New extremal results for the distance Laplacian spectral radius of trees

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Abstract

The distance Laplacian matrix of a graph G is defined as $\mathcal{L}(G) = Tr(G) - \mathcal{D}(G)$, where $Tr(G)$ and $\mathcal{D}(G)$ are, respectively, the diagonal matrix of vertex transmissions and the distance matrix of G. Inside the set $\mathcal{T}_n$ of trees with n vertices, we consider the subsets $\mathcal{NC}_n$ and $\mathcal{NS}_n$ containing non-caterpillar trees and non-starlike trees respectively, and study the graphs with maximum distance Laplacian spectral radii in $\mathcal{NC}_n$, in $\mathcal{NS}_n$, and in $\mathcal{NC}_n \cap \mathcal{NS}_n$. As a by-product, we pick out the three candidates to attain the fourth biggest maximum Laplacian spectral radius in $\mathcal{T}_n$.

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1 Introduction

In this paper, we denote by $G = (V_G, E_G)$ a simple, undirected and connected graph with vertex set $V_G = \{v_1, v_2, \ldots, v_n\}$ and edge set $E_G = \{e_1, e_2, \ldots, e_m\}$.

When two vertices u and v are adjacent, we write $u \sim v$. The neighborhood $N(v)$ of a vertex v is the set $\{u \in V_G \mid u \sim v\}$. The degree $d_G(v)$ of a vertex v is the number $|N(v)|$, and the largest vertex degree is denoted by Δ_G. When there is no risk of ambiguity we simply write $d(v)$ and Δ instead of $d_G(v)$ and Δ_G. We say that v is a pendant vertex if $d(v) = 1$. A pendant path P (of length $\ell(P) = k$) at a vertex $u \in V_G$ is a path $uu_1 \ldots u_k$ with $d_G(u) \geqslant 3$, $d_G(u_i) = 2$ for $1 \leqslant i < k$, and $d_G(u_k) = 1$.

The distance $d_G(u, v)$ between the vertices u and v is the length of a shortest path in G connecting them. The distance matrix $\mathcal{D}(G)$ of G is the $n \times n$ matrix whose (i, j)-entry is $d_G(v_i, v_j)$. The transmission $Tr_G(u)$ of a vertex u in G is $\sum_{v \in V_G} d_G(u, v)$, i.e. the sum of the distances from u to each other vertex of G.

In 2013, Aouchiche and Hansen introduced two graph matrices [2]: the *distance Laplacian* matrix $\mathcal{L}(G) = Tr(G) - \mathcal{D}(G)$ and the *distance signless Laplacian* matrix $\mathcal{Q}(G) = Tr(G) + \mathcal{D}(G)$, where $Tr(G)$ denotes the diagonal matrix of vertex transmissions of G. Being diagonally dominant, the eigenvalues of both $\mathcal{L}(G)$ and $\mathcal{Q}(G)$ are nonnegative. In particular, we denote by $\lambda(G) := \lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_n(G) = 0$ the eigenvalues of $\mathcal{L}(G)$. The largest distance Laplacian eigenvalue $\lambda(G)$ is the *distance Laplacian spectral radius* of G.

After less than ten years, the literature on these two distance Laplacian matrices is quite rich (see, for instance, [1], [7], [9], [16], [17], [18], [21]). The interest for these matrices increased

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even more when computational and numerical evidences showed that $\mathcal{L}$- and $\mathcal{Q}$-spectra could be finer invariants with respect to L and Q-spectra (here L and Q respectively denote the usual Laplacian matrix and the signless Laplacian matrix). In fact, by comparing [6, Table 1] and [3, Table 4], it is reasonable to expect that, for each order n, the number of graphs with n vertices determined by their $\mathcal{L}$- (resp. $\mathcal{Q}$)-spectrum is considerably higher than the number of those determined by their L- (resp. Q)-spectrum, even if it is still unclear whether properties like acyclicity are preserved by $\mathcal{L}$-cospectrality (this topic is discussed in [5]).

The spectral sub-branch of extremal graph theory essentially consists in identifying those objects which are extremal with respect to a fixed spectral parameter within a given class of graphs. In this context, many scholars tried to order the set $\mathcal{T}_n$ of all trees with n vertices with respect to the spectral radius of several well-known graph matrices. For instance, the list of the trees in $\mathcal{T}_n$ (with $n \geqslant 12$) attaining the first thirteen largest adjacency spectral radii can be found in [15]; similarly, one can find in [25] the list of the trees in $\mathcal{T}_n$ (with $n \geqslant 15$) attaining the first thirteen largest L- and Q-spectral radii.

In the last few years, some extremal problems concerning the distance Laplacian spectral radius have been faced and solved. For instance, it is known that the minimum and the maximum $\mathcal{L}$-spectral radius in $\mathcal{T}_n$ are only attained by the star S_n [1] and the path P_n [14] respectively.

In [14], H. Lin and B. Zhou also characterized the graph with maximum distance Laplacian spectral radius among connected graphs given clique number. The same authors found in [12] the graphs with second and third maximum $\mathcal{L}$-spectral radius in $\mathcal{T}_n$ (see Proposition 3.1 in this paper). The graphs achieving the maximum $\mathcal{L}$-spectral radius among trees in $\mathcal{T}_n$ with given maximum degree have been identified in [4]. Niu et al. detected in [19] the graphs with minimum $\mathcal{L}$-spectral radius among all bipartite graphs of fixed order with a given matching number and a given vertex connectivity, respectively. Pirzada and Khan studied the graphs minimizing the $\mathcal{L}$-spectral radius among all graphs having a sufficiently high fixed chromatic number [20]. Extremal problems concerning the $\mathcal{L}$-spectral radius of unicyclic and bicyclic graphs have been considered in [4, 11, 24].

Let $\mathcal{NC}_n$ and $\mathcal{NS}_n$ be the subsets of $\mathcal{T}_n$ containing the non-caterpillar trees and the non-starlike trees respectively. The graphs with minimum $\mathcal{L}$-spectral radius in $\mathcal{NC}_n$, $\mathcal{NS}_n$ and $\mathcal{NC}_n \cap \mathcal{NS}_n$ have been identified in [14]. Extremal results for those three sets with respect to other graph parameters can be found in [17, 22, 23]. In this paper, we identify the graphs with maximum $\mathcal{L}$-spectral radii in the same three sets $\mathcal{NC}_n$, in $\mathcal{NS}_n$ and in $\mathcal{NC}_n \cap \mathcal{NS}_n$ (see Theorems 2.8, 2.10 and 2.11). Moreover, we find the candidates destined to contend for the fourth, the fifth and the sixth maximum $\mathcal{L}$-spectral radius in $\mathcal{T}_n$ (see Theorem 3.2).

2 Maximum distance Laplacian spectral radius

We start by recalling some known results on the $\mathcal{L}$-spectral radius. As usual, we denote by P_n the path with n vertices.

Proposition 2.1. [14, Theorem 5.1] *Let G be a connected graph of order n. Then $\lambda(G) \leqslant \lambda(P_n)$. The equality holds if and only if $G \cong P_n$.*

Proposition 2.2. [8] or [1, Theorem 2.8] *Let $n \geqslant 3$. Then, $\lambda(T) \geqslant 2n-1$ for each $T \in \mathcal{T}_n$. The equality holds if and only if T is the star S_n.*

Let a and n be integers such that $1 < a < n$. We denote by $H_{n,a}$ the *broom* graph with maximum vertex degree a, i.e. the tree obtained from the path P_{n-a+1} by joining one of its pendant vertices to $a-1$ isolated vertices. Clearly, $H_{n,2} = P_n$ and $H_{n,n-1} = S_n$.

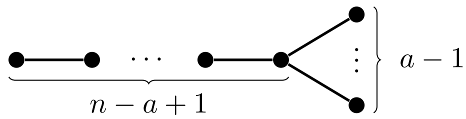

Figure 1: The broom graph $H_{n,a}$.

Proposition 2.3. [4, Theorem 5.6] *Among all trees in $\mathcal{T}_n$ with maximum vertex degree Δ, the only graph achieving the maximum $\mathcal{L}$-spectral radius is $H_{n,\Delta}$.*

Let a and b be two nonnegative integers, and let u and v be two vertices of a nontrivial connected graph F such that $d_F(u,v) \leqslant 1$. By definition, if $u \neq v$, then $u \sim v$. We denote by $F_{u,v}(a,b)$ the graph obtained by attaching a pendant path of length a at u and a pendant path of length b at v. Clearly, $F_{u,v}(0,0) = F$; moreover, if F is a tree, then $F_{u,v}(a,b)$ is a tree as well. Additionally, we set $F_u(a,b) := F_{u,u}(a,b)$.

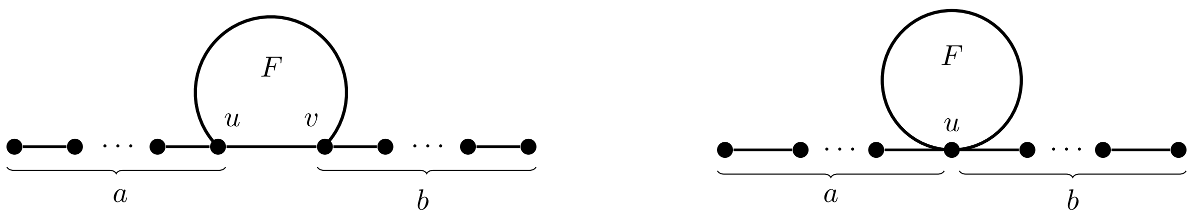

Figure 2: The graphs $F_{u,v}(a,b)$ and $F_u(a,b)$.

The proofs of our main results need three lemmas. Each of them studies how certain *graft transformations*, i.e. suitable displacements of edges, affect the $\mathcal{L}$-spectral radius.

Lemma 2.4. [4, Corollary 5.3] or [14, Corollary 3.1] *Let u be a vertex of a nontrivial connected graph F. If $k \geqslant l \geqslant 1$, then $\lambda(F_u(k,l)) < \lambda(F_u(k+1,l-1))$.*

The act of replacing a graph of type $F_u(k,l)$, where $k \geqslant l \geqslant 1$, with $F_u(k+1,l-1)$ will be called an *LZ-graft transformation (at the vertex u).*

Lemma 2.5. [4, Lemma 5.7] *Let u and v be two adjacent vertices of a connected graph $F \neq P_2$. Then, $\lambda(F_{u,v}(k,l)) < \max\{\lambda(F_{u,v}(k+1,l-1)), \lambda(F_{u,v}(k-1,l+1))\}$.*

Remark 2.6. In the statement of [4, Lemma 5.7], the restriction $|V_F| \geq 3$ is missing. A careful reading of its proof shows that the existence of a third vertex in F other than u and v is tacitly assumed. However, for $F = P_2$ the inequality

$$\lambda(F_{u,v}(k,l)) < \max\{\lambda(F_{u,v}(k+1,l-1)), \lambda(F_{u,v}(k-1,l+1))\}$$

is clearly false, since $(P_2)_{u,v}(k,l) = (P_2)_{u,v}(k+1,l-1) = (P_2)_{u,v}(k-1,l+1) = P_{k+l+2}$.

Lemma 2.7. [14, Theorem 3.2] *Let G be a graph with three induced subgraphs G_1, G_2 and G_3 such that $|V(G_i)| \geqslant 2$ for $i = 1,2,3$, $V(G_i) \cap V(G_j) = \{u\}$ for $1 \leqslant i < j \leqslant 3$ and $\cup_{i=1}^3 V(G_i) = V(G)$. For $v \in V(G_2) \setminus \{u\}$ and $y \in V(G_1) \setminus \{u\}$, let $G' = G - \{uw : w \in N_{G_3}(u)\} + \{vw : w \in N_{G_3}(u)\}$ and $G'' = G - \{uw : w \in N_{G_3}(u)\} + \{yw : w \in N_{G_3}(u)\}$. If $N_G(u) = \{y,v\} \cup N_{G_3}(u)$, then either $\lambda(G) < \lambda(G')$ or $\lambda(G) < \lambda(G'')$.*

A caterpillar is a tree such that the removal of all pendant vertices yields a path. In Section 1 we have denoted by $\mathcal{NC}_n$ the set of all non-caterpillar trees with n vertices. It is straightforward

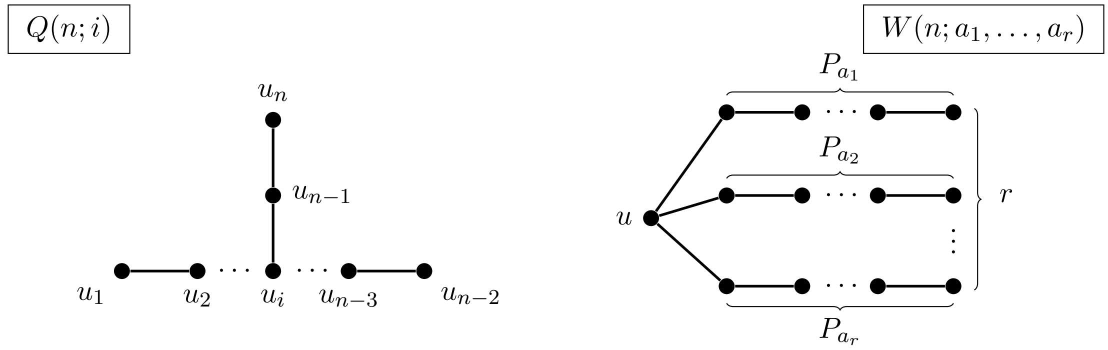

Figure 3: The graphs $Q(n;i)$ and $W(n;a_1,\dots,a_r)$.

to check that a tree $T \in \mathcal{T}_n$ belongs to $\mathcal{NC}_n$ if and only if there exists a $v \in V_T$ such that the set $\{u \in N_T(v) \mid d_T(u) \geqslant 2\}$ has more than two elements. The set $\mathcal{NC}_n$ is non-empty for $n \geqslant 7$.

In order to identify the graph maximizing the $\mathcal{L}$-spectral radius in $\mathcal{NC}_n$, we introduce the two types of graphs depicted in Fig. 3. The tree $Q(n;i)$ $(2 \leqslant i \leqslant n-3)$ is obtained by attaching a pendant path of length two to the vertex u_i of the path $P_{n-2} = u_1 \dots u_{n-2}$. The tree $W(n;a_1,\dots,a_r)$ is obtained by selecting a pendant vertex w_i on each path in the set $\{P_{a_i} \mid 1 \leqslant i \leqslant r\}$ and joining each w_i with a single vertex u. Clearly, $W(n;a_1,\dots,a_r)$ is a starlike tree is $r \geqslant 3$.

Let $G = (V_G, E_G)$ be any graph. We set $A_G = \{v \in V_G \mid d_G(v) \geqslant 3\}$.

Theorem 2.8. *Let $n \geqslant 7$. A graph attaining the maximal $\mathcal{L}$-spectral radius in $\mathcal{NC}_n$ is isomorphic to $Q(n;3)$.*

Proof. Let T be a tree with maximum $\mathcal{L}$-spectral radius in $\mathcal{NC}_n$. As for any other non-caterpillar tree, the diameter t of T is at least 4. Moreover, if $P_{t+1} = u_1u_2\dots u_{t+1}$ is a fixed diametral path of T, there exists a vertex $u_i \in V(P_{t+1}) \cap A_T$ with $3 \leqslant i \leqslant t-1$ and a vertex $u \in V(T \backslash P_{t+1})$ such that $d_T(u,u_i) = \min_{u_j \in V(P_{t+1})} d_T(u,u_j) \geqslant 2$.We now verify the following claims.

Claim 1. $A_T = \{u_i\}$.
If $|A| \geqslant 2$, we could find a vertex $w \in V(T)\backslash\{u_i\} \cap A_T$ such that

$$d_T(u_i,w) = \max_{v \in V(T) \cap A_T} d_T(u_i,v) > 0.$$

The way we chose w ensures that $d(w) \geqslant 3$ and there exist at least two pendant paths at w. We pick two pendant paths M and R at w and denote by m and r $(m \geqslant r \geqslant 1)$ their respective length. The subgraph F induced by $V(T)\backslash(V(M) \cup V(R)\backslash\{w\})$ is connected; moreover, it turns out that T is isomorphic to $F_w(m,r)$. We now consider $T' = F_w(m+1,r-1)$. By separately analyzing the cases $w \in P_{t+1}$ and $w \notin P_{t+1}$, we check that $F_w(m+1,r-1)$ is also a non-caterpillar tree. In fact, the replacement of T with T' just affects the degree of w (namely, $d_T(w)-1 \leqslant d_{T'}(w) \leqslant d_T(w)$)). Yet, by Lemma 2.4, $\lambda(T) = \lambda(F_w(m,r)) < \lambda(F_w(m+1,r-1)) = \lambda(T')$, contradicting the maximality of T in $\mathcal{NC}_n$; hence, $A = \{u_i\}$.

Claim 2. $\Delta = 3$.
Since $A = \{u_i\}$, surely $\Delta = d_T(u_i)$. Suppose $d_T(u_i) \geqslant 4$. Then, T consists of Δ pendant paths $M_1, M_2, \dots, M_\Delta$ at u_i, where $\ell(M_1) \geqslant \ell(M_2) \geqslant \cdots \geqslant \ell(M_\Delta)$. In other words, once we set $m_i := \ell(M_i)$ for $1 \leqslant i \leqslant \Delta$, the tree T is isomorphic to the starlike tree $W(n;m_1,\dots,m_\Delta)$, where $m_3 \geqslant 2$, since T is not a caterpillar. The starlike graph

$$T' = W(n;m_1,\dots,m_{\Delta-1}+1,m_\Delta-1)$$

is still in $\mathcal{NC}_n$, since it has at least three rays of length $\geqslant 2$. By Lemma 2.4, $\lambda(T) < \lambda(T')$ against the maximality of T in $\mathcal{NC}_n$. That is why $\Delta = d_T(u_i) = 3$.

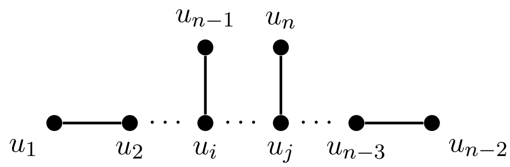

Figure 4: The graph $K(n;i,j)$.

So far, we have proved that $T \cong W(n; m_1, m_2, m_3)$ with $m_1 \geqslant m_2 \geqslant m_3 \geqslant 2$. Moreover, the maximality of T and Lemma 2.4 imply that the three graphs

$$W(n; m_1, m_2+1, m_3-1),\ \ W(n; m_1+1, m_2, m_3-1) \quad \text{and} \quad W(n; m_1+1, m_2-1, m_3)$$

are all caterpillars. This happens only if $T \cong W(n; n-5, 2, 2) \cong Q(n; 3)$. □

It is noteworthy that, in the set $\mathcal{NC}_n$, the graph $Q(n;3)$ also maximizes the distance spectral radius [23, Theorem 5.2] and the distance signless Laplacian spectral radius [17, Theorem 5.4].

A tree T is said to be non-starlike if $|A_T| \geqslant 2$. Theorem 2.10 will show that a graph maximizing the $\mathcal{L}$-spectral radius in the set $\mathcal{NS}_n$ of non-starlike trees with n vertices (which is non-empty for $n \geqslant 6$) must be searched in the set

$$\left\{ K(n; i, j) \,\middle|\, 2 \leqslant i < j \leqslant n-3, i \leqslant \left\lfloor \frac{n}{2} \right\rfloor - 1 \right\},$$

where $K(n; i, j)$ denotes the caterpillar tree obtained from a path $P_{n-2} = u_1 \ldots u_{n-2}$ by attaching two pendant vertices u_{n-1} and u_n to u_i and u_j respectively (see Fig. 4).

Lemma 2.9. *For each $n \geqslant 8$ and for all $3 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor - 1$, the following inequality holds:*

$$\lambda(K(n; i-1, i)) > \lambda(K(n; i, i+1)). \tag{1}$$

Proof. We use the vertex labeling proposed in Fig. 4. Moreover, we set $\lambda_{n,i} := \lambda(K(n; i, i+1))$. Let F be the subgraph of $K(n; i, i+1))$ induced by the vertices u_i, u_{i+1}, u_{n-1} and u_n. Clearly,

$$F \cong P_4 = xuvy \qquad \text{and} \qquad K(n; i, i+1)) \cong (P_4)_{u,v}(i-1, n-i-3),$$

where the integers $i-1$ and $n-i-3$ are both positive in the range $3 \leqslant i \leqslant \lfloor \frac{n}{2} \rfloor - 1$. Therefore, by applying Lemma 2.5, we obtain

$$\max \mathcal{S}_i > \lambda_{n,i}, \qquad \text{where } \mathcal{S}_i = \{\, \lambda_{n,i-1},\, \lambda_{n,i+1} \,\}. \tag{2}$$

For any fixed $n \geqslant 8$, the proof now proceeds by decreasing induction on i. We consider first the base case $i = \hat{\imath} := \lfloor \frac{n}{2} \rfloor - 1$. As observed above,

$$K(n; \hat{\imath}, \hat{\imath}+1)) \cong (P_4)_{u,v}\left(\left\lfloor \frac{n}{2} \right\rfloor - 2, n - \left\lfloor \frac{n}{2} \right\rfloor - 2 \right).$$

For $n = 2k$ ($k \in \mathbb{N}$), the set $\mathcal{S}_{\hat{\imath}}$ is a singleton. In fact,

$$K(n; \hat{\imath}-1, \hat{\imath}) \cong (P_4)_{u,v}(k-3, k-1) \cong (P_4)_{u,v}(k-1, k-3) \cong K(n; \hat{\imath}+1, \hat{\imath}+2).$$

Thus, by (2), $\lambda_{n,\hat{\imath}-1} > \lambda_{n,\hat{\imath}}$, proving (1) for $i = \hat{\imath}$ and n even.

For $n = 2k+1$ ($k \in \mathbb{N}$), we see that

$$K(n; \hat{\imath}+1, \hat{\imath}+2) \cong (P_4)_{u,v}(k-1, k-2) \cong (P_4)_{u,v}(k-2, k-1) \cong K(n; \hat{\imath}, \hat{\imath}+1).$$

This implies $\mathcal{S}_{\hat{\imath}} = \{\, \lambda_{n,\hat{\imath}-1},\, \lambda_{n,\hat{\imath}+1} = \lambda_{n,\hat{\imath}} \,\}$. Therefore, Inequality (2) in the case at hand holds only if $\lambda_{n,\hat{\imath}-1} > \lambda_{n,\hat{\imath}}$.

Now, let $i < \lfloor \frac{n}{2} \rfloor - 1$. The inductive hypothesis says that $\lambda_{n,i} > \lambda_{n,i+1}$. Hence, Inequality (2) yields $\lambda_{n,i-1} > \lambda_{n,i}$, ending the proof. □

Theorem 2.10. *Let $n \geqslant 6$. If a tree T in the set $\mathcal{NS}_n$ of non-starlike trees with n vertices maximizes the $\mathcal{L}$-spectral radius, then either $T \cong K(n;2,3)$ or $K(n;2,n-3)$.*

Proof. Suppose the tree T satisfies the hypothesis of the theorem. Since $T \in \mathcal{NS}_n$, then $|A_T| \geq 2$. This implies that, fixed a vertex $u \in A_T$, there exists a $v \in A_T \setminus \{u\}$ such that $d_T(u,v) \geqslant d_T(u,w)$ for all $w \in A_T$. By definition of v, in T there are (at least) two pendant path at v, say M and R, with length m and r respectively. We can assume $m \geqslant r \geqslant 1$. The subgraph F induced by $V(T)\backslash(V(M) \cup V(R)\backslash\{v\})$ is non-empty; in fact, it contains a non-trivial path P connecting u and v. Moreover, $T = F_v(m,r)$. We now consider the tree $T' = F_v(m+1, r-1)$. Note that

$$u \in A_{T'} = \begin{cases} A_T \setminus \{v\} & \text{if } d_T(v) = 3 \text{ and } r = 1, \\ A_T & \text{otherwise.} \end{cases}$$

By Lemma 2.4 and the maximality of T, the graph $T' = F_v(m+1, r-1)$ cannot belong to $\mathcal{NS}_n$. This only happens if $d_T(v) = 3$, $r = 1$, $A_{T'} = \{u\}$ and $A_T = \{u, v\}$.

Repeating the argument above starting from $v \in A_T$ instead of u, but taking into account that $|A_T| = 2$ since the beginning, we infer that $d_T(u) = 3$ as well, and, as it happens to v, the vertex u is adjacent to (at least) one pendant vertex. In other words, T is of type $K(n;i,j)$ for suitable integers i and j such that $2 \leqslant i < j \leqslant n-3$ and $i \leqslant \lfloor \frac{n}{2} \rfloor - 1$.

For the rest of the proof we refer to the vertex labeling proposed in Fig. 4. We only need to show that $i = 2$ and $j \in \{3, n-3\}$ in order to complete the proof. We distinguish two cases, depending whether $|i-j| = 1$ or not. If $|i-j| = 1$, then $T \cong K(n;2,3)$. This is immediate for $n \in \{6,7\}$, and it is a consequence of Lemma 2.9 for $n \geqslant 8$. If $|i-j| > 1$, we now prove that $T \cong K(n;2,n-3)$. Consider the trees $T' = T - u_iu_{n-1} + u_{i-1}u_{n-1}$ and $T'' = T - u_iu_{n-1} + u_{i+1}u_{n-1}$. By Lemma 2.7, we have $\lambda(T) < \max\{\lambda(T'), \lambda(T'')\}$. Since T'' is surely a nonstarlike tree, the maximality of T in $\mathcal{NS}_n$ implies $T' \notin \mathcal{NS}_n$. This happens only if $i = 2$. The argument to prove that $j = n-3$ is analogous. □

Table 1: $\lambda(K(n;2,3))$ and $\lambda(K(n;2,n-3))$.

n	7	8	9	10	11	26	33
$\lambda(K(n;2,3))$	21.6345	30.0578	39.8350	50.8858	63.1918	396.4270	646.7090
$\lambda(K(n;2,n-3))$	22.8151	31.6125	41.6612	52.9563	65.4942	401.4601	652.6599

Note that $K(n;2,3)$ and $K(n;2,n-3)$ are the same graph for $n = 6$. Data collected in Table 1 are consistent with the inequality

$$\lambda(K(n;2,3)) < \lambda(K(n;2,n-3)) \qquad \text{for } n \geq 7. \tag{3}$$

Conjecture 1. *For $n \geqslant 7$, the first and the second largest $\mathcal{L}$-spectral radius in $\mathcal{NS}_n$ are only attained by $K(n;2,n-3)$ and $K(n;2,3)$ respectively.*

We point out that, in the set $\mathcal{NS}_n$, the graph $K(n;2,n-3)$ also maximizes the distance spectral radius [23, Theorem 5.1], whereas it is dubious which graph between $K(n;2,n-3)$ and $K(n;2,3)$ maximizes the signless Laplacian spectral radius (see [17, Theorem 5.3]).

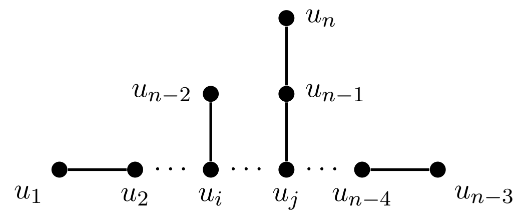

Figure 5: The graph $Y(n;i,j)$.

We now look for graphs maximizing the $\mathcal{L}$-spectral radius in the set $\mathcal{NC}_n \cap \mathcal{NS}_n$ (which is non-empty for $n \geqslant 8$), and we shall find them in the set

$$\{Y(n;i,j) \mid 2 \leqslant i < j \leqslant n-5\} \qquad \text{(see Fig. 5)}.$$

The tree $Y(n;i,j)$ is obtained from a path $P_{n-3} = u_1 \dots u_{n-3}$ by attaching a pendant vertex to u_i and a pendant path of length two to u_j.

Theorem 2.11. *Let $n \geqslant 8$. If a tree T in $\mathcal{NC}_n \cap \mathcal{NS}_n$ attains the largest $\mathcal{L}$-spectral radius, then T is one of the graphs in the set $\mathcal{Y} = \{Y(n;2,3), Y(n;2,n-5), Y(n;n-6,n-5)\}$.*

Proof. Let T be a tree in $\mathcal{NC}_n \cap \mathcal{NS}_n$ ($n \geqslant 8$) such that $\mathcal{L}(T) = \max\{\mathcal{L}(G) \mid G \in \mathcal{NC}_n \cap \mathcal{NS}_n\}$. Since T belongs in particular to $\mathcal{NS}_n$, the set $A_T = \{v \in V_T \mid d_T(v) > 2\}$ contains at least two elements. Let u be a fixed vertex in A_T and, as in the proof of Theorem 2.10, let $v = \max_{w \in V(T)} d_T(u,w)$. By definition, there exist at least two pendant paths at v. Let M_1, $M_2, \dots M_{d_t(v)-1}$ be the pendant paths at v in increasing order of their length. We denote by T' the output of an LZ-graft transformation at the vertex v involving M_1 and M_2. By Lemma 2.4 and maximality of T, the tree T' cannot belong to $\mathcal{NC}_n \cap \mathcal{NS}_n$. Now we distinguish two cases.

Case 1. T' is a starlike tree. This happens only when $d_T(v) = 3$, $\ell(M_1) = 1$ and $A_T = \{u,v\}$. Consequently there exist $d_T(u)-1$ pendant paths at u, say N_1, $N_2, \dots, N_{d_T(u)-1}$, where $\ell(N_i) \leq \ell(N_j)$ if $i < j$. Since T is not a caterpillar, surely

$$\ell(N_{d_T(u)-1}) \geqslant \ell(N_{d_T(u)-2}) \geqslant 2. \tag{4}$$

This implies that we obtain a non-starlike tree T'' if we perform an LZ-graft transformation on T at the vertex u involving N_1 and N_2. In fact $A_{T''} = \{u,v\}$. By Lemma 2.4 and maximality of T, the tree T'' is a caterpillar. This only happens if $d_T(u) = 3$ and $2 = \ell(N_1) \leqslant \ell(N_2)$. In other words, T is a tree of type $Y(n;i,j)$.

Case 2. T' is a caterpillar. Recalling how T' has been obtained from T, which is not a caterpillar, we immediately infer that $d_T(v) = 3$ and $2 = \ell(M_1) \leqslant \ell(M_2)$. Now, it is clear that A_T just contains u and v, otherwise we could perform an LZ-graft transformation at the vertex z in A_T which is at the largest distance from v, and the outcome would belong $\mathcal{NC}_n \cap \mathcal{NS}_n$ against the maximality of T. It follows that the tree T has $d_T(u)-1$ pendant paths at u. Now, LZ-graft transformations at the vertex u do not create a graph in $\mathcal{NC}_n \cap \mathcal{NS}_n$ only if $d_T(u) = 3$ and one of the pendant paths attached at u has length 1. Once again, T is a graph of type $Y(n;i,j)$.

So far, we have seen that there exist suitable i and j such that $T \cong Y(n;i,j)$ for $2 \leqslant i < j \leqslant 2n-5$ (note that $Y(n;i,2n-4)$ is a caterpillar). In order to finish the proof, we need to show that T is isomorphic to a graph in the set $\mathcal{Y}$.

Surely $i > 2$ and $|i-j| > 1$ cannot be both true. Otherwise, the two trees $\tilde{T}' = T - u_i u_{n-2} + u_{i-1}u_{n-2}$ and $\tilde{T}'' = T - u_i u_{n-2} + u_{i+1}u_{n-2}$ would be both in $\mathcal{NC}_n \cap \mathcal{NS}_n$, and one of them would have an $\mathcal{L}$-spectral radius larger $\mathcal{L}(T)$ by Lemma 2.7.

Moreover, if $i = 2$ and $|i - j| > 1$, then $j = 2n - 5$, otherwise $\hat{T}' = T - u_j u_{n-1} + u_{j-1}u_{n-1}$ and $\hat{T}'' = T - u_j u_{n-1} + u_{j+1}u_{n-1}$ would be both in $\mathcal{NC}_n \cap \mathcal{NS}_n$, and one of them would have an $\mathcal{L}$-spectral radius larger $\mathcal{L}(T)$, again by Lemma 2.7.

Finally, if $|i - j| = 1$, and $(i, j) \notin \{(2, 3), (n - 6, n - 5)\}$, we note that T is isomorphic to $(P_5)_{u,v}(i-1, n-i-4)$, where u and v are adjacent vertices of degree 2 in the path P_5, $i \geqslant 3$ and $n-i-4 \geqslant 3$. Thus, $(P_5)_{u,v}(i-2, n-i-3)$ and $(P_5)_{u,v}(i, n-i-5)$ would be both in $\mathcal{NC}_n \cap \mathcal{NS}_n$, and one of them would have an $\mathcal{L}$-spectral radius larger $\mathcal{L}(T)$, this time by Lemma 2.5. □

Clearly, for $n = 8$, we have $Y(n; 2, 3) = Y(n; 2, n-5) = Y(n; n-6, n-5)$, and $\lambda(Y(8, 2; 3)) = 25.6156$. For $n > 8$ we guess from Table 2 that $\lambda(Y(n; n - 6, n - 5)) < \lambda(Y(n; 2, 3)) < \lambda(Y(n; 2, n - 5))$. Interestingly enough, the graphs $Y(n; 2, n - 5)$ and $Y(n; 2, 3)$ are extremal in the set $\mathcal{NC}_n \cap \mathcal{NS}_n$ even respect to other graph parameters: they actually attain the first two largest distance spectral radii (see [22, Theorem 1] and [23, Theorem 5.3]) and the first two largest distance signless Laplacian spectral radii [17, Theorem 5.5].

Table 2: $\lambda(Y(n; 2, 3))$ and $\lambda(Y(n; 2, n - 5))$.

n	9	10	11	12	26	33
$\lambda(Y(n; 2, n - 5))$	35.1411	46.0244	58.2032	71.6538	390.6242	640.7190
$\lambda(Y(n; 2, 3))$	35.0266	45.8159	57.8637	71.1632	387.8626	637.0188
$\lambda(Y(n; n - 6, n - 5))$	33.3975	43.6326	55.3868	68.4721	383.2954	631.7463

3 The fourth maximum $\mathcal{L}$-spectral radius in $\mathcal{T}_n$

Let i and n be integers such that $1 < i < n - 1$. We denote by $P(n; i)$ the tree obtained from the path $P_{n-1} = u_1 \dots u_{n-1}$ by attaching a pendant vertex u_n to u_i. Recently, H. Lin and B. Zhou proved the following result.

Proposition 3.1. [12, Theorems 3.2 and 3.3] *Let $\mathcal{T}_n$ be the set of trees with n vertices with $n \geqslant 6$. The only graphs achieving the second and the third $\mathcal{L}$-spectral radius in $\mathcal{T}_n$ are the graphs $P(n; 2)$ and $P(n; 3)$ respectively.*

With the aid of Propositions 2.1, 2.2, 3.1, it is easy to order from the smallest to the largest $\mathcal{L}$-spectral radius the trees in

$$\mathcal{T}_5 = \{S_4, P(5; 2), P_5\} \qquad \text{and} \qquad \mathcal{T}_6 = \{S_5, H_{6,4}, K(6; 2, 3), P(6; 2), P(6; 3), P_n\}.$$

In fact, it turns out that

$$\lambda(S_4) < \lambda(P(5; 2)) < \lambda(P_5)$$

and

$$\lambda(S_5) < \lambda(H_{6,4}) < \lambda(K(6; 2, 3)) < \lambda(P(6; 3)) < \lambda(P(6; 2)) < \lambda(P_6),$$

since direct calculations show that $\lambda(H_{6,4}) = 15.2151$ and $\lambda(K(6; 2, 3)) = 15.2749$.

Thus, it is natural to ask which trees attain the fourth maximum $\mathcal{L}$-spectral radius in $\mathcal{T}_n$ for $n \geqslant 7$. The next theorem says that there are just three candidates.

Theorem 3.2. *Let $n \geqslant 7$ and $\mathcal{P}_n = \{P_n, P(n; 2), P(n; 3)\}$. If a tree T in the set $\mathcal{T}_n \setminus \mathcal{P}_n$ maximizes the $\mathcal{L}$-spectral radius, then $T \in \{K(n; 2, 2),\ K(n; 2, n - 3),\ P(n; 4)\}$.*

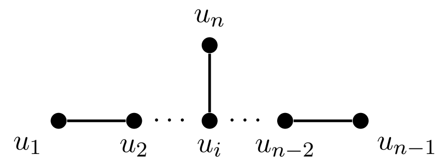

Figure 6: The graph $P(n;i)$

Proof. Let T be a tree satisfying the hypothesis of the theorem, and let $u \in V_t$ be a vertex attaining the maximum vertex degree Δ_T. Since, in particular, $T \neq P_n$, then $\Delta_T \geqslant 3$. We write $N(u) = \{u_1, u_2, \ldots, u_{\Delta_T}\}$ and, denoted by T_i the branch of T containing u_i, it is not restrictive to assume $2 \leqslant |V(T_1)| \leqslant |V(T_2)| \leqslant \cdots \leqslant |V(T_{\Delta_T})|$. Consider now the trees $T' = T - u_1u + u_1u_2$ and $T'' = T - u_1u + u_1u_3$. By Lemma 2.7 and the hypotheses on T, either T' or T'' must be in the set $\mathcal{P}_n$. It is immediately seen that neither of them could be P_n, since $T \neq P(n;2)$. This implies that $\min\{\Delta_{T'}, \Delta_{T''}\} = 3$. Moreover, since the numbers $d_T(u) - d_{T'}(u) = d_T(u) - d_{T''}(u) = 1$, we see that $\Delta_T \leqslant 4$. We now distinguish four cases, keeping in mind that the numbers $d_{T'}(u_2) - d_T(u_2)$ and $d_{T''}(u_3) - d_T(u_3)$ are both equal to 1.

Case 1. $T' = P(n;2)$. Since $T \neq P(n;3)$, the branches T_1 and T_2 both have just one edge. Thus $T = K(n;2,n-5)$.

Case 2. $T' = P(n;3)$. We consider separately the occurences $d_{T'}(u_1) = 2$ and $d_{T'}(u_1) = 3$.

Case 2.1. $d_{T'}(u_1) = 2$. In this case T_2, and *a fortiori* T_1, contains just two vertices. Now, if $d_T(u) = 3$ then $T = K(n;2,n-4)$. This case cannot occur since

$$\lambda(K(n;2,n-4)) < \max\{\lambda(K(n;2,3)), \lambda(K(n;2,n-3))\}$$

by Theorem 2.10. Therefore, $d_T(u) = 4$ and $T = K(n;2,2)$.

Case 2.2. $d_{T'}(u_1) = 3$. In this case, $d_T(u_1) = 2$ and the branches T_1 and T_3 are both paths. The inequalities $|V(T_1)| \leqslant |V(T_2)| \leqslant |V(T_3)|$ yield $T = P(n;4)$.

Case 3. $T'' = P(n;2)$. This case cannot occur. Otherwise, the vertices u_2, u and u_3 would form an induced path in T''. Analyzing the two possible instances $d_{T''} = 2$ an $d_{T''} = 3$, it is straightforward to check that n should be at most 6 contradicting the hypothesis.

Case 4. $T'' = P(n;3)$. If $d_{T''}(u_3) = 2$, then $|V(T_1)| = |V(T_2)| = |V(T_3)| = 2$. This means that $d_T(u) = 4$ and T_4, the fourth branch at u, is a path. In other words $T = K(n;2,2)$. If instead $d_{T''}(u_3) = 3$, surely $d_T(u) = 3$ and the three branches T_1, T_2 and T_3 are paths. In particular, $d_T(u_1) \in \{1,2\}$.

Case 4.1. $d_T(u_1) = 1$. Since $T \neq P(2;n)$, the vertex u_2 is not pendant in T. This implies that the branch T_3 has precisely three edges. Thus, $T = P(7;4)$ or $T = P(8;4)$.

Case 4.2. $d_T(u_2) = 1$. We are supposing $T'' = P(n;3)$, and the branches rooted in u_3 containing u_1 and u_2 have at least two edges. This implies $|E_{T_3}| = 2$ and $T = Q(7;2)$ (see Fig. 3). This case does not occur, since an LZ-graft transformation at u would convert $Q(7;2)$ in $P(7;4)$, which has a larger $\mathcal{L}$-spectral radius.

Summarizing the results coming from our case analysis, we see that T is one of the three graphs in the set $T \in \{K(n;2,2),\ K(n;2,n-3),\ P(n;4)\}$, as claimed. $\square$

Data in Table 3, together with Theorem 3.2, drive us to state the following conjecture.

Conjecture 2. *For $n \geqslant 16$, $K(n;2,n-3)$, $P(n;4)$ and $K(n;2,2)$ are the only trees in $\mathcal{T}_n$ respectively attaining the fourth, the fifth and the sixth largest $\mathcal{L}$-spectral radius.*

It is somehow instructive to compare the data in Tables 1-3 with those in Table 4. As predicted by Propositions 2.1 and 2.2, $\lambda(S_n) < \lambda(T) < \lambda(P_n)$ for every T appearing in the first column of Tables 1-3.

Table 3: $\lambda(K(n;2,n-3))$, $\lambda(P(n;4))$ and $\lambda(K(n;2,2))$.

n	8	9	10	11	15	16	26	33
$\lambda(K(n;2,n-3))$	31.6125	41.6612	52.9563	65.4942	**128.0212**	**146.7373**	401.4601	652.6599
$\lambda(P(n;4))$	33.0841	42.7659	53.8105	66.1520	**128.0929**	**146.6855**	400.6764	651.0278
$\lambda(K(n;2,2))$	31.3575	41.2918	52.4684	64.8864	126.9452	145.5503	399.3205	650.0007

Table 4: $\lambda(P_n)$ and $\lambda(S_n)$.

n	8	9	10	11	12	15	16	26	33
$\lambda(P_n)$	38.4457	48.8051	60.3856	73.1869	87.2086	136.5950	155.4972	411.6068	663.4548
$\lambda(S_n)$	15	17	19	21	23	29	31	51	65

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