviously, this method is not suited to calculate the Laplacian Estrada index of the general graphs. So, it is interesting to consider the index for the non-bipartite graphs.

Let $G$ be a graph with $n$ vertices and $m$ edges. If $n = m$, then we call $G$ an unicyclic graph. Let $S_n^3$ be the unicyclic graph obtained by adding an edge to the star graph $S_n$. In this paper, we will show that $S_n^3$ is the unique unicyclic graph on $n$ vertices with maximal Laplacian Estrada index.

2 Main Results

Let $G$ be a graph with $n$ vertices and let $G^* = G + e$ be the graph obtained from $G$ by inserting a new edge $e$ into $G$.

Lemma 1 [1, 3] The Laplacian eigenvalues of $G$ and $G^*$ interlace, that is, $\mu_1(G^*) \geq \mu_1(G) \geq \mu_2(G^*) \geq \mu_2(G) \geq \cdots \geq \mu_n(G^*) = \mu_n(G) = 0$.

Lemma 2 [15] Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$, and $N_u$ be the set of neighbors of $u$. Then

$$\mu_1(G) \leq \max\{d_G(u) + d_G(v) - |N_u \cap N_v| : uv \in E(G)\}.$$ 

Let $s(G) = \max\{d_G(u) + d_G(v) - |N_u \cap N_v| : uv \in E(G)\}$ and $n(G) = |V(G)|$. Clearly, if $G$ is an unicyclic graph with $n$ vertices, then $s(G) \leq n$.

Lemma 3 Let $G$ be an unicyclic graph with $n \geq 8$ vertices and $s(G) \leq n(G) - 2$. Then $LEE(G) \leq LEE(S_n^3)$ with equality if and only if $G \cong S_n^3$. 

Proof. By induction on \( n \) to prove it. From the Appendix table of [2], there are 57 unicyclic graphs on 8 vertices of \( s(G) \) not greater than 6. We give Table 1 for the LEE of these graphs, in which we use the same graph labels as the Appendix table of [2]. It implies that the result holds for \( n = 8 \).

\[
\begin{array}{cccccc}
\text{Label} & \text{LEE} & \text{Label} & \text{LEE} & \text{Label} & \text{LEE} \\
1 & 134.7549405 & 16 & 186.9609149 & 36 & 262.8445145 \\
2 & 160.1365435 & 17 & 195.4963498 & 40 & 375.5477041 \\
3 & 162.8965473 & 18 & 194.0249743 & 46 & 148.2025007 \\
4 & 161.8648960 & 19 & 197.9591155 & 47 & 171.0874842 \\
5 & 185.7915381 & 20 & 196.4963498 & 48 & 173.6518608 \\
6 & 167.9367951 & 21 & 200.5709879 & 49 & 177.5303931 \\
7 & 189.8493511 & 22 & 273.9601119 & 50 & 180.1005287 \\
8 & 188.0623938 & 24 & 221.0272062 & 51 & 171.2211615 \\
9 & 187.0766847 & 25 & 225.1528983 & 52 & 173.6518608 \\
10 & 191.4014165 & 26 & 262.3182544 & 53 & 204.5253414 \\
11 & 166.9477426 & 27 & 229.4185558 & 54 & 194.2417996 \\
12 & 249.2712699 & 28 & 229.5574315 & 55 & 200.5944661 \\
13 & 213.8766018 & 29 & 269.3362990 & 56 & 232.4648707 \\
14 & 217.8546022 & 31 & 285.4468880 & 57 & 200.4666498 \\
15 & 254.8665304 & 33 & 289.9695503 & 58 & 239.4760009 \\
\end{array}
\]

We now suppose that \( n \geq 9 \) and the result is true for graphs with vertex number less than \( n \). Let \( G \) be a graph with \( n \) vertices. Suppose \( G \cong C_n \). Then \( \mu_1(C_n) \leq 4 \) and \( LEE(G) \leq \mu_1(C_n) \leq 4 \). Note that \( LEE(S_n) = e^n + e^3 + e^1 + \cdots + e^0 > e^n \). Let \( f(n) = e^n - n \cdot e^4 \). Note that \( f'(n) = e^n - n > 0 \), and \( f(7) = e^7 - 7e^4 > e^4 > 0 \). Hence, \( LEE(S_n) > e^n > n e^4 \geq LEE(G) \). Suppose \( G \not\cong C_n \). Then \( G \) must have a pendent vertex. Let \( wt \in E(G) \) with \( d_G(w) = 1 \) and \( G' = G - w \), then \( s(G') \leq s(G) \leq n - 2 \) and \( G = G' \cup \{w\} \). Let \( Spec(G') = \{\mu_1, \mu_2, \cdots, \mu_{n-1}\} \) be the Laplacian spectra of \( G' \), then

\[
LEE(G' \cup \{w\}) = \mu_1 + \mu_2 + \cdots + \mu_{n-1} + e^0.
\]

Note that \( \mu_1(H) + \mu_2(H) + \cdots + \mu_n(H) = 2m \) for any graph \( H \) and \( m \) denotes the number of edges in \( H \). By Lemma 1, then we can assume that the Laplacian spectra of \( G \), is

\[
Spec(G) = \{\mu_1 + x_1, \mu_2 + x_2, \cdots, \mu_{n-1} + x_{n-1}, 0\},
\]

where \( x_i \geq 0 \) and \( \sum_{i=1}^{n-1} x_i = 2 \).

Case 1. \( s(G') \leq n(G') - 2 = n - 3 \). Then

\[
LEE(G) = \sum_{i=1}^{n-1} e^{\mu_1 + x_i} + e^0 \leq e^{\mu_1 + 2} + \sum_{i=2}^{n-1} e^{\mu_i} + e^0
\]

\[
= e^{\mu_1 + 2} - e^{\mu_1} + e^0 + \sum_{i=1}^{n-1} e^{\mu_i}
\]

\[
= e^{\mu_1 + 2} - e^{\mu_1} + e^0 + LEE(G')
\]
By the induction hypothesis, \( LEE(G') \leq LEE(S^3_{n-1}) \) with equality if and only if \( G' \cong S^3_{n-1} \). Now by Lemma 2, \( \mu_1 \leq s(G') \leq n - 3 \), and we have

\[
LEE(G) \leq e^{\mu_1+2} - e^{\mu_1} + e^0 + LEE(S^3_{n-1}) \\
= e^{\mu_1+2} - e^{\mu_1} + e^0 + (e^{n-1} + e^3 + (n-4)e^1 + e^0) \\
= LEE(S^3_n) - [e^n - e^{n-1} + e^1 - e^0 - (e^{\mu_1+2} - e^{\mu_1})] \\
\leq LEE(S^3_n) - [e^n - e^{n-1} + e^1 - e^0 - (e^{n-2} - e^{n-3})] \\
= LEE(S^3_n) - (e - 1)e^{n-3}(e^2 - e - 1) \\
< LEE(S^3_n).
\]

**Case 2.** For any pendent vertex \( w \), \( s(G - w) = n - 2 \). Then \( s(G) = n - 2 \) since \( n - 2 = s(G - w) \leq s(G) \leq n - 2 \). That is, \( s(G - w) = s(G) = n - 2 \) for any pendent vertex \( w \).

Suppose that \( uv \in E(G) \) such that \( d_G(u) + d_G(v) - |N_u \cap N_v| = s(G) \).

**Subcase 2.1.** \( u, v \) have no common neighbor. Suppose without loss of generality that \( d_G(u) = y + 1 \geq x + 1 = d_G(v) \). Then \( d_G(u) + d_G(v) = s(G) = n - 2 \), \( x + y = n - 4 \), and \( G \) can be viewed as the connected graph obtained from a double star \( S(x + 1, y + 1) \) and two isolated vertices by adding three edges to them such that each of the three edges is not incident to \( u \) and \( v \), where a double star \( S(a, b) \) is the tree obtained from the stars \( S_a \) and \( S_b \) by joining their centers an edge. Let \( d_G(z_1) = \max\{d_G(z) | z \in V(G) \setminus \{u, v\} \} \). Then \( d_G(z_1) \leq 4 \).

Suppose \( x \geq 4 \). Then \( d_G(u) \geq d_G(v) \geq 5 \), and there must exists a pendent vertex adjacent to \( u \) in \( G \). Let \( w_1 \) be an any pendent vertex at \( u \), then \( s(G - w_1) = s(G) - 1 = n - 3 \), a contradiction.

Suppose \( x = 3 \). If \( d_G(z_1) = 4 \), then \( z_1 \in V(S(x + 1, y + 1)) \setminus \{u, v\} \) and the new three edges are all incident to \( z_1 \). Suppose that \( z_1 \) is adjacent to \( v \), there must exist a pendent vertex, say \( w_2 \), adjacent to \( v \), and then \( s(G - w_2) = s(G) - 1 = n - 3 \), a contradiction. If \( d_G(z_1) \leq 3 \), then \( d_G(u) \geq d_G(v) \geq 4 > d_G(z_1) \), and there must exist a pendent vertex, say \( w_3 \), that incident to \( u \) or \( v \). Clearly, \( s(G - w_3) < s(G) = n - 2 \), a contradiction again.

Suppose \( x = 2 \). Then \( y = n - 6 \geq 3 > x \). Clearly, there is no pendent vertex \( w_4 \) adjacent to \( u \) in \( G \). Otherwise, \( s(G - w_4) = s(G) - 1 \). A contradiction. If \( n \geq 11 \), then \( y = n - 6 \geq 5 \) and there must exist a pendent vertex \( w_5 \) adjacent to \( v \), and consequently \( s(G - w_5) = s(G) - 1 \), a contradiction. So \( 9 \leq n \leq 10 \). If \( n = 10 \), then \( y = 4 \). Since there are no pendent vertices adjacent to \( u \), there exists at least a pendent vertex \( w_6 \).
adjacent to \( v \). Clearly, \( s(G - w_6) = s(G) - 1 \), a contradiction. If \( n = 9 \), note the condition \( s(G - w) = s(G) = 7 \) for any pendent vertex \( w \) of \( G \), then \( G \) must be \( H_1 \) or \( H_2 \) in fig.1. By direct computation, the result follows.

Suppose \( x = 1 \). Then \( y = n - 4 - 1 \geq 4 \). If \( n \geq 10 \), then there exists a pendent vertex \( w_7 \) at \( u \) in \( G \). Clearly, \( s(G - w_7) < s(G) \), a contradiction. Thus \( n = 9 \) and \( G \cong H_3 \), where \( H_3 \) is shown as in Fig.1. It is easy to prove the result by direct computation.

By combining Cases 1 and 2, the result follows. \( \square \)

**Lemma 4** Let \( G \) be an unicyclic graph with \( n \geq 8 \) vertices and \( s(G) = n - 1 \). Then \( \text{LEE}(G) \leq \text{LEE}(S^3_n) \) with equality if and only if \( G \cong S^3_n \).

*Proof.* Suppose that \( uv \) be the edges such that \( d_G(u) + d_G(v) - |N_u \cap N_v| = n - 1 \).

If \( u \) and \( v \) have no common neighbors, then \( G \) can be viewed as the connected graph obtained from a double star \( S(a, b)(a + b = n - 1) \) and an isolated vertex by adding two
edges such that the two new edges are not incident to both $u$ and $v$. Then $G$ must be one of graphs in Fig.2 and Fig.3.

If $u$ and $v$ have a common neighbor, then $G$ can be viewed as the connected graph obtained by $G'$ and an isolated vertex by adding two edges such that the two new edges are not incident to both $u$ and $v$, where $G'$ is the graph obtained from a triangle $C_3 = zuvz$ by joining respectively $x$ and $y$ isolated vertices to $u$ and $v$, where $x + y = n - 4$. Thus $G$ must be one of graphs in Fig.4.

Note the fact that $G_i (i = 1, 2, \ldots , 9)$ has Laplacian eigenvalues 1 with multiplicity at least $n_1 + n_2 - 2$ and 0 with multiplicity 1. If $n_1 + n_2 = n - 6$, then we suppose
that \( \mu_1, \mu_2, \mu_3, \mu_4, \mu_5, \mu_6, \mu_7 \) are the remaining Laplacian eigenvalues of \( G \), then
\[
\mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_5 + \mu_6 + \mu_7 = 2n - (n - 8) \cdot 1 - 0 = n + 8.
\]
By Lemma 2, it follows that \( \mu_1 \leq s(G) = n - 1 \). So, we have that for \( n - 1 \geq 9 \),
\[
LEE(G_i) = e^\mu_1 + e^\mu_2 + e^\mu_3 + e^\mu_4 + e^\mu_5 + e^\mu_6 + e^\mu_7 + (n - 8)e^1 + e^0
\leq e^{n-1} + e^0 + 5e^0 + (n - 8)e^1 + e^0
< e^n + e^3 + 5e^1 + (n - 8)e^1 + e^0
= LEE(S'_n)
\]
and for \( n - 1 \leq 9 \),
\[
LEE(G_i) \leq e^{n-1} + e^{n-1} + e^{10-n} + 4e^0 + (n - 8)e^1 + e^0
< e^n + e^3 + e^1 + 4e^1 + (n - 8)e^1 + e^0
= LEE(S'_n)
\]
Similarly, we can prove the result for the cases \( n_1 + n_2 = n - 4 \) and \( n_1 + n_2 = n - 5 \), and then complete the proof.

![Figure 5 Graphs G10, G11 and G12.](image)

**Lemma 5** Let \( G \) be the unicyclic graph with \( n \geq 9 \) vertices and \( s(G) = n \). Then \( LEE(G) \leq LEE(S'_n) \) with equality if and only if \( G \cong S'_n \).

**Proof.** Since \( s(G) = n \), \( G \) is a type of graphs in Fig.5. By direct computation we can obtain that the Laplacian characteristic polynomials of \( G_{10}, G_{11} \) and \( G_{12} \) are respectively
\[
L_{G_{10}}(x) = x(x - 1)^{n-5}[x^4 - (n + 5)x^3 + (n_1n_2 + 6n + 4)x^2 - (3n_1n_2 + 10n - 4)x + 4n]
L_{G_{11}}(x) = x(x - 1)^{n-4}[x^3 - (n + 2)x^2 + (n + 1 + n_1n_2 + 2n_1)x - n]
L_{G_{12}}(x) = x(x - 1)^{n-5}[x^4 - (n + 5)x^3 + (5n + n_1n_2 + 7)x^2 - (7n + 2n_1n_2 + 3)x + 3n].
\]
Then we can obtain that \( G_{10} \) has Laplacian eigenvalues 1 with multiplicity \( n - 5 \), 0 with multiplicity 1, and the largest Laplacian eigenvalue less than \( n - 1 \). By a similar proof of Lemma 4, it follows that \( LEE(G_{10}) < LEE(S'_n) \). Similarly, we also can prove that \( LEE(G_{11}) < LEE(S'_n) \) for \( n_1 \geq 1, n_2 \geq 0 \), and \( LEE(G_{12}) < LEE(S'_n) \) for \( n_1, n_2 \geq 1 \) and \( n \geq 9 \). If \( n_1 = 0 \), then \( G_{12} \cong S'_n \). Thus we complete the proof. \( \square \)
By Lemmas 3, 4 and 5 it follows

**Theorem 1** Let $G$ be a connected graph with $n$ vertices and $n$ edges, where $n \geq 9$. Then

$$\text{Lee}(G) \leq e^n + e^3 + (n - 3)e + 1$$

with equality if and only if $G \cong S_n^3$.

**References**


