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ORDERING THE NON-STARLIKE TREES WITH LARGE REVERSE WIENER INDICES

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Abstract. The reverse Wiener index of a connected graph G is defined as

$$\Lambda(G) = \frac{1}{2}n(n-1)d - W(G),$$

where n is the number of vertices, d is the diameter, and $W(G)$ is the Wiener index (the sum of distances between all unordered pairs of vertices) of G. We determine the n-vertex non-starlike trees with the first four largest reverse Wiener indices for $n \geqslant 8$, and the n-vertex non-starlike non-caterpillar trees with the first four largest reverse Wiener indices for $n \geqslant 10$.

Keywords: distance, diameter, Wiener index, reverse Wiener index, trees, starlike trees, caterpillars

MSC 2010: 05C12, 05C35, 05C90

1. Introduction

Let G be a simple connected graph. The Wiener index $W(G)$ of G is the sum of distances between all unordered pairs of vertices of G [11], [20]. It is one of the oldest graph invariants studied extensively and thoroughly both in chemistry, e.g., [16], [18], [19] and in mathematics (under different names), e.g., [6], [7], [8], [10], [17].

Balaban *et al.* [2] proposed a novel variant of the Wiener index named the reverse Wiener index. For a connected graph G with n vertices, it is defined as [2]

$$\Lambda(G) = \frac{1}{2}n(n-1)d - W(G),$$

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where d is the diameter of G. The reverse Wiener index found applications in QSPR studies, see [2], [12]. Some mathematical properties of the reverse Wiener index have been established in [3], [9], [13], [14], [15], [21], see [22], [23] for a survey.

We note that the study of the reverse Wiener index is equivalent to the study of the difference between the diameter and the average distance [1], [4], [5].

A tree with exactly one vertex of degree at least three is said to be starlike. Otherwise, it is non-starlike. A caterpillar is a tree such that deleting all the pendent vertices (vertices of degree one) yields a path. A tree that is not a caterpillar is said to be a non-caterpillar tree.

In [13], we determined the n-vertex trees with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{1}{2}n \rfloor$, where $n \geqslant 5$. In [14], we determined the n-vertex non-caterpillar trees with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{1}{2}(n-3) \rfloor$, where $n \geqslant 8$. All these extremal trees are starlike. Therefore it is of interest to study the reverse Wiener indices of non-starlike trees.

In this paper, we determine the n-vertex non-starlike trees with the first four largest reverse Wiener indices for $n \geqslant 8$, and the n-vertex non-starlike non-caterpillar trees with the first four largest reverse Wiener indices for $n \geqslant 10$.

2. Preliminaries

Let T be a tree with a vertex set $V(T)$ and an edge set $E(T)$. For $e \in E(T)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ denote the number of vertices of T lying on the two sides of the edge e, respectively. It is well-known that [20], [6]

$$W(T) = \sum_{e \in E(T)} n_{T,1}(e) n_{T,2}(e).$$

Let v be a vertex of degree $r+1$ in a tree T (which is not a star) with a unique non-pendent neighbor u and pendent neighbors $v_1, v_2, \ldots, v_r$. Let $\sigma(T; u, v)$ be the tree obtained from T by removing edges $vv_1, vv_2, \ldots, vv_r$ and adding new edges $uv_1, uv_2, \ldots, uv_r$. We say that $\sigma(T; u, v)$ is a σ-transformation of T at u and v.

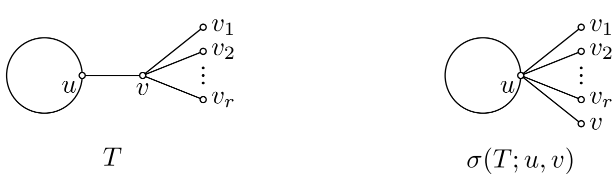

Figure 1. σ-transformation applied to T at u and v.

Lemma 2.1. *Let T be a tree and v a vertex of T with a unique non-pendent neighbor u and at least one pendent neighbor. Then*

$$W(\sigma(T;u,v)) < W(T).$$

Proof. Let $v_1, v_2, \ldots, v_r$ be the pendent neighbors of v. Let $n = |V(T)|$. Obviously, $n \geqslant r+3$. It is easily seen that

$$\begin{aligned} W(T) - W(\sigma(T;u,v)) &= n_{T,1}(uv)n_{T,2}(uv) - n_{\sigma(T;u,v),1}(uv)n_{\sigma(T;u,v),2}(uv) \\ &= (r+1)(n-r-1) - (n-1) \\ &= r(n-r-2) > 0, \end{aligned}$$

from which the result follows. □

For $u, v \in V(T)$, $d_T(u,v)$ denotes the distance between the vertices u and v in T. For $u \in V(T)$ and $A \subseteq V(T)$, let $d_T(u|A)$ be the sum of all distances from u to the vertices in A, i.e., $d_T(u|A) = \sum\limits_{v \in A} d_T(u,v)$.

Let P_n be the n-vertex path.

Lemma 2.2. *Let $P_{d+1} = v_0 v_1 \ldots v_d$. Then $d_{P_{d+1}}(v_i|P_{d+1}) \leqslant d_{P_{d+1}}(v_j|P_{d+1})$ for $|i - \frac{1}{2}d| \leqslant |j - \frac{1}{2}d|$.*

Proof. It is easily seen that

$$d_{P_{d+1}}(v_i|P_{d+1}) = \sum_{s=1}^{i} s + \sum_{s=1}^{d-i} s = i^2 - di + \frac{d(d+1)}{2},$$

which is symmetrical for $i = \frac{1}{2}d$. □

Let G be a connected graph with a subgraph H. For $u \in V(G)$, the distance from u to H is defined as the minimum distance between u and the vertices of H.

Lemma 2.3. *Let T be a tree with $P_{d+1} = v_0 v_1 \ldots v_d$ as its subgraph. For $u \in V(T)$, let h be the distance from u to P_{d+1}. If $h \geqslant 1$, then*

$$d_T(u|P_{d+1}) = h(d+1) + d_T(v_{i'}|P_{d+1}),$$

where $v_{i'} \in V(P_{d+1})$ with $h = d_T(u, v_{i'})$.

P r o o f. Obviously, $d_T(v_{i'}|P_{d+1}) = \sum\limits_{s=1}^{i'} s + \sum\limits_{s=1}^{d-i'} s$. Then we have

$$\begin{aligned} d_T(u|P_{d+1}) = \sum_{s=h}^{h+i'} s + \sum_{s=h+1}^{h+d-i'} s &= (i'+1)h + \sum_{s=1}^{i'} s + (d-i')h + \sum_{s=1}^{d-i'} s \\ &= h(d+1) + d_T(v_{i'}|P_{d+1}), \end{aligned}$$

as desired. □

Lemma 2.4. *Let T be a tree with a diameter-achieving path $P = v_0v_1\dots v_d$. Let v_s and v_t with $0 < s < t < d$ be two vertices of degree at least three such that all internal vertices (if any) of the path connecting them have degree two. Form a tree T' by removing the edges outside P incident with v_s to v_t and a tree T'' by removing the edges outside P incident with v_t to v_s. Then*

$$\min\{W(T'), W(T'')\} < W(T).$$

P r o o f. Let n_s or n_t be the number of vertices of the tree containing v_s or v_t resulting from T by deleting the edge v_sv_{s+1} or $v_{t-1}v_t$, respectively. Let $a+1$ or $b+1$ be the number of vertices of the tree containing v_s or v_t resulting from T by deleting edges $v_{s-1}v_s$ and v_sv_{s+1} or $v_{t-1}v_t$ and v_tv_{t+1}, respectively. Let $c = t - s$. Let $n = |V(T)|$. Then $n = n_s + n_t + c - 1$. It is easily seen that

$$\begin{aligned} W(T) - W(T') &= \sum_{i=0}^{c-1} [(n_t+i)(n-n_t-i) - (n_t+a+i)(n-n_t-a-i)] \\ &= \sum_{i=0}^{c-1} a(2n_t+2i+a-n) = ac(2n_t+c-1+a-n) \\ &= ac(n_t-n_s+a). \end{aligned}$$

Similarly,

$$W(T) - W(T'') = bc(n_s - n_t + b).$$

Therefore $W(T') < W(T)$ if $n_t \geqslant n_s$, and $W(T'') < W(T)$ if $n_s \geqslant n_t$. □

3. Reverse Wiener indices of non-starlike trees

Let $\mathcal{NS}_{n,d}$ be the class of non-starlike trees with n vertices and diameter d, where $3 \leqslant d \leqslant n-3$. Let $N_{n,d}$ be the tree obtained from the path $P_{d+1} = v_0v_1\dots v_d$ by attaching $n-d-2$ pendent vertices to $v_{\lfloor d/2\rfloor}$ and one pendent vertex to $v_{\lfloor d/2\rfloor+1}$. See Figure 2.

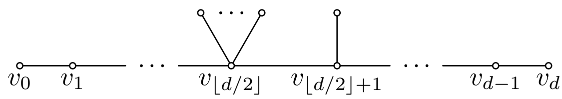

Figure 2. The tree $N_{n,d}$.

Theorem 3.1. *Let $T \in \mathcal{NS}_{n,d}$, where $3 \leqslant d \leqslant n-3$. Then*

$$W(T) \geqslant \frac{d(d+1)(d+2)}{6} + (n-d-1)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big) + 2\Big\lfloor\frac{d}{2}\Big\rfloor + (n+1)(n-d-2) + 2$$

with equality if and only if $T = N_{n,d}$.

Proof. Note that $W(P_{d+1}) = \frac{1}{6}d(d+1)(d+2)$. By Lemma 2.3, we have

$$\begin{aligned}
W(N_{n,d}) &= W(P_{d+1}) + (n-d-2)(d+1+d_{N_{n,d}}(v_{\lfloor d/2\rfloor}|P_{d+1}))\\
&\quad + (d+1+d_{N_{n,d}}(v_{\lfloor d/2\rfloor+1}|P_{d+1})) + 2\binom{n-d-2}{2} + 3(n-d-2)\\
&= W(P_{d+1}) + (n-d-2)d_{N_{n,d}}(v_{\lfloor d/2\rfloor}|P_{d+1}) + d_{N_{n,d}}(v_{\lfloor d/2\rfloor+1}|P_{d+1})\\
&\quad + (n-d-1)(d+1) + (n-d)(n-d-2)\\
&= W(P_{d+1}) + (n-d-2)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big)\\
&\quad + \Big[\Big(\Big\lfloor\frac{d}{2}\Big\rfloor+1\Big)^2 - d\Big(\Big\lfloor\frac{d}{2}\Big\rfloor+1\Big) + \frac{d(d+1)}{2}\Big]\\
&\quad + (n-d-1)(d+1) + (n-d)(n-d-2)\\
&= \frac{d(d+1)(d+2)}{6} + (n-d-1)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big)\\
&\quad + 2\Big\lfloor\frac{d}{2}\Big\rfloor + (n+1)(n-d-2) + 2.
\end{aligned}$$

Let T be a tree in $\mathcal{NS}_{n,d}$ with a minimum Wiener index. We need only to show that $T = N_{n,d}$. Let $P = v_0v_1\dots v_d$ be a diameter-achieving path of T.

Suppose that there exists a vertex in T (outside P), the distance from which to P is at least two. Let u be such a vertex, the distance from which to P is maximal. Then u is pendent. Let $uvw\dots$ be the shortest path from u to P. Note that

$\sigma(T;w,v) \in \mathcal{NS}_{n,d}$. By Lemma 2.1 we have $W(\sigma(T;w,v)) < W(T)$, a contradiction. It follows that T is a caterpillar.

Since $T \in \mathcal{NS}_{n,d}$, there are at least two vertices on P of degree at least three.

If there are at least three vertices on P of degree at least three, then for two such vertices with minimal distance, say v_s and v_t on P, by Lemma 2.4 we may relocate the observed pendent edges (edges incident to the pendent vertices) outside P in such a way that the edges which were previously attached at v_s are now attached at v_t, or, conversely, to obtain a tree in $\mathcal{NS}_{n,d}$ with a Wiener index smaller than T, a contradiction.

Hence there are exactly two vertices, say v_i and v_j on P of degree at least three. Suppose without loss of generality that $1 \leqslant i \leqslant \lfloor \frac{1}{2}d \rfloor$ and $|i - \frac{1}{2}d| \leqslant |j - \frac{1}{2}d|$. If $(i,j) \neq \left(\frac{1}{2}(d-1), \frac{1}{2}(d+1)\right)$ for odd d and $(i,j) \neq \left(\frac{1}{2}d, \frac{1}{2}d \pm 1\right)$ for even d, then move all the pendent neighbors of v_i or v_j outside P to $v_{\lfloor d/2 \rfloor}$ or $v_{\lfloor d/2 \rfloor+1}$, respectively, to obtain a tree $T^* \in \mathcal{NS}_{n,d}$. Let a or b be the number of pendent neighbors outside P at v_i or v_j, respectively. By Lemmas 2.2 and 2.3,

$$\begin{aligned} W(T) - W(T^*) &= a[(d+1+d_T(v_i|P)) - (d+1+d_T(v_{\lfloor d/2 \rfloor}|P))] \\ &\quad + b[(d+1+d_T(v_j|P)) - (d+1+d_T(v_{\lfloor d/2 \rfloor+1}|P))] \\ &\quad + ab|j-i| - ab \\ &= a(d_T(v_i|P) - d_T(v_{\lfloor d/2 \rfloor}|P)) + b(d_T(v_j|P) - d_T(v_{\lfloor d/2 \rfloor+1}|P)) \\ &\quad + ab(|j-i|-1) > 0, \end{aligned}$$

a contradiction. Hence $(i,j) = \left(\lfloor \frac{1}{2}d \rfloor, \lfloor \frac{1}{2}d \rfloor + 1\right)$ or $\left(\frac{1}{2}d, \frac{1}{2}d - 1\right)$. For the case $(i,j) = \left(\frac{1}{2}d, \frac{1}{2}d - 1\right)$, we may turn to the first case by relabeling the vertices of the path P conversely. Hence T has exactly two vertices $v_{\lfloor d/2 \rfloor}$ and $v_{\lfloor d/2 \rfloor+1}$ of degree at least three on P. Then

$$\begin{aligned} W(T) &= W(P) + a(d+1+d_T(v_{\lfloor d/2 \rfloor}|P)) \\ &\quad + b(d+1+d_T(v_{\lfloor d/2 \rfloor+1}|P)) + 2\binom{a}{2} + 2\binom{b}{2} + 3ab \\ &= W(P) + ad_T(v_{\lfloor d/2 \rfloor}|P) + bd_T(v_{\lfloor d/2 \rfloor+1}|P) \\ &\quad + (a+b)(d+1) + a(a-1) + b(b-1) + 3ab \\ &= W(P_{d+1}) + (a+b)\Big(\Big\lfloor \frac{d}{2} \Big\rfloor^2 - d\Big\lfloor \frac{d}{2} \Big\rfloor + \frac{d(d+1)}{2}\Big) \\ &\quad + 2b\Big\lfloor \frac{d}{2} \Big\rfloor - bd + b + (a+b)(a+b+d) + ab \\ &= \frac{d(d+1)(d+2)}{6} + (n-d-1)\Big(\Big\lfloor \frac{d}{2} \Big\rfloor^2 - d\Big\lfloor \frac{d}{2} \Big\rfloor + \frac{d(d+1)}{2}\Big) \\ &\quad + (n-d-1)(n-1) + b\Big(2\Big\lfloor \frac{d}{2} \Big\rfloor - d + 1 + a\Big), \end{aligned}$$

which is minimal for fixed n and d if and only if

$$b\Big(2\Big\lfloor\frac{d}{2}\Big\rfloor-d+1+a\Big)=\begin{cases}ab+b & \text{if } d \text{ is even,}\\ ab & \text{if } d \text{ is odd}\end{cases}$$

is minimal (for positive integers a and b with $a+b=n-d-1$) if and only if $b=1$ if d is even and $a=1$ or $b=1$ if d is odd. Thus $T=N_{n,d}$. $\square$

Lemma 3.2. *For $3\leqslant d\leqslant n-4$, we have $\Lambda(N_{n,d})<\Lambda(N_{n,d+1})$.*

Proof. By Theorem 3.1,

$$\begin{aligned}\Lambda(N_{n,d+1})-\Lambda(N_{n,d})&=\frac{n(n-1)}{2}-W(N_{n,d+1})+W(N_{n,d})\\&=\frac{n(n-1)}{2}+\Big\lfloor\frac{d}{2}\Big\rfloor^2+2\Big(\Big\lfloor\frac{d}{2}\Big\rfloor-\Big\lfloor\frac{d+1}{2}\Big\rfloor\Big)\\&\quad+(n-2)\Big\lfloor\frac{d+1}{2}\Big\rfloor+2d-nd+2\\&\geqslant\frac{n(n-1)}{2}+\Big\lfloor\frac{d}{2}\Big\rfloor^2+(n-2)\Big\lfloor\frac{d+1}{2}\Big\rfloor-(n-2)d\\&\geqslant\frac{n(n-1)}{2}+\Big\lfloor\frac{d}{2}\Big\rfloor^2+(n-2)\cdot\frac{d}{2}-(n-2)d\\&=\frac{n(n-1)}{2}+\Big\lfloor\frac{d}{2}\Big\rfloor^2-\frac{(n-2)d}{2}\\&>0,\end{aligned}$$

from which the result follows. $\square$

By Theorem 3.1 and Lemma 3.1, we have

Theorem 3.3. *Let T be an n-vertex non-starlike tree with $n\geqslant 6$. Then*

$$\Lambda(T)\leqslant\Lambda(N_{n,n-3})$$

with equality if and only if $T=N_{n,n-3}$.

Let $N_{n,n-3}(i,j)$ be the tree formed from the path $P_{n-2}=v_0v_1\dots v_{n-3}$ by attaching a pendent vertex at vertices v_i and v_j, respectively, where $1\leqslant i\leqslant\lfloor\frac{1}{2}(n-3)\rfloor$ and $i<j\leqslant n-4$. By symmetry, $N_{n,n-3}(i,j)=N_{n,n-3}(n-3-j,n-3-i)$ for $\lfloor\frac{1}{2}(n-3)\rfloor<j\leqslant n-4$ and thus, if n is even, then we may further restrict i and j as $i<j\leqslant\frac{1}{2}(n-4)$ or $n-3-i\leqslant j\leqslant n-4$. Similarly, if n is odd, then we may further restrict i and j as (a) $1\leqslant i\leqslant\frac{1}{2}(n-5)$, and $i<j\leqslant\frac{1}{2}(n-5)$ or $n-3-i\leqslant j\leqslant n-4$, or (b) $i=\frac{1}{2}(n-3)$ and $\frac{1}{2}(n-3)<j\leqslant n-4$. Clearly, $N_{n,n-3}=N_{n,n-3}(\lfloor\frac{1}{2}(n-3)\rfloor,\lfloor\frac{1}{2}(n-3)\rfloor+1)$.

It is easily seen that

$$\begin{aligned}W(N_{n,n-3}(i,j)) &= W(P_{n-2})+2(n-2)+d_{N_{n,n-3}(i,j)}(v_i|P_{n-2})\\&\quad+d_{N_{n,n-3}(i,j)}(v_j|P_{n-2})+j-i+2\\&= W(P_{n-2})+2(n-2)+i^2-(n-3)i+\frac{1}{2}(n-3)(n-2)\\&\quad+j^2-(n-3)j+\frac{1}{2}(n-3)(n-2)+j-i+2\\&= W(P_{n-2})+i^2-(n-2)i+j^2-(n-4)j+n(n-3)+4,\end{aligned}$$

and then

$$\begin{aligned}\Lambda(N_{n,n-3}(i,j)) &= \frac{1}{3}(n+1)(n-1)(n-3)-n(n-3)\\&\quad-i^2+(n-2)i-j^2+(n-4)j-4.\end{aligned}$$

Let $[a,b]^0$ be the set of integers in the interval $[a,b]$. Let

$$\mathcal{U}_n^{\mathrm{e}}=\left\{(s,t)\colon\ s\in\left[-\frac{n-6}{2},0\right]^0,\ t\in[s+1,0]^0\cup\left[-s+1,\frac{n-4}{2}\right]^0\right\}$$

for even $n\geqslant 6$, and

$$\begin{aligned}\mathcal{U}_n^{\mathrm{o}}=&\left\{(s,t)\colon\ s\in\left[-\frac{n-5}{2},-1\right]^0,\ t\in[s+1,-1]^0\cup\left[-s,\frac{n-5}{2}\right]^0\right\}\\&\cup\left\{(0,t)\colon\ t\in\left[1,\frac{n-5}{2}\right]^0\right\}\end{aligned}$$

for odd $n\geqslant 7$.

For even n and $(s,t)\in\mathcal{U}_n^{\mathrm{e}}$, let $i_s=\frac{1}{2}(n-4+2s)$, $j_t=\frac{1}{2}(n-4+2t)$, and $f(s,t)=(s-1)^2+t^2$. For odd n and $(s,t)\in\mathcal{U}_n^{\mathrm{o}}$, let $i_s=\frac{1}{2}(n-3+2s)$, $j_t=\frac{1}{2}(n-3+2t)$, and $g(s,t)=s(s-1)+t(t+1)$. Clearly, $N_{n,n-3}=N_{n,n-3}(i_0,j_1)$. For $(s,t)\in\mathcal{U}_n^{\mathrm{e}}\cup\mathcal{U}_n^{\mathrm{o}}$,

$$\begin{aligned}\Lambda(N_{n,n-3}(i_s,j_t)) &= \frac{1}{3}(n+1)(n-1)(n-3)-n(n-3)\\&\quad-i_s^2+(n-2)i_s-j_t^2+(n-4)j_t-4\\&=\begin{cases}\frac{1}{3}(n+1)(n-1)(n-3)-\frac{1}{2}n^2\\\qquad-(s-1)^2-t^2+1 & \text{for even } n,\\\frac{1}{3}(n+1)(n-1)(n-3)-\frac{1}{2}n^2\\\qquad-s(s-1)-t(t+1)+\frac{1}{2} & \text{for odd } n\end{cases}\\&=\begin{cases}\frac{1}{3}(n+1)(n-1)(n-3)-\frac{1}{2}n^2+1-f(s,t) & \text{for even } n,\\\frac{1}{3}(n+1)(n-1)(n-3)-\frac{1}{2}n^2+\frac{1}{2}-g(s,t) & \text{for odd } n.\end{cases}\end{aligned}$$

Lemma 3.4. *Let T be an n-vertex non-starlike tree different from $N_{n,n-3}$ with diameter $n-3$, where $n \geqslant 8$. If n is even and $T \neq N_{n,n-3}(i_{-1}, j_0)$, $N_{n,n-3}(i_0, j_2)$, $N_{n,n-3}(i_{-1}, j_2)$, then*

$$\begin{aligned}\Lambda(N_{n,n-3}(i_{-1}, j_0)) &> \Lambda(N_{n,n-3}(i_0, j_2)) \\ &> \Lambda(N_{n,n-3}(i_{-1}, j_2)) \\ &> \Lambda(T),\end{aligned}$$

while if n is odd and $T \neq N_{n,n-3}(i_{-1}, j_1)$, $N_{n,n-3}(i_0, j_2)$, $N_{n,n-3}(i_{-2}, j_{-1})$, $N_{n,n-3}(i_{-1}, j_2)$, then

$$\begin{aligned}\Lambda(N_{n,n-3}(i_{-1}, j_1)) &> \Lambda(N_{n,n-3}(i_0, j_2)) = \Lambda(N_{n,n-3}(i_{-2}, j_{-1})) \\ &> \Lambda(N_{n,n-3}(i_{-1}, j_2)) \\ &> \Lambda(T).\end{aligned}$$

Proof. Obviously, any n-vertex non-starlike tree with diameter $n-3$ is of the form $N_{n,n-3}(i_s, j_t)$, where $(s,t) \in \mathcal{U}_n^{\mathrm{e}}$ for even n and $(s,t) \in \mathcal{U}_n^{\mathrm{o}}$ for odd n.

Case 1. n is even. It is easily seen that

$$f(0,1) = 2 < f(-1,0) = 4 < f(0,2) = 5 < f(-1,2) = 8.$$

Suppose that $(s,t) \neq (0,1), (-1,0), (0,2), (-1,2)$. We have $s \in [-\frac{1}{2}(n-6), -2]^0$ and then $f(s,t) \geqslant 9 + t^2 > 8$, or $t \in [3, \frac{1}{2}(n-4)]^0$ and then $f(s,t) \geqslant 9 + (s-1)^2 > 8$. Since $\Lambda(N_{n,n-3}(i_s, j_t)) = \frac{1}{3}(n+1)(n-1)(n-3) - \frac{1}{2}n^2 + 1 - f(s,t)$ and $T \neq N_{n,n-3} = N_{n,n-3}(i_0, j_1)$, $N_{n,n-3}(i_{-1}, j_0)$, $N_{n,n-3}(i_0, j_2)$, $N_{n,n-3}(i_{-1}, j_2)$, we have

$$\begin{aligned}\Lambda(N_{n,n-3}(i_0, j_1)) &> \Lambda(N_{n,n-3}(i_{-1}, j_0)) \\ &> \Lambda(N_{n,n-3}(i_0, j_2)) \\ &> \Lambda(N_{n,n-3}(i_{-1}, j_2)) \\ &> \Lambda(T).\end{aligned}$$

Case 2. n is odd. It is easily seen that

$$g(0,1) = 2 < g(-1,1) = 4 < g(0,2) = g(-2,-1) = 6 < g(-1,2) = 8.$$

Suppose that $(s,t) \neq (0,1), (-1,1), (0,2), (-2,-1), (-1,2)$. We have $(s,t) = (-2,2)$ and then $g(s,t) = 12 > 8$, or $s \in [-\frac{1}{2}(n-5), -3]^0$ and then $g(s,t) \geqslant 12 + t(t+1) > 8$, or $t \in [3, \frac{1}{2}(n-5)]^0$ and then $g(s,t) \geqslant 12 + s(s-1) > 8$. Since $\Lambda(N_{n,n-3}(i_s, j_t)) = \frac{1}{3}(n+1)(n-1)(n-3) - \frac{1}{2}n^2 + \frac{1}{2} - g(s,t)$ and $T \neq N_{n,n-3} =$

$N_{n,n-3}(i_0,j_1)$,$N_{n,n-3}(i_{-1},j_1)$, $N_{n,n-3}(i_0,j_2)$, $N_{n,n-3}(i_{-2},j_{-1})$, $N_{n,n-3}(i_{-1},j_2)$, we have

$$\begin{aligned}\Lambda(N_{n,n-3}(i_0,j_1)) &> \Lambda(N_{n,n-3}(i_{-1},j_1))\\ &> \Lambda(N_{n,n-3}(i_0,j_2)) = \Lambda(N_{n,n-3}(i_{-2},j_{-1}))\\ &> \Lambda(N_{n,n-3}(i_{-1},j_2))\\ &> \Lambda(T).\end{aligned}$$

The result follows by combining Cases 1 and 2. □

Note that $N_{6,3}$ (see Figure 3) is the only 6-vertex non-starlike tree, and $N_{7,4}$, $N_{7,4}(1,3)$, and $N_{7,3}$ (see Figure 3) are all the 7-vertex non-starlike trees. It is easily seen that $\Lambda(N_{7,4}) = 38 > \Lambda(N_{7,4}(1,3)) = 36 > \Lambda(N_{7,3}) = 21$.

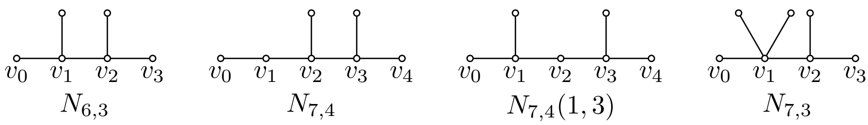

Figure 3. The non-starlike trees with 6 or 7 vertices.

Theorem 3.5. *Let T be an n-vertex non-starlike tree with $n \geqslant 8$, and $T \neq N_{n,n-3}$.*

(i) *If n is even and $T \neq N_{n,n-3}\left(\frac{1}{2}(n-6),\frac{1}{2}(n-4)\right)$, $N_{n,n-3}\left(\frac{1}{2}(n-4),\frac{1}{2}n\right)$, $N_{n,n-3}\left(\frac{1}{2}(n-6),\frac{1}{2}n\right)$, then*

$$\begin{aligned}\Lambda\Big(N_{n,n-3}\Big(\frac{n-6}{2},\frac{n-4}{2}\Big)\Big) &> \Lambda\Big(N_{n,n-3}\Big(\frac{n-4}{2},\frac{n}{2}\Big)\Big)\\ &> \Lambda\Big(N_{n,n-3}\Big(\frac{n-6}{2},\frac{n}{2}\Big)\Big)\\ &> \Lambda(T);\end{aligned}$$

(ii) *If n is odd and $T \neq N_{n,n-3}\left(\frac{1}{2}(n-5),\frac{1}{2}(n-1)\right)$, $N_{n,n-3}\left(\frac{1}{2}(n-3),\frac{1}{2}(n+1)\right)$, $N_{n,n-3}\left(\frac{1}{2}(n-7),\frac{1}{2}(n-5)\right)$, $N_{n,n-3}\left(\frac{1}{2}(n-5),\frac{1}{2}(n+1)\right)$, then*

$$\begin{aligned}\Lambda\Big(N_{n,n-3}\Big(\frac{n-5}{2},\frac{n-1}{2}\Big)\Big) &> \Lambda\Big(N_{n,n-3}\Big(\frac{n-3}{2},\frac{n+1}{2}\Big)\Big) = \Lambda\Big(N_{n,n-3}\Big(\frac{n-7}{2},\frac{n-5}{2}\Big)\Big)\\ &> \Lambda\Big(N_{n,n-3}\Big(\frac{n-5}{2},\frac{n+1}{2}\Big)\Big)\\ &> \Lambda(T).\end{aligned}$$

Proof. Note that

$$\begin{aligned}
W(N_{n,n-4}) &= \frac{(n-2)(n-3)(n-4)}{6} + 3\Big(\Big\lfloor\frac{n-4}{2}\Big\rfloor^2 - (n-4)\Big\lfloor\frac{n-4}{2}\Big\rfloor \\
&\quad + \frac{(n-4)(n-3)}{2}\Big) + 2\Big\lfloor\frac{n-4}{2}\Big\rfloor + 2(n+1) + 2 \\
&= \frac{(n-2)(n-3)(n-4)}{6} + 3\Big\lfloor\frac{n-4}{2}\Big\rfloor^2 - 3(n-4)\Big\lfloor\frac{n-4}{2}\Big\rfloor + 2\Big\lfloor\frac{n-4}{2}\Big\rfloor \\
&\quad + \frac{3n^2-17n}{2} + 22 \\
&= \begin{cases} \frac{1}{6}(n-2)(n-3)(n-4) + \frac{3}{4}n(n-2) + 6 & \text{for even } n, \\ \frac{1}{6}(n-2)(n-3)(n-4) + \frac{3}{4}n(n-2) + \frac{23}{4} & \text{for odd } n. \end{cases}
\end{aligned}$$

We have

$$\Lambda(N_{n,n-4}) - \Lambda(N_{n,n-3}(i_s,j_t)) = \begin{cases} -\frac{1}{4}(n^2+2n+16) + f(s,t) & \text{for even } n, \\ -\frac{1}{4}(n^2+2n+13) + g(s,t) & \text{for odd } n. \end{cases}$$

Then

$$\begin{aligned}
\Lambda(N_{n,n-4}) - \Lambda(N_{n,n-3}(i_{-1},j_2)) &= \begin{cases} -\frac{1}{4}(n^2+2n+16) + f(-1,2) & \text{for even } n, \\ -\frac{1}{4}(n^2+2n+13) + g(-1,2) & \text{for odd } n \end{cases} \\
&\leqslant \begin{cases} -\frac{1}{4}(8^2+2\times 8+16) + 8 < 0 & \text{for even } n, \\ -\frac{1}{4}(9^2+2\times 9+13) + 8 < 0 & \text{for odd } n, \end{cases}
\end{aligned}$$

i.e., $\Lambda(N_{n,n-4}) < \Lambda(N_{n,n-3}(i_{-1},j_2))$. Now the result follows from Lemma 3.2. □

4. Reverse Wiener indices of non-starlike non-caterpillar trees

Let $\mathcal{NSC}_{n,d}$ be the class of non-starlike non-caterpillar trees with n vertices and diameter d, where $4 \leqslant d \leqslant n-4$. Let $\widetilde{N}_{n,d}$ be the tree obtained from the path $P_{d+1} = v_0v_1\ldots v_d$ by attaching $n-d-4$ pendent vertices and a path P_2 to the vertex $v_{\lfloor d/2\rfloor}$ and attaching one pendent vertex to the vertex $v_{\lfloor d/2\rfloor+1}$, see Figure 4.

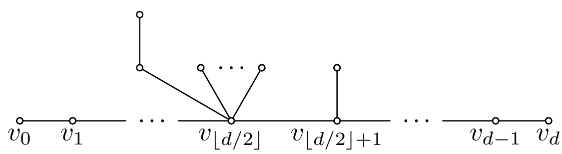

Figure 4. The tree $\widetilde{N}_{n,d}$.

Theorem 4.1. *Let $T \in \mathcal{NSC}_{n,d}$, where $4 \leqslant d \leqslant n-4$. Then*

$$W(T) \geqslant \frac{d(d+1)(d+2)}{6} + (n-d-1)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big) + 2\Big\lfloor\frac{d}{2}\Big\rfloor + (n+1)(n-d-1) - 2$$

with equality if and only if $T = \widetilde{N}_{n,d}$.

Proof. By direct calculation, we have

$$\begin{aligned}
W(\widetilde{N}_{n,d}) &= W(P_{d+1}) + [2(d+1) + d_{\widetilde{N}_{n,d}}(v_{\lfloor d/2\rfloor}|P_{d+1})] \\
&\quad + (n-d-3)(d+1+d_{\widetilde{N}_{n,d}}(v_{\lfloor d/2\rfloor}|P_{d+1})) \\
&\quad + (d+1+d_{\widetilde{N}_{n,d}}(v_{\lfloor d/2\rfloor+1}|P_{d+1})) + 2\binom{n-d-3}{2} \\
&\quad + 3(n-d-4) + 1 + 3(n-d-3) + 4 \\
&= W(P_{d+1}) + (n-d-2)d_{\widetilde{N}_{n,d}}(v_{\lfloor d/2\rfloor}|P_{d+1}) + d_{\widetilde{N}_{n,d}}(v_{\lfloor d/2\rfloor+1}|P_{d+1}) \\
&\quad + (n-d)(d+1) + (n-d)(n-d-4) + 3(n-d-3) + 5 \\
&= W(P_{d+1}) + (n-d-2)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big) \\
&\quad + \Big[\Big(\Big\lfloor\frac{d}{2}\Big\rfloor+1\Big)^2 - d\Big(\Big\lfloor\frac{d}{2}\Big\rfloor+1\Big) + \frac{d(d+1)}{2}\Big] \\
&\quad + n^2 - nd - 4 \\
&= \frac{d(d+1)(d+2)}{6} + (n-d-1)\Big(\Big\lfloor\frac{d}{2}\Big\rfloor^2 - d\Big\lfloor\frac{d}{2}\Big\rfloor + \frac{d(d+1)}{2}\Big) \\
&\quad + 2\Big\lfloor\frac{d}{2}\Big\rfloor + (n+1)(n-d-1) - 2.
\end{aligned}$$

Let T be a tree in $\mathcal{NSC}_{n,d}$ with minimum Wiener index. We need only to show that $T = \widetilde{N}_{n,d}$. Let $P = v_0v_1\ldots v_d$ be a diameter-achieving path of T.

Suppose that there exists a vertex in T (outside P), the distance from which to P is at least three. Let w be such a vertex, the distance from which to P is maximal. Then w is pendent. Let $wvu\ldots$ be the shortest path from w to P. Note that $\sigma(T;u,v) \in \mathcal{NSC}_{n,d}$. By Lemma 2.1, we have $W(\sigma(T;u,v)) < W(T)$, a contradiction. Thus the maximal distance from the vertices outside P to P is two. Suppose that there are at least two vertices of degree at least two outside P. For any such vertex, say z, with z' denoting its neighbor on P, we have $\sigma(T;z',z) \in \mathcal{NSC}_{n,d}$ and by Lemma 2.1, $W(\sigma(T;z',z)) < W(T)$, a contradiction. It follows that there is exactly one vertex, say x, of degree at least two outside P.

Let s be the number of pendent neighbors of x. If $s > 1$, we obtain a tree $T' \in \mathcal{NSC}_{n,d}$ from T by moving $s-1$ pendent neighbors of x to its neighbor on P.

Obviously $n-s>3$. Then

$$\begin{aligned} W(T)-W(T') &= (s+1)(n-s-1)-2(n-2) \\ &= (s-1)(n-s-3)>0, \end{aligned}$$

a contradiction. Thus the only vertex outside P of degree at least two has degree two.

If there are at least three vertices of degree at least three on P, then for two such vertices with minimal distance, by Lemma 2.4 we obtain a tree in $\mathcal{NSC}_{n,d}$ with a Wiener index smaller than T, a contradiction. It follows that there are exactly two vertices, say v_i and v_j, of degree at least three on P. Note that there is exactly one vertex x outside P having degree two, and all other vertices outside P are pendent. Suppose without loss of generality that x is a neighbor of v_i. Let a or b be the number of pendent neighbors of v_i or v_j, respectively, outside P, where $a \geqslant 0$ and $b \geqslant 1$.

If $|i-\frac{1}{2}d| > |j-\frac{1}{2}d|$, then by moving all the pendent neighbors (if such exist) outside P of v_i to v_j and the pendent neighbor of x to a pendent neighbor of v_j, we obtain a tree $T_1 \in \mathcal{NSC}_{n,d}$, and by Lemma 2.2, it is easily seen that

$$W(T)-W(T_1) = (a+1)(d_T(v_i|P)-d_T(v_j|P)) + (a+1)(b-1)|i-j| > 0,$$

a contradiction. Thus $|i-\frac{1}{2}d| \leqslant |j-\frac{1}{2}d|$.

If $b \geqslant 2$, then by moving all but one pendent neighbors of v_j outside P to v_i, we have a tree $T_2 \in \mathcal{NSC}_{n,d}$, and by Lemma 2.2, it is easily seen that

$$W(T)-W(T_2) = (b-1)(d_T(v_j|P)-d_T(v_i|P)) + (a+1)(b-1)|i-j| > 0,$$

a contradiction. Thus $b=1$, i.e., v_i has $n-d-4$ pendent neighbors and one neighbor x of degree two (outside P), and v_j has exactly one pendent neighbor (outside P). Then

$$\begin{aligned} W(T) = {} & W(P) + [2(d+1) + d_T(v_i|P)] \\ & + (n-d-3)(d+1+d_T(v_i|P)) \\ & + (d+1+d_T(v_j|P)) + 2\binom{n-d-3}{2} \\ & + 3(n-d-4) + 1 + (n-d-3)(|i-j|+2) + (|i-j|+3) \\ = {} & W(P_{d+1}) + (n-d-2)d_T(v_i|P) + d_T(v_j|P) \\ & + (n-d)(d+1) + (n-d)(n-d-4) + 2(n-d-3) + 4 \\ & + (n-d-2)|i-j|, \end{aligned}$$

which is minimal for fixed n and d if and only if

$$F(i,j) = (n-d-2)d_T(v_i|P) + d_T(v_j|P) + (n-d-2)|i-j|$$

is minimal. By Lemma 2.2, if d is even, $F(i,j)$ is minimal if and only if $i = \frac{1}{2}d$ and $j = \frac{1}{2}d \pm 1$, while if d is odd, $F(i,j)$ is minimal if and only if $i = \frac{1}{2}(d \pm 1)$ and $j = \frac{1}{2}(d \mp 1)$. Thus $T = \widetilde{N}_{n,d}$. □

Lemma 4.2. *For $4 \leqslant d \leqslant n-5$, we have $\Lambda(\widetilde{N}_{n,d}) < \Lambda(\widetilde{N}_{n,d+1})$.*

Proof. As in the proof of Lemma 3.1, we have

$$\begin{aligned}\Lambda(\widetilde{N}_{n,d+1}) - \Lambda(\widetilde{N}_{n,d}) &= \frac{n(n-1)}{2} - W(\widetilde{N}_{n,d+1}) + W(\widetilde{N}_{n,d}) \\ &= \frac{n(n-1)}{2} + \Big\lfloor \frac{d}{2} \Big\rfloor^2 + 2\Big\lfloor \frac{d}{2} \Big\rfloor - 2\Big\lfloor \frac{d+1}{2} \Big\rfloor \\ &\quad + (n-2)\Big\lfloor \frac{d+1}{2} \Big\rfloor + 2d - nd + 2 > 0,\end{aligned}$$

from which the result follows. □

By Theorem 4.1 and Lemma 4.1, we have

Theorem 4.3. *Let T be an n-vertex non-starlike non-caterpillar tree with $n \geqslant 8$. Then*

$$\Lambda(T) \leqslant \Lambda(\widetilde{N}_{n,n-4})$$

with equality if and only if $T = \widetilde{N}_{n,n-4}$.

Let $\widetilde{N}_{n,n-4}(i,j)$ be the tree formed from the path $P_{n-3} = v_0 v_1 \ldots v_{n-4}$ by attaching a path on two vertices and a pendent vertex at vertices v_i and v_j, respectively, where $2 \leqslant i \leqslant \lfloor \frac{1}{2}(n-4) \rfloor$, $1 \leqslant j \leqslant n-5$ and $j \neq i$. By symmetry, if n is even and $i = \frac{1}{2}(n-4)$, then we may restrict ourselves to $\frac{1}{2}(n-4) < j \leqslant n-5$. Clearly, $\widetilde{N}_{n,n-4} = \widetilde{N}_{n,n-4}(\lfloor \frac{1}{2}(n-4) \rfloor, \lfloor \frac{1}{2}(n-4) \rfloor + 1)$. It is easily seen that

$$\begin{aligned}W(\widetilde{N}_{n,n-4}(i,j)) &= W(P_{n-3}) + 4(n-3) + 2d_{\widetilde{N}_{n,n-4}(i,j)}(v_i|P_{n-3}) \\ &\quad + d_{\widetilde{N}_{n,n-4}(i,j)}(v_j|P_{n-3}) + 2|i-j| + 6 \\ &= W(P_{n-3}) + \frac{3}{2}(n-3)(n-4) + 4n - 6 + 2[i^2 - (n-4)i] \\ &\quad + [j^2 - (n-4)j] + 2|i-j|,\end{aligned}$$

and then

$$\begin{aligned}\Lambda(\widetilde{N}_{n,n-4}(i,j)) &= \frac{1}{6}(n-4)(2n^2 - 7n + 21) - 4n + 6 \\ &\quad - 2[i^2 - (n-4)i] - [j^2 - (n-4)j] - 2|i-j|.\end{aligned}$$

Let

$$\mathcal{C}_n^{\mathrm{e}} = \Big\{(s,t)\colon\ s \in \Big[-\frac{n-8}{2}, -1\Big]^0,\ t \in \Big[-\frac{n-6}{2}, \frac{n-6}{2}\Big]^0,\ s \neq t\Big\} \\ \cup \Big\{(0,t)\colon\ t \in \Big[1, \frac{n-6}{2}\Big]^0\Big\}$$

for even $n \geqslant 8$, and

$$\mathcal{C}_n^{\mathrm{o}} = \Big\{(s,t)\colon\ s \in \Big[-\frac{n-9}{2}, 0\Big]^0,\ t \in \Big[-\frac{n-7}{2}, \frac{n-5}{2}\Big]^0,\ s \neq t\Big\}$$

for odd $n \geqslant 9$.

For even n and $(s,t) \in \mathcal{C}_n^{\mathrm{e}}$, let $i_s = \frac{1}{2}(n-4+2s)$, $j_t = \frac{1}{2}(n-4+2t)$, and $f_2(s,t) = 2s^2+t^2+2|s-t|$. For odd n and $(s,t) \in \mathcal{C}_n^{\mathrm{o}}$, let $i_s = \frac{1}{2}(n-5+2s)$, $j_t = \frac{1}{2}(n-5+2t)$, and $g_2(s,t) = 2s(s-1)+t(t-1)+2|s-t|$. Clearly, $\widetilde{N}_{n,n-4} = \widetilde{N}_{n,n-4}(i_0, j_1)$. For $(s,t) \in \mathcal{C}_n^{\mathrm{o}} \cup \mathcal{C}_n^{\mathrm{e}}$,

$$\begin{aligned}
\Lambda(\widetilde{N}_{n,n-4}(i_s, j_t)) &= \frac{1}{6}(n-4)(2n^2-7n+21) - 4n + 6 \\
&\quad - 2[i_s^2 - (n-4)i_s] - [j_t^2 - (n-4)j_t] - 2|i_s - j_t| \\
&= \begin{cases} \frac{1}{6}(n-4)(2n^2-7n+21) + \frac{3}{4}n^2 - 10n + 18 & \\ \qquad -2s^2 - t^2 - 2|s-t| & \text{for even } n, \\ \frac{1}{6}(n-4)(2n^2-7n+21) + \frac{3}{4}n^2 - 10n + \frac{69}{4} & \\ \qquad -2s(s-1) - t(t-1) - 2|s-t| & \text{for odd } n \end{cases} \\
&= \begin{cases} \frac{1}{6}(n-4)(2n^2-7n+21) + \frac{3}{4}n^2 - 10n + 18 & \\ \qquad -f_2(s,t) & \text{for even } n, \\ \frac{1}{6}(n-4)(2n^2-7n+21) + \frac{3}{4}n^2 - 10n + \frac{69}{4} & \\ \qquad -g_2(s,t) & \text{for odd } n. \end{cases}
\end{aligned}$$

Lemma 4.4. *Let T be an n-vertex non-starlike non-caterpillar tree with diameter $d = n-4$, where $n \geqslant 10$ and $T \neq \widetilde{N}_{n,n-4}$. If n is even, and $T \neq \widetilde{N}_{n,n-4}(i_{-1}, j_0)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_1)$, $\widetilde{N}_{n,n-4}(i_0, j_2)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_{-2})$, then*

$$\begin{aligned}
\Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_0)) &> \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1)) \\
&> \Lambda(\widetilde{N}_{n,n-4}(i_0, j_2)) = \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_{-2})) \\
&> \Lambda(T),
\end{aligned}$$

while if n is odd and $T \neq \widetilde{N}_{n,n-4}(i_0, j_{-1})$, $\widetilde{N}_{n,n-4}(i_0, j_2)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_0)$, $\widetilde{N}_{n,n-4}$ (i_{-1}, j_1), then

$$\begin{aligned}
\Lambda(\widetilde{N}_{n,n-4}(i_0, j_{-1})) &> \Lambda(\widetilde{N}_{n,n-4}(i_0, j_2)) = \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_0)) \\
&> \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1)) \\
&> \Lambda(T).
\end{aligned}$$

P r o o f. Obviously, any n-vertex non-starlike non-caterpillar tree with diameter $d = n-4$ is of the form $\widetilde{N}_{n,n-4}(i_s, j_t)$, where $(s,t) \in \mathcal{C}_n^{\mathrm{e}}$ for even n and $(s,t) \in \mathcal{C}_n^{\mathrm{o}}$ for odd n.

C a s e 1. n is even. It is easily seen that

$$f_2(0,1) = 3 < f_2(-1,0) = 4 < f_2(-1,1) = 7 < f_2(0,2) = f_2(-1,-2) = 8.$$

Suppose that $(s,t) \neq (0,1), (-1,0), (-1,1), (0,2), (-1,-2)$. Since $2|s-t| \geqslant 2$, we have $(s,t) = (-1,2)$ and then $f_2(-1,2) = 12 > 8$, or $s \in [-\frac{1}{2}(n-8), -2]^0$ and then $f_2(s,t) \geqslant 10 + t^2 > 8$, or $t \in [-\frac{1}{2}(n-6), -3]^0$ and then $f_2(s,t) \geqslant 11 + 2s^2 > 8$, or $t \in [3, \frac{1}{2}(n-6)]^0$ and then $f_2(s,t) \geqslant 11 + 2s^2 > 8$. Since $\Lambda(\widetilde{N}_{n,n-4}) = \frac{1}{6}(n-4)(2n^2 - 7n + 21) + \frac{3}{4}n^2 - 10n + 18 - f_2(s,t)$ and $T \neq \widetilde{N}_{n,n-4} = \widetilde{N}_{n,n-4}(i_0, j_1)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_0)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_1)$, $\widetilde{N}_{n,n-4}(i_0, j_2)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_{-2})$, we have

$$\begin{aligned}\Lambda(\widetilde{N}_{n,n-4}(i_0, j_1)) &> \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_0)) \\ &> \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1)) \\ &> \Lambda(\widetilde{N}_{n,n-4}(i_0, j_2)) = \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_{-2})) \\ &> \Lambda(T).\end{aligned}$$

C a s e 2. n is odd. It is easily seen that

$$g_2(0,1) = 2 < g_2(0,-1) = 4 < g_2(0,2) = g_2(-1,0) = 6 < g_2(-1,1) = 8.$$

Suppose that $(s,t) \neq (0,1), (0,-1), (0,2), (-1,0), (-1,1)$. Since $2|s-t| \geqslant 2$, we have $(s,t) = (-1,2)$ and then $g_2(-1,2) = 12 > 8$, or $s \in [-\frac{1}{2}(n-9), -2]^0$ and then $g_2(s,t) \geqslant 14 + t(t-1) > 8$, or $t \in [-\frac{1}{2}(n-7), -2]^0$ and then $g_2(s,t) \geqslant 6 + 2s(s-1) + 2|s-t| > 8$, or $t \in [3, \frac{1}{2}(n-5)]^0$ and then $g_2(s,t) \geqslant 6 + 2s(s-1) + 2|s-t| > 8$. Since $\Lambda(\widetilde{N}_{n,n-4}) = \frac{1}{6}(n-4)(2n^2 - 7n + 21) + \frac{3}{4}n^2 - 10n + \frac{69}{4} - g_2(s,t)$ and $T \neq \widetilde{N}_{n,n-4}(i_0, j_1)$, $\widetilde{N}_{n,n-4}(i_0, j_{-1})$, $\widetilde{N}_{n,n-4}(i_0, j_2)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_0)$, $\widetilde{N}_{n,n-4}(i_{-1}, j_1)$, we have

$$\begin{aligned}\Lambda(\widetilde{N}_{n,n-4}(i_0, j_1)) &> \Lambda(\widetilde{N}_{n,n-4}(i_0, j_{-1})) \\ &> \Lambda(\widetilde{N}_{n,n-4}(i_0, j_2)) = \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_0)) \\ &> \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1)) \\ &> \Lambda(T).\end{aligned}$$

The result follows by combining Cases 1 and 2. □

Note that $\widetilde{N}_{8,4}$ (see Figure 5) is the only 8-vertex non-starlike non-caterpillar tree, and $\widetilde{N}_{9,5}$, $\widetilde{N}_{9,5}(2,1)$, $\widetilde{N}_{9,5}(2,4)$, and $\widetilde{N}_{9,4}$ (see Figure 5) are all the 9-vertex non-starlike non-caterpillar trees. It is easily seen that $\Lambda(\widetilde{N}_{9,5}) = 86 > \Lambda(\widetilde{N}_{9,5}(2,1)) = 84 > \Lambda(\widetilde{N}_{9,5}(2,4)) = 82 > \Lambda(\widetilde{N}_{9,4}) = 58$.

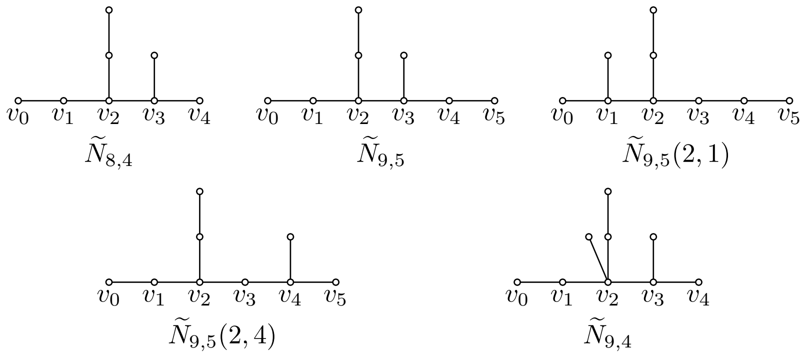

Figure 5. The non-starlike non-caterpillar trees with 8 or 9 vertices.

Theorem 4.5. *Let T be an n-vertex non-starlike non-caterpillar tree with $n \geqslant 10$, and $T \neq \widetilde{N}_{n,n-4}$.*

(i) *If n is even and $T \neq \widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-6), \frac{1}{2}(n-4)\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-6), \frac{1}{2}(n-2)\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-4), \frac{1}{2}n\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-6), \frac{1}{2}(n-8)\bigr)$, then*

$$\begin{aligned}\Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-6}{2}, \frac{n-4}{2}\Bigr)\Bigr) &> \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-6}{2}, \frac{n-2}{2}\Bigr)\Bigr)\\ &> \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-4}{2}, \frac{n}{2}\Bigr)\Bigr)\\ &= \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-6}{2}, \frac{n-8}{2}\Bigr)\Bigr)\\ &> \Lambda(T);\end{aligned}$$

(ii) *If n is odd and $T \neq \widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-5), \frac{1}{2}(n-7)\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-5), \frac{1}{2}(n-1)\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-7), \frac{1}{2}(n-5)\bigr)$, $\widetilde{N}_{n,n-4}\bigl(\frac{1}{2}(n-7), \frac{1}{2}(n-3)\bigr)$, then*

$$\begin{aligned}\Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-5}{2}, \frac{n-7}{2}\Bigr)\Bigr) &> \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-5}{2}, \frac{n-1}{2}\Bigr)\Bigr)\\ &= \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-7}{2}, \frac{n-5}{2}\Bigr)\Bigr)\\ &> \Lambda\Bigl(\widetilde{N}_{n,n-4}\Bigl(\frac{n-7}{2}, \frac{n-3}{2}\Bigr)\Bigr)\\ &> \Lambda(T).\end{aligned}$$

P r o o f. Note that

$$\begin{aligned}W(\widetilde{N}_{n,n-5}) &= \frac{(n-3)(n-4)(n-5)}{6} + 4\Bigl[\Bigl\lfloor\frac{n-5}{2}\Bigr\rfloor^2 - (n-5)\Bigl\lfloor\frac{n-5}{2}\Bigr\rfloor\Bigr] + 2\Bigl\lfloor\frac{n-5}{2}\Bigr\rfloor\\ &\quad + 2(n-4)(n-5) + 4(n+1) - 2\\ &= \frac{1}{6}(n-3)(n-4)(n-5) + n(n-3) + 12.\end{aligned}$$

Then

$$\Lambda(\widetilde{N}_{n,n-5}) - \Lambda(\widetilde{N}_{n,n-4}(i_s, j_t)) = \begin{cases} -\frac{1}{4}(n^2+2n+24) + f_2(s,t) & \text{for even } n, \\ -\frac{1}{4}(n^2+2n+21) + g_2(s,t) & \text{for odd } n. \end{cases}$$

Thus

$$\Lambda(\widetilde{N}_{n,n-5}) - \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_{-2})) = -\frac{1}{4}(n^2+2n+24)+8 \leqslant -\frac{1}{4}(10^2+20+24)+8 < 0$$

for even n, and

$$\begin{aligned} \Lambda(\widetilde{N}_{n,n-5}) - \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1)) &= -\frac{1}{4}(n^2+2n+21)+8 \\ &\leqslant -\frac{1}{4}(11^2+22+21)+8 < 0 \end{aligned}$$

for odd n. Then $\Lambda(\widetilde{N}_{n,n-5}) < \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_{-2}))$ for even n and $\Lambda(\widetilde{N}_{n,n-5}) < \Lambda(\widetilde{N}_{n,n-4}(i_{-1}, j_1))$ for odd n. Now the result follows from Lemma 4.2. □

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