On the first two largest distance Laplacian eigenvalues of unicyclic graphs

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Abstract

The distance Laplacian eigenvalues of a connected graph $G$ are the eigenvalues of its distance Laplacian matrix $L(G)$, defined as $L(G) = \text{Tr}(G) - D(G)$, where $\text{Tr}(G)$ is the diagonal matrix of vertex transmissions of $G$, and $D(G)$ is the distance matrix of $G$. In this paper, we determine the unique unicyclic graphs with maximum largest distance Laplacian eigenvalue and minimum second largest distance Laplacian eigenvalue, respectively.

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1 Introduction

We consider simple and undirected graphs. Let $G$ be a connected graph of order $n$ with vertex set $V(G)$ and edge set $E(G)$.

The distance matrix of $G$ is the $n \times n$ matrix $D(G) = (d_G(u, v))_{u, v \in V(G)}$, where $d_G(u, v)$ denotes the distance between vertices $u$ and $v$ in $G$, i.e., the length of a shortest path from $u$ to $v$ in $G$. The spectrum of a distance matrix, arisen from a data communication problem studied by Graham and Pollack [5] in 1971, has been studied extensively, see the recent survey [2].

For $u \in V(G)$, the transmission of $u$ in $G$, denoted by $\text{Tr}_G(u)$, is defined as the sum of distances from $u$ to all other vertices of $G$, i.e., the row sum of $D(G)$ indexed by vertex $u$. Let $\text{Tr}(G)$ be the diagonal matrix of vertex transmissions of $G$.

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The distance Laplacian matrix of $G$ is defined as $L(G) = \text{Tr}(G) - D(G)$, see [1]. The distance Laplacian eigenvalues of $G$ are the eigenvalues of $L(G)$, denoted by $\lambda_1(G), \ldots, \lambda_n(G)$, arranged in the nonincreasing order, where $n = |V(G)|$. Note that $L(G)$ is positive semidefinite and $\lambda_n(G) = 0$. The largest distance Laplacian eigenvalue of $G$ (i.e., $\lambda_1(G)$) is known as the distance Laplacian spectral radius of $G$.

Aouchiche and Hansen [3] showed that the star is the unique tree with minimum distance Laplacian spectral radius. More results on distance Laplacian spectral radius may be found in [3, 8, 9, 11]. Tian et al. [14] studied lower bounds for $\lambda_1(G)$ and $\lambda_2(G)$. Aouchiche and Hansen [1] showed that the distance Laplacian eigenvalues do not increase when an edge is added, and $\lambda_{n-1}(G) \geq n$ for $n \geq 3$ with equality if and only if the complement of $G$ is disconnected. Nath and Paul [10] characterized the (connected) graphs $G$ of order $n \geq 5$ whose complements are trees or unicyclic graphs having $\lambda_{n-1}(G) = n + 1$.

In [3], Aouchiche and Hansen proposed several conjectures on $\lambda_1(G)$ and $\lambda_2(G)$, and some were settled in [7, 9, 12, 13, 14]. For unicyclic graphs, they also proposed the following two conjectures about the first two largest distance Laplacian eigenvalues ($\lambda_1(G)$ and $\lambda_2(G)$).

**Conjecture 1.1.** If $G$ is a unicyclic graph of order $n \geq 4$, then $\lambda_1(G) \leq \lambda_1(K_{n,3})$ with equality if and only if $G \cong K_{n,3}$, where $K_{n,3}$ is the graph obtained by adding an edge between a vertex of a triangle and a terminal vertex of a path on $n - 3$ vertices (see Fig. 1).

**Conjecture 1.2.** If $G$ is a unicyclic graph of order $n \geq 6$, then $\lambda_2(G) \geq \lambda_2(S^+_n)$ with equality if and only if $G \cong S^+_n$, where $S^+_n$ is the graph obtained by adding an edge to the star $S_n$ of order $n$.

The remainder of this paper is organized as follows. Section 2 introduces several basic concepts and notations, and some lemmas are also been presented there. In Section 3, we show that $K_{n,3}$ is the unique unicyclic graph of order $n \geq 4$ with maximum largest distance Laplacian eigenvalue, and thus Conjecture 1.1 follows. Section 4 establishes properties of the second largest distance Laplacian eigenvalues of unicyclic graphs with some particular structures. Finally, in Section 5, by considering Conjecture 1.2, we show that $S^+_n$ is the unique unicyclic graph of order $n \geq 7$ with minimum second largest distance Laplacian eigenvalue, but for $n = 6$, besides $S^+_n$, the graph obtained by attaching a pendant vertex to a vertex of a pentagon is also a unicyclic graph with minimum second largest distance Laplacian eigenvalue.

## 2 Preliminaries

Let $G$ be a connected graph with $V(G) = \{v_1, \ldots, v_n\}$. A column vector $x = (x_{v_1}, \ldots, x_{v_n})^\top \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex $v_i$ to $x_{v_i}$, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \ldots, n$. Then

$$x^\top L(G)x = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)(x_u - x_v)^2.$$
In particular, if \( x \) is a unit eigenvector corresponding to \( \lambda_1(G) \), then we have the following eigenequation of \( G \) at \( u \) for each \( u \in V(G) \):

\[
(\lambda_1(G) - Tr_G(u))x_u = - \sum_{v \in V(G)} d_G(u, v)x_v,
\]

or equivalently,

\[
\lambda_1(G)x_u = \sum_{v \in V(G)} d_G(u, v)(x_u - x_v).
\]

For a unit column vector \( x \in \mathbb{R}^n \), by Rayleigh’s principle, we have \( \lambda_1(G) \geq x^\top\mathcal{L}(G)x \) with equality if and only if \( x \) is a unit eigenvector of \( \mathcal{L}(G) \) corresponding to \( \lambda_1(G) \). From this or the interlacing theorem [6, pp. 185–186], we immediately have the following result.

**Lemma 2.1.** Let \( G \) be a connected graph and \( Tr_{\text{max}}(G) \) be the maximum vertex transmission of \( G \). Then \( \lambda_1(G) \geq Tr_{\text{max}}(G) \).

Note that \( 1_n = (1, \ldots, 1)^\top \) is an eigenvector of \( \mathcal{L}(G) \) corresponding to \( \lambda_n(G) = 0 \).

For \( n \geq 2 \), if \( x \) is an eigenvector of \( \mathcal{L}(G) \) corresponding to \( \lambda_1(G) \), then \( x^\top 1_n = 0 \).

Let \( G \) be a graph. For \( u \in V(G) \), let \( N_G(v) \) be the set of neighbors of \( v \) in \( G \), and \( \delta_G(v) \) the degree of \( v \) in \( G \). For \( U \subseteq V(G) \), let \( G[U] \) be the subgraph of \( G \) induced by \( U \). For a subset \( E_1 \) of \( E(G) \), \( G - E_1 \) denotes the graph obtained from \( G \) by deleting all the edges in \( E_1 \), and in particular, we write \( G - xy \) instead of \( G - \{xy\} \) if \( E_1 = \{xy\} \). For a subset \( E_2 \) of \( E(\overline{G}) \), where \( \overline{G} \) is the complement of \( G \), \( G + E_2 \) denotes the graph obtained from \( G \) by adding all edges in \( E_2 \), and in particular, we write \( G + xy \) instead of \( G + \{xy\} \) if \( E_2 = \{xy\} \).

**Lemma 2.2.** [1] Let \( G \) be a connected graph with \( u, v \in V(G) \). If \( u \) and \( v \) are non-adjacent in \( G \), then \( \lambda_1(G + uv) \leq \lambda_1(G) \).

A path \( u_1 \ldots u_r \) (with \( r \geq 2 \)) in a graph \( G \) is called a pendant path (of length \( r - 1 \)) at \( u_1 \) if \( \delta_G(u_1) \geq 3 \), the degrees of \( u_2, \ldots, u_{r-1} \) (if exist) are all equal to 2 in \( G \), and \( \delta_G(u_r) = 1 \). If \( P \) is a pendant path of \( G \) at \( u \) with length \( r \geq 1 \), we say \( G \) is obtained from \( H \) by attaching a pendant path \( P \) of length \( r \) at \( u \), where \( H = G[V(G) \setminus (V(P) \setminus \{u\})] \).

In particular, if the pendant path of length 1 is attached to a vertex \( u \) of \( H \), then we also say that a pendant vertex is attached to \( u \).

For a nontrivial connected graph \( G \) with \( u \in V(G) \), and positive integers \( k \) and \( l \), let \( G_u(k, l) \) be the graph obtained from \( G \) by attaching two pendant paths of lengths \( k \) and \( l \), respectively, at \( u \), and in particular, let \( G_u(k, 0) \) be the graph obtained from \( G \) by attaching a pendant path of length \( k \) at \( u \).

**Lemma 2.3.** [9] Let \( G \) be a nontrivial connected graph with \( u \in V(G) \). For \( k \geq l \geq 1 \), \( \lambda_1(G_u(k, l)) < \lambda_1(G_u(k + 1, l - 1)) \).

For a connected graph \( G \) with \( u, v \in V(G) \), and positive integers \( k \) and \( l \), where \( \delta_G(u), \delta_G(v) \geq 2 \), let \( G_{u,v}(k, l) \) be the graph obtained from \( G \) by attaching a pendant path of length \( k \) at \( u \), and a pendant path of length \( l \) at \( v \), and in particular, let \( G_{u,v}(k, 0) \) be the graph obtained from \( G \) by attaching a pendant path of length \( k \) at \( u \).
Lemma 2.4. [9] Let $G$ be a connected graph with $uv \in E(G)$. If $N_{G-uv}(u) = N_{G-uv}(v) \neq \emptyset$ and $k \geq l \geq 1$, then $\lambda_1(G_{u,v}(k,l)) < \lambda_1(G_{u,v}(k+1,l-1))$.

For an $n \times n$ real symmetric matrix $M$, let $\lambda_1(M)$ and $\lambda_2(M)$ be the largest and the second largest eigenvalues of $M$, respectively. From interlacing theorem [6, pp. 185–186], we have the following lemma.

Lemma 2.5. Let $N$ be an $n \times n$ real symmetric matrix, and $M$ a principal submatrix of $N$ with order $m$ with $2 \leq m \leq n$. Then $\lambda_2(N) \geq \lambda_2(M)$.

Lemma 2.6. [1] Let $G$ be a connected graph with an independent set $S$ such that $N_G(u) = N_G(v)$ for any $u, v \in S$. Then for $u \in S$, $\text{Tr}_G(u) + 2$ is a distance Laplacian eigenvalue of $G$ with multiplicity at least $|S| - 1$.

For a connected graph $G$ with $u, v \in V(G)$, let $\mathcal{L}(G)[u, v]$ be the principal submatrix of $\mathcal{L}(G)$ indexed by $u$ and $v$.

Let $P_n$ and $C_n$ be the path and the cycle on $n$ vertices, respectively.

## 3 Maximum largest distance Laplacian eigenvalue of unicyclic graphs

Let $G_n$ be the graph as shown in Fig. 1.

![Graphs G_n and Ki_{n,3}](image)

Fig. 1: The graphs $G_n$ and $Ki_{n,3}$ in Lemma 3.1.

Lemma 3.1. For $n \geq 6$, $\lambda_1(G_n) < \lambda_1(Ki_{n,3})$.

Proof. If $n = 6, \ldots, 16$, then the results follow from Table 1.

In what following, we suppose that $n \geq 17$.

Let $x$ be a unit eigenvector of $\mathcal{L}(G_n)$ corresponding to $\lambda_1(G_n)$. By direct calculation, we have $\text{Tr}_{G_n}(v_1) = \frac{n^2-n-4}{2}$, $\text{Tr}_{G_n}(v_{n-2}) = \frac{n^2-5n+12}{2}$, $\text{Tr}_{G_n}(v_{n-1}) = \frac{n^2-3n+8}{2}$ and $\text{Tr}_{G_n}(v_n) = \frac{n^2-5n+16}{2}$.

From the label of vertices in $G_n$ and $Ki_{n,3}$ in Fig. 1, note that $Ki_{n,3} = G_n - \{v_{n-3}v_n\} + \{v_{n-2}v_n, v_{n-1}v_n\}$. As we pass from $G_n$ to $Ki_{n,3}$, the distance between $v_n$ and $v_i$ with $1 \leq i \leq n - 3$ is increased by 1, the distance between $v_n$ and $v_{n-2}$ is decreased by 1, the distance between $v_n$ and $v_{n-1}$ is decreased by 2, and the distance between any other vertex pair remains unchanged. Note that $\sum_{i=1}^{n} x_{v_i} = 0$ and $\sum_{i=1}^{n} x_{v_i}^2 = 1$. Then

$$\lambda_1(Ki_{n,3}) - \lambda_1(G_n)$$
First, by Eqs. (3.2) and (3.3),

\[
\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) x_{v_{n-2}} = -2x_{v_{n-2}} - \sum_{i=1}^{n-3} d_{G_n}(v_{n-2}, v_i) x_{v_i},
\]

(3.2)

\[
\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) x_{v_{n-1}} = -3x_{v_{n-1}} - \sum_{i=1}^{n-3} (d_{G_n}(v_{n-2}, v_i) + 1) x_{v_i},
\]

(3.3)

\[
\lambda_1(G_n) - Tr_{G_n}(v_n) x_{v_n} = -2x_{v_{n-2}} - 3x_{v_{n-1}} - \sum_{i=1}^{n-3} d_{G_n}(v_{n-2}, v_i) x_{v_i}.
\]

(3.4)

From the eigenequations of \(G_n\) at \(v_{n-2}, v_{n-1}\) and \(v_n\), we have

\[
\sum_{i=1}^{n-3} (x_{v_i} - x_{v_{n-1}})^2 - (x_{v_n} - x_{v_{n-2}})^2 - 2(x_{v_n} - x_{v_{n-1}})^2
\]

\[
= \sum_{i=1}^{n-3} (x_{v_i}^2 - 2x_{v_i} x_{v_{n-1}} + x_{v_{n-1}}^2) - (x_{v_n}^2 - 2x_{v_n} x_{v_{n-2}} + x_{v_{n-2}}^2) - 2(x_{v_n}^2 - 2x_{v_n} x_{v_{n-1}} + x_{v_{n-1}}^2)
\]

\[
= (n - 6) x_{v_n}^2 + \sum_{i=1}^{n-3} x_{v_i} + 2x_{v_n} \left(- \sum_{i=1}^{n-3} x_{v_i} + x_{v_{n-2}} + 2x_{v_{n-1}}\right) - x_{v_{n-2}}^2 - 2x_{v_{n-1}}^2
\]

\[
= (n - 6) x_{v_n}^2 + 1 - \sum_{i=2}^{n} x_{v_i} + 2x_{v_n} \left( \sum_{i=2}^{n} x_{v_i} + x_{v_{n-2}} + 2x_{v_{n-1}}\right) - x_{v_{n-2}}^2 - 2x_{v_{n-1}}^2
\]

\[
= (n - 5) x_{v_n}^2 + 1 + 2x_{v_n} \left( 2x_{v_{n-2}} + 3x_{v_{n-1}}\right) - 2x_{v_{n-2}}^2 - 3x_{v_{n-1}}^2.
\]

(3.1)
\[
(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))x_{v_{n-2}} = (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2)x_{v_{n-1}}.
\]  
(3.5)

From Lemma 2.1, we have
\[
\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) \geq Tr_{\max}(G_n) - Tr_{G_n}(v_{n-2})
\]
\[
\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_{n-2})
\]
\[
= 2n - 8
\]
\[
> 4
\]

and
\[
\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2 \geq Tr_{\max}(G_n) - Tr_{G_n}(v_{n-1}) - 2
\]
\[
\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_{n-1}) - 2
\]
\[
= n - 8
\]
\[
> 4.
\]

So \(x_{v_{n-2}}\) and \(x_{v_{n-1}}\) possess the same sign from Eq. (3.5).

Without loss of generality, we suppose that \(x_{v_{n-2}} \geq x_{v_{n-1}}\).

On the other hand, by Eqs. (3.3) and (3.4),
\[
\begin{align*}
(\lambda_1(G_n) - Tr_{G_n}(v_n))x_v &= (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}))x_{v_{n-1}} - 3x_{v_{n-1}} + 3x_v - 3x_{v_{n-1}} - x_{v_{n-2}} \\
&= (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}))x_{v_{n-1}} - 2x_{v_{n-1}} + 3x_v - 3x_{v_{n-1}} - x_{v_{n-2}} \\
&= 2x_v - 4x_{v_{n-1}} - 2x_{v_{n-2}},
\end{align*}
\]
i.e.,
\[
(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_v - (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 4)x_{v_{n-1}} = -2x_{v_{n-2}} \geq -2x_{v_{n-1}},
\]
which implies that
\[
(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_v \geq (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 6)x_{v_{n-1}} \geq 0.
\]

From Lemma 2.1, we have
\[
\begin{align*}
\lambda_1(G_n) - Tr_{G_n}(v_n) - 2 &\geq Tr_{\max}(G_n) - Tr_{G_n}(v_n) - 2 \\
&\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_n) - 2 \\
&= 2n - 12 \\
&> 0.
\end{align*}
\]
Thus $x_{v_n} \geq 0$.
Furthermore, by Eqs. (3.2) and (3.4),
\[
(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))x_{v_{n-2}} - (\lambda_1(G_n) - Tr_{G_n}(v_n))x_{v_n} = 2x_{v_{n-2}} + 2x_{v_{n-1}} - 2x_{v_n},
\]
i.e.,
\[
(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) - 4)x_{v_{n-2}} - (\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_{v_n} = 2(x_{v_{n-1}} - x_{v_{n-2}}).
\]
(3.6)
Noting that $Tr_{G_n}(v_{n-2}) + 4 = Tr_{G_n}(v_n) + 2$, by Eq. (3.6), we have
\[
(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) - 4)(x_{v_{n-2}} - x_{v_n}) = 2(x_{v_{n-1}} - x_{v_{n-2}}) \geq 0,
\]
which implies that $x_{v_{n-2}} \geq x_{v_n}$.
In conclusion, we get $x_{v_{n-1}} \geq x_{v_{n-2}} \geq x_{v_n} \geq 0$.
Now by (3.1), we have
\[
\lambda_1(K_{i_n,3}) - \lambda_1(G_n) \geq (n - 5)x_{v_n}^2 + 1 + 2x_{v_n}(2x_{v_{n-2}} + 3x_{v_{n-1}}) - 2x_{v_{n-2}}^2 - 3x_{v_{n-1}}^2
\]
\[
\geq (n - 5)x_{v_n}^2 + 1 + 2x_{v_n}(2x_{v_{n-2}} + 3x_{v_{n-1}}) - 2x_{v_{n-2}}^2 - 3x_{v_{n-1}}^2
\]
\[
\geq (n + 5)x_{v_n}^2 + 1 - 5x_{v_{n-1}}^2
\]
\[
\geq 22x_{v_n}^2 + 1 - 5x_{v_{n-1}}^2.
\]
(3.7)
Let
\[
f(t) = 2(t - Tr_{G_n}(v_{n-2}) - 2)(t - Tr_{G_n}(v_{n-1}) - 2) - 4(t - Tr_{G_n}(v_n - 2))
\]
\[
- (t - Tr_{G_n}(v_n) - 2)(t - Tr_{G_n}(v_{n-2}))
\]
\[
= 2\left( t - \frac{n^2 - 5n + 16}{2} \right)\left( t - \frac{n^2 - 3n + 12}{2} \right) - 4\left( t - \frac{n^2 - 5n + 12}{2} \right)
\]
\[
- \left( t - \frac{n^2 - 5n + 20}{2} \right)\left( t - \frac{n^2 - 5n + 12}{2} \right)
\]
\[
= t^2 - (n^2 - 3n + 16)t + \frac{n^4 - 6n^3 + 37n^2 - 96n + 240}{4}.
\]
It is easily verified that $\frac{n^2 - 3n + 16 \pm \sqrt{\frac{n^2 + 1}{2}}}{2}$ are the two roots of $f(t) = 0$.
By interlacing theorem,
\[
\lambda_1(G_n) \geq \lambda_1(\mathcal{L}(G_n)[v_1, v_{n-1}]) = \frac{n^2 - 2n + 2 + \sqrt{5n^2 - 28n + 52}}{2}
\]
\[
> \frac{n^2 - 3n + 16 + 2\sqrt{n^2 + 4}}{2}
\]
for $n \geq 17$, which implies that $f(\lambda_1(G_n)) > 0$, equivalently,
\[
\frac{2(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) - 2)(\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2) - 4(\lambda_1(G_n) - Tr_{G_n}(v_n - 2))}{(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))} > 1
\]
for $n \geq 17$. 

Together with Eqs. (3.5) and (3.6), we may deduce

\[
2x_{v_n} = \frac{2(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) - 2)(\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2) - 4(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))}{(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))} x_{v_{n-1}} \geq x_{v_{n-1}}.
\]

Finally, from (3.7), we conclude that

\[
\lambda_1(K_{i,n,3}) - \lambda_1(G_n) \geq 22x_{v_n} + 1 - 5x_{v_{n-1}} \geq 2x_{v_n} + 1 > 0,
\]

implying that \(\lambda_1(K_{i,n,3}) > \lambda_1(G_n)\), as desired. □

**Theorem 3.1.** Let \(G\) be a unicyclic graph of order \(n \geq 3\). Then \(\lambda_1(G) \leq \lambda_1(K_{i,n,3})\) with equality if and only if \(G \cong K_{i,n,3}\).

**Proof.** It is trivial when \(n = 3\). Suppose that \(n \geq 4\). Let \(G\) be a unicyclic graph of order \(n\) with maximum distance Laplacian spectral radius. Let \(l\) be the length of the unique cycle in \(G\).

Suppose that \(G \cong C_n\). From [1], we have

\[
\lambda_1(C_n) = \begin{cases} 
\frac{n^2}{4} + \csc^2 \frac{\pi}{n} & \text{if } n \text{ is even}, \\
\frac{n^2 - 1}{4} + \frac{1}{4} \csc^2 \frac{\pi}{2n} & \text{if } n \text{ is odd}.
\end{cases}
\]

If \(n = 4, 5\), then by direct calculation,

\[
\lambda_1(C_4) = 6 < 7 \approx \lambda_1(K_{i,4,3}), \quad \lambda_1(C_5) \approx 8.6180 < 12.2361 \approx \lambda_1(K_{i,5,3}).
\]

Suppose that \(n \geq 6\). Let \(w_1\) and \(w_2\) be, respectively, the pendant vertex and a vertex of degree 2 on the triangle in \(K_{i,n,3}\). Note that \(Tr_{K_{i,n,3}}(w_1) = \frac{n^2 - n - 2}{2}\) and \(Tr_{K_{i,n,3}}(w_2) = \frac{n^2 - 3n + 4}{2}\). Let \(M\) be the principal submatrix of \(L(K_{i,n,3})\) indexed by \(w_1\) and \(w_2\). By interlacing theorem,

\[
\lambda_1(K_{i,n,3}) \geq \lambda_1(M) = \frac{n^2 - 2n + 1 + \sqrt{(n - 3)^2 + 4(n - 2)^2}}{2}.
\]

It is easily verified that \(\frac{2n^2}{\pi^2} > \csc^2 \frac{\pi}{n}\) and \(\frac{2n^2}{\pi^2} > \frac{1}{4} \csc^2 \frac{\pi}{2n}\). Then

\[
\lambda_1(K_{i,n,3}) \geq \frac{n^2 - 2n + 1 + \sqrt{(n - 3)^2 + 4(n - 2)^2}}{2} > \frac{n^2}{4} + \frac{2n^2}{\pi^2} > \lambda_1(C_n),
\]

which is a contradiction to the maximality of \(\lambda_1(G) = \lambda_1(C_n)\). Thus \(3 \leq l \leq n - 1\).

Suppose that \(l \geq 5\). Assume that \(w_1\) is a vertex of degree at least 3 lying on the unique cycle in \(G\). Let \(uv\) be the edge on the cycle in \(G\) such that \(d_G(u, w_1), d_G(v, w_1) \geq 2\). Let \(G' = G - uv\). By Lemmas 2.2, 2.3 and 3.1, we have

\[
\lambda_1(G) \leq \lambda_1(G') \leq \lambda_1(G_n) < \lambda_1(K_{i,n,3}),
\]

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which is a contradiction to the maximality of $\lambda_1(G)$. Thus $l = 3, 4$.

Suppose that $l = 4$. By Lemma 2.3, $G \cong C_n(l_1, l_2, l_3, l_4)$, where $C_n(l_1, l_2, l_3, l_4)$ is the graph obtained from a quadrangle $C_4 = w_1w_2w_3w_4w_1$ by attaching a pendant path of length $l_i$ at $w_i$, $l_1 + l_2 + l_3 + l_4 + 4 = n$ and $l_i \geq 0$ for $1 \leq i \leq 4$. Suppose without loss of generality that $l_1 = \max\{l_i : 1 \leq i \leq 4\}$ and $l_2 \geq l_4$. Suppose that $l_1 \geq 2$. Let $G' = G - w_2w_3$. By Lemmas 2.2, 2.3 and 3.1, we have

\[ \lambda_1(G) \leq \lambda_1(G') \leq \lambda_1(G_n) < \lambda_1(K_{i_{n,3}}), \]

which is a contradiction to the maximality of $\lambda_1(G)$. Suppose that $l_1 = 1$. If $l_2 = 1$, then as above, we may deduce that $\lambda_1(G) < \lambda_1(K_{i_{n,3}})$, which is a contradiction again. If $l_2 = 0$, then also $l_4 = 0$, and thus $G \cong C_5(1, 0, 0, 0)$ or $C_6(1, 0, 1, 0)$. By direct calculation,

\[ \lambda_1(G) = \lambda_1(C_5(1, 0, 0, 0)) \approx 10.8951 < 12.2361 \approx \lambda_1(K_{i_{5,3}}) \]

and

\[ \lambda_1(G) = \lambda_1(C_6(1, 0, 1, 0)) \approx 16.6056 < 18.7130 \approx \lambda_1(K_{i_{6,3}}), \]

also a contradiction.

Thus $l = 3$. By Lemmas 2.3 and 2.4, $G \cong K_{i_{n,3}}$, as desired. \qed

We remark that Bapat et al. [4] gave an independent and different proof for the above theorem very recently.

4 Second largest distance Laplacian eigenvalues of unicyclic graphs with particular structures

The eccentricity of $u$ in $G$ is defined to be the largest distance from $u$ to other vertex. Denote by $d(G)$ or $d$ the diameter of $G$. Recall that the diameter of $G$ is actually the largest eccentricity among all vertices of $G$.

**Lemma 4.1.** Let $G$ be a unicyclic graph of order $n \geq 7$ and $G \not\cong S_n^+$. If there are at least three pendant vertices of $G$ sharing a common neighbor, then $\lambda_2(G) > 2n - 1$.

**Proof.** Since there are at least three pendant vertices of $G$ sharing a common neighbor, we may assume that $v$ is a vertex among such pendant vertices. Denote by $s$ the eccentricity of $v$ in $G$. Clearly, $s \geq 3$ because $G \not\cong S_n^+$.

First by Lemma 2.6, we know that $Tr_G(v) + 2$ is a distance Laplacian eigenvalue of $G$ with multiplicity at least 2, which implies that $\lambda_2(G) \geq Tr_G(v) + 2$. On the other hand, it is easily seen that

\[
Tr_G(v) \geq (1 + 2 + \cdots + s) + 2(n - s - 1) \\
= 2n + \frac{s^2}{2} - \frac{3}{2}s - 2 \\
\geq 2n + \frac{3^2}{2} - \frac{3}{2} \cdot 3 - 2 \\
= 2n - 2.
\]

Now it follows that

\[ \lambda_2(G) \geq Tr_G(v) + 2 \geq 2n > 2n - 1, \]

as desired. \qed
Lemma 4.2. Let $G$ be a unicyclic graph of order $n \geq 8$, where $u$ is a pendant vertex of $G$ with unique neighbor $v$. Suppose that the eccentricity of $u$ in $G$ is $s \geq 6$. If $\delta_G(v) = 2, 3$ or $4$, then $\lambda_2(G) > 2n - 1$.

Proof. First suppose that $\delta_G(v) = 2$. By Lemma 2.5, we have

$$\lambda_2(G) \geq \lambda_2(L(G)[u,v]) > Tr_G(v) - 1.$$  

On the other hand, it is easily seen that

$$Tr_G(v) \geq (1 + 1 + 2 + \cdots + s - 1) + 2(n - s - 1)$$
$$= 2n + \frac{s^2}{2} - \frac{5}{2} s - 1$$
$$\geq 2n + \frac{6^2}{2} - \frac{5}{2} \cdot 6 - 1$$
$$= 2n + 2.$$  

Then we get

$$\lambda_2(G) > Tr_G(v) - 1 \geq 2n + 1 > 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$.

If $\delta_G(v) = 3$, then similarly we have $Tr_G(v) \geq 2n + 1$, and thus

$$\lambda_2(G) > Tr_G(v) - 1 \geq 2n > 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$.

If $\delta_G(v) = 4$, then similarly we have $Tr_G(v) \geq 2n$, and thus

$$\lambda_2(G) > Tr_G(v) - 1 \geq 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$.

Lemma 4.3. Let $G$ be a unicyclic graph of order $n \geq 7$, where $d = 5$, and $u$ is a pendant vertex of $G$ with unique neighbor $v$. Suppose that $\delta_G(v) = 3$, and there is a diametrical path $P$ of $G$ such that $u$ is an end vertex of $P$. If there are at least two vertices, say $x, y$, in $G$ outside $P$ such that $d_G(v, x) = d_G(v, y) = 3$, or there is at least one vertex, say $z$, in $G$ outside $P$ such that $d_G(v, z) = 4$, then $\lambda_2(G) > 2n - 1$.

Proof. Similar to the proof of Lemma 4.2, if there are at least two vertices, say $x, y$, in $G$ outside $P$ such that $d_G(v, x) = d_G(v, y) = 3$, then we have

$$Tr_G(v) \geq (1 + 1 + 2 + 3 + 4) + 1 + 2 \cdot 3 + 2(n - 9) = 2n,$$

and if there is at least one vertex, say $z$, in $G$ outside $P$, such that $d_G(v, z) = 4$, then we have

$$Tr_G(v) \geq (1 + 1 + 2 + 3 + 4) + 1 + 4 + 2(n - 8) = 2n.$$  

Now it follows that

$$\lambda_2(G) \geq \lambda_2(L(G)[u,v]) > Tr_G(v) - 1 \geq 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$, as desired. \qed
If $u$ is a pendant vertex of $G$ whose unique neighbor $v$ is of degree 2, and $w$ is the unique neighbor of $v$ in $G$ different from $u$, then the local structure of $G$ induced by vertices $u, v, w$ is said to be a pendant $P_3$ of $G$.

If two pendant vertices $x$ and $y$ possess a common neighbor $z$ in $G$, then the local structure of $G$ induced by vertices $x, y, z$ is said to be an outer $P_3$ of $G$.

If $G$ is a unicyclic graph of maximum degree 3 obtainable by attaching some pendant vertices to some vertices of a cycle, then $G$ is said to be a sun graph.

For a unicyclic graph $G$, it is easily seen that if $G$ contains neither pendant nor outer $P_3$, then $G$ would be either a cycle or a sun graph.

4.1 Unicyclic graphs with pendant $P_3$

First, we focus on the unicyclic graphs with pendant $P_3$.

**Lemma 4.4.** Let $G$ be a unicyclic graph of order $n \geq 7$. If there are at least two pendant $P_3$’s of $G$ attached to the same vertex, then $\lambda_2(G) > 2n - 1$.

**Proof.** Denote by $u$ and $v$ the two pendant vertices in such two pendant $P_3$’s in $G$.

By Lemma 2.5, we know that

$$\lambda_2(G) \geq \lambda_2(\mathcal{L}(G)[u, v]) = Tr_G(v) - 4.$$

On the other hand, it is easily seen that

$$Tr_G(v) \geq (1 + 2 + 3 + 4) + 3(n - 5) = 3n - 5.$$  

Then

$$\lambda_2(G) \geq Tr_G(v) - 4 \geq 3n - 9 > 2n - 1$$

for $n \geq 9$.

If $n = 7$ or 8, then $G$ is a graph as shown in Fig. 2. For the first two graphs, $\lambda_2(G) > 2n - 1$ follows from direct calculation, and for the remaining three graphs, noting that there is at least one vertex different from $u$ with distance 4 from itself to $v$, we have $Tr_G(v) \geq 3n - 4$, and thus

$$\lambda_2(G) \geq Tr_G(v) - 4 \geq 3n - 8 > 2n - 1$$

for $n = 8$. 

Fig. 2: The graphs in Lemma 4.4 when $n = 7$ or 8.
Lemma 4.5. Let $G$ be a unicyclic graph of order $n \geq 7$, where $d = 5$. Suppose that there exists pendant $P_3$ in $G$, where $u$ and $v$ are, respectively, the vertices of degrees one and two in such pendant $P_3$. If there is a diametrical path $P$ of $G$ such that $u$ is an end vertex of $P$, and there is at least one vertex, say $w$, in $G$ outside $P$ such that $d_G(v, w) \geq 3$, then $\lambda_2(G) > 2n - 1$.

Proof. First by Lemma 2.5, we have

$$\lambda_2(G) \geq \lambda_2(L(G)[u, v]) > Tr_G(v) - 1.$$ 

On the other hand, it is easily seen that

$$Tr_G(v) \geq (1 + 1 + 2 + 3 + 4) + 3 + 2(n - 7) = 2n.$$ 

Now it follows that

$$\lambda_2(G) \geq \lambda_2(L(G)[u, v]) > Tr_G(v) - 1 \geq 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$, as desired. \hfill \Box

Lemma 4.6. Let $G$ be a unicyclic graph of order $n \geq 8$, where $d = 4$. Suppose that there exists pendant $P_3$ in $G$, where $u$ and $v$ are, respectively, the vertices of degrees one and two in such pendant $P_3$. If there is a diametrical path $P$ of $G$ such that $u$ is an end vertex of $P$, and there are at least three vertices, say $x, y, z$, in $G$ outside $P$ such that $d_G(v, x) = d_G(v, y) = d_G(v, z) = 3$, then $\lambda_2(G) > 2n - 1$.

Proof. Similar to the proof of Lemma 4.5, we have

$$Tr_G(v) \geq (1 + 1 + 2 + 3) + 3 \cdot 3 + 2(n - 8) = 2n,$$

and thus

$$\lambda_2(G) \geq \lambda_2(L(G)[u, v]) > Tr_G(v) - 1 \geq 2n - 1,$$

i.e., $\lambda_2(G) > 2n - 1$, as desired. \hfill \Box

4.2 Unicyclic graphs with outer $P_3$

Next we consider the unicyclic graphs with outer $P_3$.

Lemma 4.7. Let $G$ be a unicyclic graph of order $n \geq 7$. If there are at least two vertex-disjoint outer $P_3$’s in $G$, then $\lambda_2(G) > 2n - 1$.

Proof. Denote by $u$ a pendant vertex of an outer $P_3$ of $G$, and $v$ a pendant vertex of another outer $P_3$ of $G$. Let $s = d_G(u, v)$. Clearly, $s \geq 3$.

By Lemma 2.6, we know that both $Tr_G(u) + 2$ and $Tr_G(v) + 2$ are distance Laplacian eigenvalues of $G$, which implies that

$$\lambda_2(G) \geq \min\{Tr_G(u) + 2, Tr_G(v) + 2\}.$$ 

It is easily seen that

$$Tr_G(u) \geq (1 + 2 + \cdots + s) + 2(n - s - 1)$$
\[
= 2n + \frac{s^2}{2} - \frac{3}{2}s - 2 \\
\geq 2n + \frac{3^2}{2} - \frac{3}{2} \cdot 3 - 2 \\
= 2n - 2.
\]

Similarly, we have \(Tr_G(v) \geq 2n - 2\). Thus we can get that
\[
\lambda_2(G) \geq \min\{Tr_G(u) + 2, Tr_G(v) + 2\} \geq 2n > 2n - 1,
\]
as desired.

**Lemma 4.8.** Let \(G\) be a unicyclic graph of order \(n \geq 7\). Suppose that there exists outer \(P_3\) in \(G\), where \(u\) and \(v\) are the two pendant vertices in such outer \(P_3\). Let \(s\) be the eccentricity of \(u\) in \(G\), where \(s = 4\) or \(5\). Denote by \(w\) the unique neighbor of \(u\) in \(G\). If \(\delta_G(w) = 3\) or \(4\), then \(\lambda_2(G) > 2n - 1\).

**Proof.** First suppose that \(\delta_G(w) = 3\). By Lemma 2.5, we know that
\[
\lambda_2(G) \geq \lambda_2(\mathcal{L}(G)[u,v]) = Tr_G(u) - 2.
\]
On the other hand, it is easily seen that
\[
Tr_G(u) \geq (1 + 2 + \cdots + s) + 2 + 3(n - s - 2) \\
= 3n + \frac{s^2}{2} - \frac{5}{2}s - 4 \\
= \begin{cases} 
3n - 6 & \text{if } s = 4, \\
3n - 4 & \text{if } s = 5.
\end{cases}
\]
Then
\[
\lambda_2(G) \geq Tr_G(u) - 2 \geq 3n - 8 > 2n - 1
\]
for \(s = 4\) and \(n \geq 8\), and
\[
\lambda_2(G) \geq Tr_G(u) - 2 \geq 3n - 6 > 2n - 1
\]
for \(s = 5\) and \(n \geq 7\). In particular, if \(s = 4\) and \(n = 7\), then \(G\) is a graph as shown in Fig. 3, and thus \(\lambda_2(G) > 2n - 1\) follows from direct calculation.

![Fig. 3: The graphs in Lemma 4.8 when \(\delta_G(w) = 3\), \(s = 4\) and \(n = 7\).](image)

The proof for \(\delta_G(w) = 4\) when \(s = 4\) and \(n \geq 9\), or \(s = 5\) and \(n \geq 7\) can be deduced similarly. In particular, if \(s = 4\) and \(n = 7\) or \(8\), then together with Lemmas 4.1 and 4.7, we may assume that \(G\) is a graph as shown in Fig. 4, and thus \(\lambda_2(G) > 2n - 1\) follows from direct calculation.

Now the result follows. \(\square\)
Lemma 4.9. Let $G$ be a unicyclic graph of order $n \geq 7$. Suppose that $d = 4$, or $d = 5$ and there is no pendant $P_3$ in $G$. If there exists outer $P_3$ in $G$, then $\lambda_2(G) > 2n - 1$.

Proof. Denote by $u$ and $v$ the two pendant vertices of an outer $P_3$ of $G$, and $w$ the unique neighbor of $v$ in $G$. Let $s$ be the eccentricity of $u$ in $G$.

First suppose that there exists pendant $P_3$ in $G$. Then $d = 4$ from the hypothesis. Denote by $x$ and $y$, respectively, the vertices of degrees one and two in such pendant $P_3$.

Suppose that $s = 4$. Then we may choose a diametrical path of $G$ such that $u$ is an end vertex of such diametrical path. In this case, together with Lemma 4.1, we only need to consider the cases that $\delta_G(w) = 3$ if $w$ lies outside the unique cycle of $G$, and $\delta_G(w) = 4$ if $w$ lies on the unique cycle of $G$. Now $\lambda_2(G) > 2n - 1$ follows from Lemma 4.8.

Suppose that $s < 4$. Then the unique neighbor of $y$ in $G$ different from $x$ is actually $w$, otherwise $d_G(u, x) \geq 4$, i.e., $s \geq 4$, which is a contradiction. Moreover, by Lemmas 4.1, 4.4, 4.6 and 4.7, we only need to consider when $G$ is a graph as shown in Fig. 5, and thus $\lambda_2(G) > 2n - 1$ follows from direct calculation.

Next suppose that there is no pendant $P_3$ in $G$. By Lemmas 4.1 and 4.7, we only need to consider the cases that $\delta_G(w) = 3$ if $w$ lies outside the unique cycle of $G$, and $\delta_G(w) = 4$ if $w$ lies on the unique cycle of $G$. If $s = 4$ or 5, then $\lambda_2(G) > 2n - 1$ follows from Lemma 4.8. If $s = 3$, then by Lemma 4.7, we only need to consider when $G$ is a graph as shown in Fig. 6, and thus $\lambda_2(G) > 2n - 1$ follows from direct calculation. If $s = 2$, then $G \cong S_n^+$, and $d = 2$, which is a contradiction to the hypothesis that $d = 4$ or 5.

Now the result follows. \qed
5 Minimum second largest distance Laplacian eigenvalue of unicyclic graphs

We are now ready to give the unique unicyclic graphs whose second largest distance Laplacian eigenvalue is minimum.

**Theorem 5.1.** Let $G$ be a unicyclic graph of order $n \geq 6$. Then $\lambda_2(G) \geq 2n - 1$ with equality if and only if $G \cong S^+_6$ or the graph obtained by attaching a pendant vertex to a vertex of a pentagon for $n = 6$, and $G \cong S^+_n$ for $n \geq 7$.

**Proof.** Suppose that $G \cong C_n$. From [1], we have

$$\lambda_2(C_n) = \begin{cases} \frac{n^2}{4} + \csc^2 \frac{\pi}{n} & \text{if } n \text{ is even}, \\ \frac{n^2}{4} + \frac{1}{4} \csc^2 \frac{\pi}{2n} & \text{if } n \text{ is odd}. \end{cases}$$

So it is easily seen that $\lambda_2(C_n) > 2n - 1$.

In the following, suppose that $G \not\cong C_n$. Since $G \not\cong C_n$, we may choose a diametrical path of $G$, say $P = v_0v_1 \ldots v_d$, such that $v_0$ is a pendant vertex of $G$.

**Case 1.** $d \geq 6$.

If $\delta_G(v_1) \geq 5$, then $\lambda_2(G) > 2n - 1$ follows from Lemma 4.1. If $\delta_G(v_1) = 2, 3$ or $4$, then $\lambda_2(G) > 2n - 1$ follows from Lemma 4.2.

**Case 2.** $d = 5$.

First suppose that there exists no pendant $P_3$ in $G$. By Lemma 4.9, we only need to consider the graphs without outer $P_3$, which implies that $G$ is a sun graph. By Lemma 4.3, we only need to consider the graphs as shown in Fig. 7, and $\lambda_2(G) > 2n - 1$ follows from direct calculation.

![Fig. 7: The graphs in Theorem 5.1 when $d = 5$ without pendant $P_3$.](image)

Next suppose that there exists pendant $P_3$ in $G$. Denote by $u$ and $v$, respectively, the vertices of degrees one and two in such pendant $P_3$ of $G$.

Suppose that the eccentricity of $u$ in $G$ is 5. Then we may choose a diametrical path $Q$ of $G$ such that $u$ is an end vertex of $Q$. By Lemma 4.5, we only need to consider the case that the distance between $v$ and each vertex outside $Q$ in $G$ is exactly 2. It means that the unique cycle of $G$ is of length at most 4. Together with Lemma 4.3, we may assume that $G$ is a graph as shown in Fig. 8, and $\lambda_2(G) > 2n - 1$ follows from direct calculation.

If the eccentricity of $u$ in $G$ is 3 (4, respectively), then it is easily seen that the diameter of $G$ must be 3 (4, respectively), which would lead to a contradiction to the hypothesis that $d = 5$.

**Case 3.** $d = 4$.

By Lemma 4.9, we only need to consider the graphs without outer $P_3$. It implies that either there exists pendant $P_3$ in $G$, or $G$ is a sun graph.
First suppose that there exists no pendant $P_3$ in $G$, i.e., $G$ is a sun graph. Then we only need to consider $G$ is a graph as shown in Fig. 9, and $\lambda_2(G) > 2n - 1$ follows from direct calculation.

Next suppose that there exists pendant $P_3$ in $G$. Denote by $u$ and $v$, respectively, the vertices of degrees one and two in such pendant $P_3$ of $G$.

Suppose that the eccentricity of $u$ in $G$ is 4. Then we may choose a diametrical path $Q$ of $G$ such that $u$ is an end vertex of $Q$. By Lemmas 4.4 and 4.6, we only need to consider the case that $G$ is a graph as shown in Fig. 10, and $\lambda_2(G) > 2n - 1$ follows from direct calculation.

If the eccentricity of $u$ in $G$ is 3, then it is easily seen that the diameter of $G$ must be 3, which is a contradiction to the hypothesis that $d = 4$.

**Case 4.** $d = 3$.

It is easily seen that $G$ is a graph of the form as shown in Fig. 11.

For the first type of graphs in Fig. 11, from Lemmas 4.1 and 4.7, we only need to consider the four possibilities that $(a, b) = (0, 0), (0, 1), (0, 2),$ or $(1, 0)$.

For the second type of graphs in Fig. 11, from Lemmas 4.1 and 4.7, we only need to consider the three possibilities that $(a, b) = (0, 1), (0, 2),$ or $(1, 0)$.

For the third type of graphs in Fig. 11, from Lemmas 4.1 and 4.7, we only need to consider the four possibilities that $(a, b) = (0, 1), (2, 0), (1, 0),$ or $(1, 1)$.

For the fourth type of graphs in Fig. 11, from Lemmas 4.1 and 4.7, we only need to consider the three possibilities that $(a, b, c) = (0, 0, 1), (0, 0, 2),$ or $(0, 1, 0)$.

By direct calculations for the above possible graphs, we have $\lambda_2(G) \geq 2n - 1$ with equality if and only if $n = 6$, and $G$ is the 6-vertex graph obtained by attaching a pendant vertex to a vertex of a pentagon.

**Case 5.** $d = 2$. 

Clearly $G \cong S_n^+$, and $\lambda_2(G) = 2n - 1$.
Combining all the above five cases, the result follows. \hfill \Box

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**References**


