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 $\mathcal{L}(G)$, defined as $\mathcal{L}(G) = Tr(G) - D(G)$, where $Tr(G)$ 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 $Tr_G(u)$, 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 $Tr(G)$ be the diagonal matrix of vertex transmissions of G.

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The distance Laplacian matrix of G is defined as $\mathcal{L}(G) = Tr(G) - D(G)$, see [1]. The distance Laplacian eigenvalues of G are the eigenvalues of $\mathcal{L}(G)$, denoted by $\lambda_1(G), \ldots, \lambda_n(G)$, arranged in the nonincreasing order, where $n = |V(G)|$. Note that $\mathcal{L}(G)$ 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 eigenvelues ($\lambda_1(G)$ and $\lambda_2(G)$).

Conjecture 1.1. *If G is a unicyclic graph of order $n \geq 4$, then $\lambda_1(G) \leq \lambda_1(Ki_{n,3})$ with equality if and only if $G \cong Ki_{n,3}$, where $Ki_{n,3}$ 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 $Ki_{n,3}$ 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

$$x^\top \mathcal{L}(G) x = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)(x_u - x_v)^2.$$

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 $Tr_{\max}(G)$ be the maximum vertex transmission of G. Then $\lambda_1(G) \geq Tr_{\max}(G)$.*

Note that $\mathbf{1}_n = (\underbrace{1,\dots,1}_{n})^\top$ 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 $x^\top \mathbf{1}_n = 0$.

Let G be a graph. For $v \in V(G)$, 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 nonadjacent in G, then $\lambda_1(G + uv) \leq \lambda_1(G)$.*

A path $u_1 \dots u_r$ (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 $u_2, \dots, u_{r-1}$ (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 $N_{G-uv}(u) = N_{G-uv}(v) \neq \varnothing$ 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 $u \in S$, $Tr_G(u) + 2$ 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.

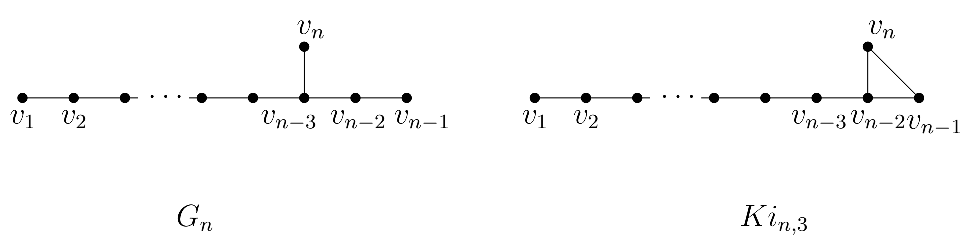

Fig. 1: The graphs G_n and $Ki_{n,3}$ in Lemma 3.1.

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 $Tr_{G_n}(v_1) = \frac{n^2-n-4}{2}$, $Tr_{G_n}(v_{n-2}) = \frac{n^2-5n+12}{2}$, $Tr_{G_n}(v_{n-1}) = \frac{n^2-3n+8}{2}$ and $Tr_{G_n}(v_n) = \frac{n^2-5n+16}{2}$.

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

$$\lambda_1(Ki_{n,3}) - \lambda_1(G_n)$$

Table 1: $\lambda_1(G_n)$ and $\lambda_1(Ki_{n,3})$ for $n = 6, \ldots, 16$.

n	6	7	8	9	10	11
$\lambda_1(G_n)$	17.6056	24.9373	33.6659	43.6796	54.95	67.4664
$\lambda_1(Ki_{n,3})$	18.7130	26.4296	35.3836	45.5731	56.9962	69.6512
n	12	13	14	15	16	
$\lambda_1(G_n)$	81.2235	96.2178	112.4472	129.9099	148.6044	
$\lambda_1(Ki_{n,3})$	83.5368	98.6518	114.9952	132.5661	151.3638	

$$\begin{aligned}
&\geq x^\top(\mathcal{L}(Ki_{n,3}) - \mathcal{L}(G_n))x \\
&= \sum_{i=1}^{n-3}(x_{v_n} - x_{v_i})^2 - (x_{v_n} - x_{v_{n-2}})^2 - 2(x_{v_n} - x_{v_{n-1}})^2 \\
&= \sum_{i=1}^{n-3}(x_{v_n}^2 - 2x_{v_n}x_{v_i} + x_{v_i}^2) - (x_{v_n}^2 - 2x_{v_n}x_{v_{n-2}} + x_{v_{n-2}}^2) - 2(x_{v_n}^2 - 2x_{v_n}x_{v_{n-1}} + x_{v_{n-1}}^2) \\
&= (n-6)x_{v_n}^2 + \sum_{i=1}^{n-3} x_{v_i}^2 + 2x_{v_n}\left(-\sum_{i=1}^{n-3} x_{v_i} + x_{v_{n-2}} + 2x_{v_{n-1}}\right) - x_{v_{n-2}}^2 - 2x_{v_{n-1}}^2 \\
&= (n-6)x_{v_n}^2 + 1 - \sum_{i=n-2}^{n} x_{v_i}^2 + 2x_{v_n}\left(\sum_{i=n-2}^{n} x_{v_i} + x_{v_{n-2}} + 2x_{v_{n-1}}\right) - x_{v_{n-2}}^2 - 2x_{v_{n-1}}^2 \\
&= (n-5)x_{v_n}^2 + 1 + 2x_{v_n}\left(2x_{v_{n-2}} + 3x_{v_{n-1}}\right) - 2x_{v_{n-2}}^2 - 3x_{v_{n-1}}^2. \qquad (3.1)
\end{aligned}$$

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

$$(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))x_{v_{n-2}} = -2x_{v_n} - x_{v_{n-1}} - \sum_{i=1}^{n-3} d_{G_n}(v_{n-2}, v_i)x_{v_i}, \qquad (3.2)$$

$$(\lambda_1(G_n) - Tr_{G_n}(v_{n-1}))x_{v_{n-1}} = -3x_{v_n} - x_{v_{n-2}} - \sum_{i=1}^{n-3}(d_{G_n}(v_{n-2}, v_i) + 1)x_{v_i}, \qquad (3.3)$$

$$(\lambda_1(G_n) - Tr_{G_n}(v_n))x_{v_n} = -2x_{v_{n-2}} - 3x_{v_{n-1}} - \sum_{i=1}^{n-3} d_{G_n}(v_{n-2}, v_i)x_{v_i}. \qquad (3.4)$$

First, by Eqs. (3.2) and (3.3),

$$\begin{aligned}
&(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))x_{v_{n-2}} - (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}))x_{v_{n-1}} \\
&= \sum_{i=1}^{n-3} x_{v_i} + x_{v_n} - x_{v_{n-1}} + x_{v_{n-2}} \\
&= (-x_{v_{n-2}} - x_{v_{n-1}} - x_{v_n}) + x_{v_n} - x_{v_{n-1}} + x_{v_{n-2}}
\end{aligned}$$

$$= \quad -2x_{v_{n-1}},$$

i.e.,

$$(\lambda_1(G_n) - Tr_{G_n}(v_{n-2}))x_{v_{n-2}} = (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2)x_{v_{n-1}}. \tag{3.5}$$

From Lemma 2.1, we have

$$\begin{aligned}
\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) &\geq Tr_{\max}(G_n) - Tr_{G_n}(v_{n-2}) \\
&\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_{n-2}) \\
&= 2n - 8 \\
&> 4
\end{aligned}$$

and

$$\begin{aligned}
\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 2 &\geq Tr_{\max}(G_n) - Tr_{G_n}(v_{n-1}) - 2 \\
&\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_{n-1}) - 2 \\
&= n - 8 \\
&> 4.
\end{aligned}$$

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 $x_{v_{n-2}}$ and $x_{v_{n-1}}$ are both non-negative. Note that

$$Tr_{G_n}(v_{n-2}) < Tr_{G_n}(v_{n-1}) + 2.$$

Then by Eq. (3.5), $x_{v_{n-2}} \leq x_{v_{n-1}}$.

On the other hand, by Eqs. (3.3) and (3.4),

$$\begin{aligned}
&(\lambda_1(G_n) - Tr_{G_n}(v_n))x_{v_n} - (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}))x_{v_{n-1}} \\
= \; &\sum_{i=1}^{n-3} x_{v_i} + 3x_{v_n} - 3x_{v_{n-1}} - x_{v_{n-2}} \\
= \; &(-x_{v_{n-2}} - x_{v_{n-1}} - x_{v_n}) + 3x_{v_n} - 3x_{v_{n-1}} - x_{v_{n-2}} \\
= \; &2x_{v_n} - 4x_{v_{n-1}} - 2x_{v_{n-2}},
\end{aligned}$$

i.e.,

$$(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_{v_n} - (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 4)x_{v_{n-1}} \quad = \quad -2x_{v_{n-2}} \geq -2x_{v_{n-1}},$$

which implies that

$$(\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_{v_n} \geq (\lambda_1(G_n) - Tr_{G_n}(v_{n-1}) - 6)x_{v_{n-1}} \geq 0.$$

From Lemma 2.1, we have

$$\begin{aligned}
\lambda_1(G_n) - Tr_{G_n}(v_n) - 2 &\geq Tr_{\max}(G_n) - Tr_{G_n}(v_n) - 2 \\
&\geq Tr_{G_n}(v_1) - Tr_{G_n}(v_n) - 2 \\
&= 2n - 12 \\
&> 0.
\end{aligned}$$

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.,

$$\begin{aligned} & (\lambda_1(G_n) - Tr_{G_n}(v_{n-2}) - 4)x_{v_{n-2}} - (\lambda_1(G_n) - Tr_{G_n}(v_n) - 2)x_{v_n} \\ = \;& 2(x_{v_{n-1}} - x_{v_{n-2}}). \end{aligned} \tag{3.6}$$

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

$$\begin{aligned} \lambda_1(Ki_{n,3}) - \lambda_1(G_n) \;&\geq\; (n-5)x_{v_n}^2 + 1 + 2x_{v_n}\left(2x_{v_{n-2}} + 3x_{v_{n-1}}\right) - 2x_{v_{n-2}}^2 - 3x_{v_{n-1}}^2 \\ &\geq\; (n-5)x_{v_n}^2 + 1 + 2x_{v_n}\left(2x_{v_n} + 3x_{v_n}\right) - 2x_{v_{n-1}}^2 - 3x_{v_{n-1}}^2 \\ &\geq\; (n+5)x_{v_n}^2 + 1 - 5x_{v_{n-1}}^2 \\ &\geq\; 22x_{v_n}^2 + 1 - 5x_{v_{n-1}}^2. \end{aligned} \tag{3.7}$$

Let

$$\begin{aligned} f(t) \;&=\; 2(t - Tr_{G_n}(v_{n-2}) - 2)(t - Tr_{G_n}(v_{n-1}) - 2) - 4(t - Tr_{G_n}(v_{n-2})) \\ &\quad -(t - Tr_{G_n}(v_n) - 2)(t - Tr_{G_n}(v_{n-2})) \\ &=\; 2\left(t - \frac{n^2-5n+16}{2}\right)\left(t - \frac{n^2-3n+12}{2}\right) - 4\left(t - \frac{n^2-5n+12}{2}\right) \\ &\quad - \left(t - \frac{n^2-5n+20}{2}\right)\left(t - \frac{n^2-5n+12}{2}\right) \\ &=\; t^2 - (n^2-3n+16)t + \frac{n^4-6n^3+37n^2-96n+240}{4}. \end{aligned}$$

It is easily verified that $\frac{n^2-3n+16\pm 2\sqrt{n^2+4}}{2}$ are the two roots of $f(t) = 0$.

By interlacing theorem,

$$\begin{aligned} \lambda_1(G_n) \geq \lambda_1(\mathcal{L}(G_n)[v_1, v_{n-1}]) \;&=\; \frac{n^2-2n+2+\sqrt{5n^2-28n+52}}{2} \\ &>\; \frac{n^2-3n+16+2\sqrt{n^2+4}}{2} \end{aligned}$$

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

$$\begin{aligned}
& 2x_{v_n} \\
= & \frac{2(\lambda_1(G_n)-Tr_{G_n}(v_{n-2})-2)(\lambda_1(G_n)-Tr_{G_n}(v_{n-1})-2)-4(\lambda_1(G_n)-Tr_{G_n}(v_{n-2}))}{(\lambda_1(G_n)-Tr_{G_n}(v_n)-2)(\lambda_1(G_n)-Tr_{G_n}(v_{n-2}))}x_{v_{n-1}} \\
\geq & x_{v_{n-1}}.
\end{aligned}$$

Finally, from (3.7), we conclude that

$$\lambda_1(Ki_{n,3})-\lambda_1(G_n) \geq 22x_{v_n}^2+1-5x_{v_{n-1}}^2 \geq 2x_{v_n}^2+1>0,$$

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

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

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,

$$\lambda_1(C_4)=6<7\approx\lambda_1(Ki_{4,3}),$$

$$\lambda_1(C_5)\approx 8.6180<12.2361\approx\lambda_1(Ki_{5,3}).$$

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 $Ki_{n,3}$. Note that $Tr_{Ki_{n,3}}(w_1)=\frac{n^2-n-2}{2}$ and $Tr_{Ki_{n,3}}(w_2)=\frac{n^2-3n+4}{2}$. Let M be the principal submatrix of $\mathcal{L}(Ki_{n,3})$ indexed by w_1 and w_2. By interlacing theorem,

$$\lambda_1(Ki_{n,3}) \geq \lambda_1(M)=\frac{n^2-2n+1+\sqrt{(n-3)^2+4(n-2)^2}}{2}.$$

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

$$\lambda_1(Ki_{n,3}) \geq \frac{n^2-2n+1+\sqrt{(n-3)^2+4(n-2)^2}}{2}>\frac{n^2}{4}+\frac{2n^2}{\pi^2}>\lambda_1(C_n),$$

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

$$\lambda_1(G) \leq \lambda_1(G') \leq \lambda_1(G_n) < \lambda_1(Ki_{n,3}),$$

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

$$\lambda_1(G) \leq \lambda_1(G') \leq \lambda_1(G_n) < \lambda_1(Ki_{n,3}),$$

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 $\lambda_1(G) < \lambda_1(Ki_{n,3})$, 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,

$$\lambda_1(G) = \lambda_1(C_5(1, 0, 0, 0)) \approx 10.8951 < 12.2361 \approx \lambda_1(Ki_{5,3})$$

and

$$\lambda_1(G) = \lambda_1(C_6(1, 0, 1, 0)) \approx 16.6056 < 18.7130 \approx \lambda_1(Ki_{6,3}),$$

also a contradiction.

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

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 $G \ncong S_n^+$. 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 $G \ncong S_n^+$.

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

$$\begin{aligned} Tr_G(v) &\geq (1 + 2 + \cdots + s) + 2(n - s - 1) \\ &= 2n + \frac{s^2}{2} - \frac{3}{2}s - 2 \\ &\geq 2n + \frac{3^2}{2} - \frac{3}{2} \cdot 3 - 2 \\ &= 2n - 2. \end{aligned}$$

Now it follows that

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

as desired. $\square$

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

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

On the other hand, it is easily seen that

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

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

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

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

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 $n = 8$. □

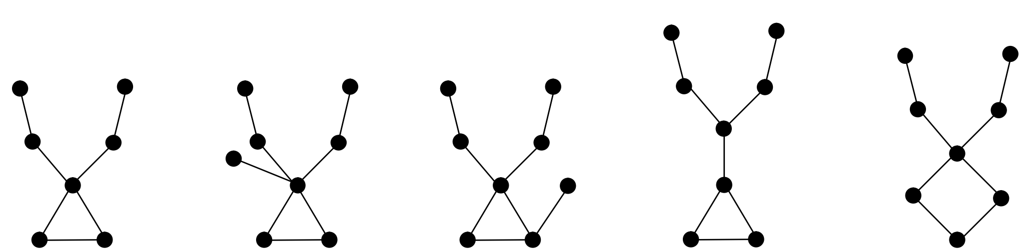

Fig. 2: The graphs in Lemma 4.4 when $n = 7$ or 8.

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

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

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

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

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

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

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

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

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

$$Tr_G(u) \geq (1 + 2 + \cdots + s) + 2(n - s - 1)$$

$$
\begin{aligned}
&= 2n + \frac{s^2}{2} - \frac{3}{2}s - 2 \\
&\geq 2n + \frac{3^2}{2} - \frac{3}{2} \cdot 3 - 2 \\
&= 2n - 2.
\end{aligned}
$$

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

$$
\begin{aligned}
Tr_G(u) &\geq (1 + 2 + \cdots + s) + 2 + 3(n - s - 2) \\
&= 3n + \frac{s^2}{2} - \frac{5}{2}s - 4 \\
&= \begin{cases} 3n - 6 & \text{if } s = 4, \\ 3n - 4 & \text{if } s = 5. \end{cases}
\end{aligned}
$$

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.

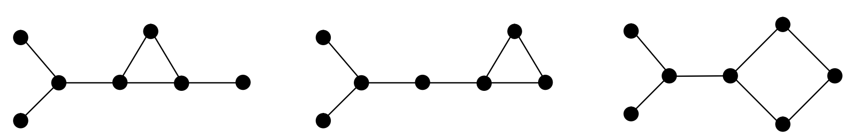

Fig. 3: The graphs in Lemma 4.8 when $\delta_G(w) = 3$, $s = 4$ and $n = 7$.

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. □

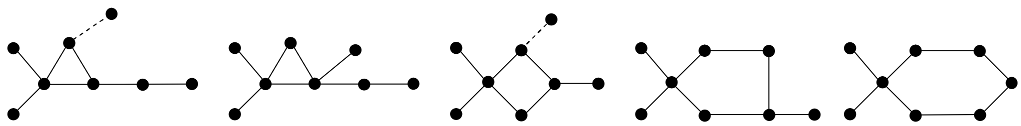

Fig. 4: The graphs in Lemma 4.8 when $\delta_G(w) = 4$, $s = 4$ and $n = 7$ or 8.
(The dashed line represents the edge may exist or not exist.)

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.

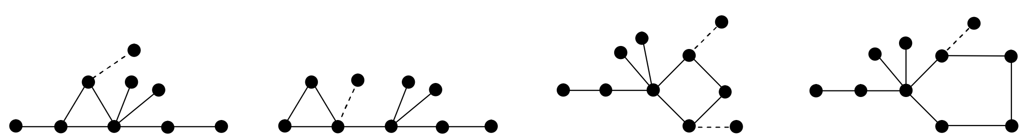

Fig. 5: The graphs in Lemma 4.9 when there exists pendant P_3 in G.

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.

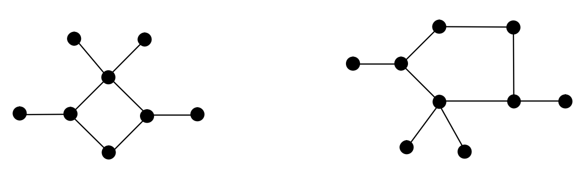

Fig. 6: The graphs in Lemma 4.9 when there is no pendant P_3 in G.

Now the result follows. □

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

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

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

In the following, suppose that $G \ncong C_n$. Since $G \ncong C_n$, we may choose a diametrical path of G, say $P = v_0 v_1 \ldots v_d$, 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.

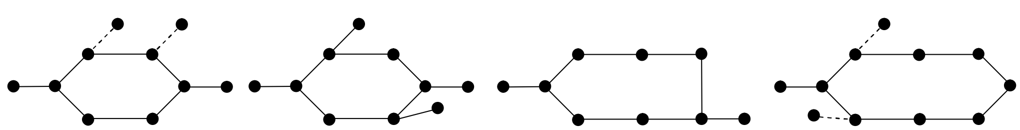

Fig. 7: The graphs in Theorem 5.1 when $d = 5$ without pendant P_3.

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.

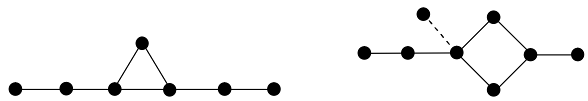

Fig. 8: The graphs in Theorem 5.1 when $d = 5$ with pendant P_3.

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.

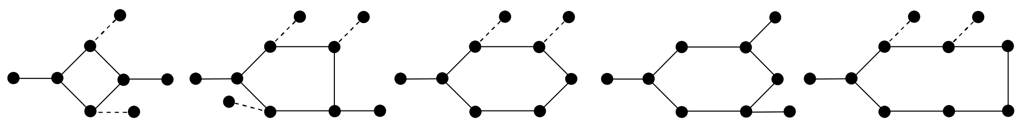

Fig. 9: The graphs in Theorem 5.1 when $d = 4$ without pendant P_3.

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.

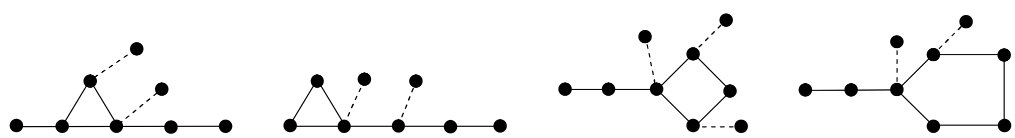

Fig. 10: The graphs in Theorem 5.1 when $d = 4$ with pendant P_3.

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. $d = 2$.

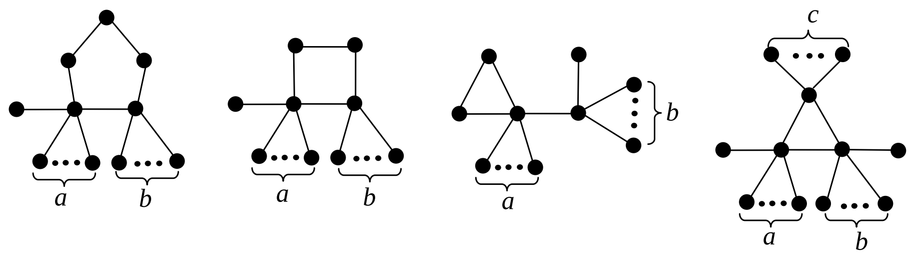

Fig. 11: The graphs in Theorem 5.1 when $d = 3$.

Clearly $G \cong S_n^+$, and $\lambda_2(G) = 2n - 1$.

Combining all the above five cases, the result follows. □

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