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Ordering trees having small reverse Wiener indices

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Abstract. The Wiener index $W(G)$ of a connected graph G is defined as the sum of distances between all unordered pairs of vertices of G. As a variation of the Wiener index, the reverse Wiener index of G is defined as $\Lambda(G) = \frac{1}{2}n(n-1)d - W(G)$, where n is the number of vertices, and d is the diameter of G. It is known that the star is the unique n-vertex tree with the smallest reverse Wiener index. We now determine the second and the third smallest reverse Wiener indices of n-vertex trees, and characterize the trees whose reverse Wiener indices attain these values for $n \geq 5$.

1. Introduction

Let G be a simple connected graph. The Wiener index of G is defined as the sum of distances between all unordered pairs of vertices of G, denoted by $W(G)$ [14, 15, 28]. The Wiener index is one of the oldest and the most useful molecular descriptors used to explain various chemical and physical properties of molecules and to correlate the structure of molecules with their biological activity [17, 22, 25, 26]. It also found applications in other fields such as social science and architecture, and among others, it is known as the total status, the distance, or the transmission of a graph [3, 12, 13, 21, 24]. Equivalently, the average distance or mean distance $\mu(G) = \frac{2}{n(n-1)}W(G)$ (where $n = |V(G)|$) has also been studied [1, 5–8, 10]. The mathematical properties of Wiener index for trees can be found in the review [9] and in the recent references [11, 23, 27].

In 2000, Balaban *et al.* [2] proposed a variant of the Wiener index, the reverse Wiener index. The reverse Wiener index of G is defined as [2]

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

where n is the number of vertices and d is the diameter of G. The reverse Wiener index is also a useful structure–descriptor, with applications in quantitative structure–property relationship studies, as demonstrated in [2, 16]. Zhang and Zhou [29] showed that the path P_n and the star S_n are respectively the unique n-vertex trees with the largest and the smallest reverse Wiener indices. Cai and Zhou [4] determined the trees with the largest reverse Wiener index within some subclasses of trees. Luo and Zhou determined in [20] the n-vertex trees for $n \geq 5$ with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n}{2} \rfloor + 1$,

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and determined in [19] the n-vertex trees that are not caterpillars (trees for which the removal of pendant vertices results in a path) for $n \geq 8$ with the first a few largest reverse Wiener indices. Li and Zhou [18] determined the n-vertex non-starlike trees with the first four largest reverse Wiener indices for $n \geq 8$, and the n-vertex non-starlike non-caterpillar trees with the first four largest reverse Wiener indices for $n \geq 10$. See the surveys [30, 31] for more results on the reverse Wiener index.

If G is a connected graph with diameter d, then the study of the reverse Wiener index $\Lambda(G)$ is equivalent to the study of $d - \mu(G)$, the difference between the diameter and the average distance.

A k-cyclic graph is a connected graph with cyclomatic number k. If G is a connected graph with m edges and diameter d, then [4]

$$\Lambda(G) \geq (d-1)m$$

with equality if and only if $d \leq 2$. This implies that among n-vertex connected graphs, the complete graph K_n is the unique graph with the smallest reverse Wiener index, and the $(k-2)$-cyclic graphs of diameter two are the unique graph(s) with the kth smallest reverse Wiener index for $k = 2, 3, \ldots, n-1$, respectively.

In this paper, we determine the second and the third smallest reverse Wiener indices of n-vertex trees and characterize the trees whose reverse Wiener indices attain these values for $n \geq 5$.

2. Preliminaries

Let T be a tree with vertex set $V(T)$ and edge set $E(T)$. For any $e \in E(T)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ respectively denote the number of vertices of T lying on the two sides of the edge e. For a long time it is known [14, 28] that

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

A vertex is pendant if it is of degree one. Let $\mathcal{T}_n$ be the set of the trees on n vertices. A center of a tree is a vertex whose eccentricity (the maximum distance from it to any other vertex) is minimal. Let $\mathcal{CT}_n$ be the set of trees T in $\mathcal{T}_n$ such that one center of T has at least one pendant neighbor.

For a tree T with $v \in V(T)$, $T - v$ denotes the subgraph of T obtained by deleting the vertex v and its incident edge(s). And for $u, v \in V(T)$, if u and v are adjacent in T, then $T - uv$ denotes the graph obtained from T by deleting the edge uv, and if u and v are not adjacent in T, then $T + uv$ denotes the graph obtained from T by adding an edge uv.

We need the following two lemmas from [29], and for completeness, we include their proofs.

Lemma 2.1. *Let $T \in \mathcal{CT}_n$ with diameter $d \geq 4$. Then there is a tree $T^* \in \mathcal{T}_n \setminus \mathcal{CT}_n$ with the same diameter as T such that $\Lambda(T^*) < \Lambda(T)$.*

Proof. Let v be a center of T with at least one pendant neighbor, say w. Obviously, there is at least one subtree T_1 in $T - v$ not containing w that possesses $n_1 \leq \frac{n}{2} - 1$ vertices. Let v_1 be the neighbor of v in T_1. Let T' be the tree formed from T by deleting edge vw and adding edge wv_1. Note that both T and T' have diameter d. Then

$$\Lambda(T') - \Lambda(T) = W(T) - W(T') = n_1(n - n_1) - (n_1 + 1)(n - n_1 - 1) < 0,$$

and thus $\Lambda(T') < \Lambda(T)$. Iterating the transformation from T to T' will finally yield the tree T^* as required. □

Lemma 2.2. *Let $T \in \mathcal{T}_n \setminus \mathcal{CT}_n$ with diameter $d \geq 4$. Then there is a tree $T^* \in \mathcal{CT}_n$ with diameter $d - 2$ such that $\Lambda(T^*) < \Lambda(T)$.*

Proof. Let v be a center of T with neighbors $v_1, v_2, \ldots, v_p$. For $i = 1, 2, \ldots, p$, let T_i be the subtree in $T - v$ with $v_i \in V(T_i)$, $v_{i1}, v_{i2}, \ldots, v_{ir_i}$ be the neighbors of v_i in T_i, and $n_i = |V(T_i)|$. Let T^* be the tree formed from T by deleting edges v_iv_{ij} and adding edges vv_{ij} for all $i = 1, 2 \ldots, p$ and $j = 1, 2, \ldots, r_i$. Obviously, $T^* \in \mathcal{CT}_n$. It is easily seen that

$$\begin{aligned}
\Lambda(T^*) - \Lambda(T) &= -n(n-1) + W(T) - W(T^*) \\
&= -n(n-1) + \sum_{i=1}^{p} n_i(n - n_i) - p(n-1) \\
&\le -n(n-1) + (n-1)\sum_{i=1}^{p} n_i - p(n-1) \\
&= -n(n-1) + (n-1)(n-1) - p(n-1) \\
&= -(n-1)(1+p) < 0,
\end{aligned}$$

as desired. □

Denote by S_n the n-vertex star. An n-vertex tree of diameter 4 may be constructed as follows: For some integer $k \ge 2$, it is obtained from the star S_{k+1} with center v_0 and pendant vertices $v_1, v_2, \ldots, v_k$ by attaching m_i pendant vertices to v_i for $i = 0, 1, \ldots, k$, where $m_0 \ge 0$, $m_i \ge 1$ for $i = 1, \ldots, k$, and $\sum_{i=0}^{k} m_i + k + 1 = n$. If there are s distinct (positive) numbers $n_1 < n_2 < \cdots < n_s$ among the numbers $m_1, m_2, \ldots, m_k$, where n_i appears b_i times for $i = 1, 2, \ldots, s$, then such a tree is denoted by $T_{n,k}\big(n_0; n_1^{[b_1]}, n_2^{[b_2]}, \ldots, n_s^{[b_s]}\big)$ with $n_0 = m_0$, where $k \ge 2$, $\sum_{i=1}^{s} b_i = k$ and $\sum_{i=1}^{s} b_i n_i = n - n_0 - k - 1$. If $n_0 = 0$, then we write it simply $T_{n,k}\big(n_1^{[b_1]}, n_2^{[b_2]}, \ldots, n_s^{[b_s]}\big)$.

Obviously, for an integer $n \ge 2$, there is a unique positive integer q such that $q^2 < n \le (q+1)^2$, and thus n may be written as

$$n = q^2 + r \text{ with } r = 1, 2, \ldots, 2q+1. \tag{1}$$

It is easily seen that

$$\begin{aligned}
W\left(T_{n,k}\left(n_0; n_1^{[b_1]}, n_2^{[b_2]}, \ldots, n_s^{[b_s]}\right)\right) &= 1 \cdot (n-1) \cdot (n-1-k) + \sum_{i=1}^{s} b_i(n_i+1)(n-n_i-1) \\
&= (n-1)^2 - (n-1)k + n\sum_{i=1}^{s} b_i(n_i+1) - \sum_{i=1}^{s} b_i(n_i+1)^2 \\
&= (n-1)^2 - (n-1)k + n(n-n_0-1) - 2(n-n_0-k-1) - k - \sum_{i=1}^{s} b_i n_i^2 \\
&= (n-1)(2n-3) - (n-2)k - (n-2)n_0 - \sum_{i=1}^{s} b_i n_i^2.
\end{aligned}$$

Lemma 2.3. *Let $T = T_{n,k}\left(n_0; n_1^{[b_1]}, n_2^{[b_2]}, \ldots, n_s^{[b_s]}\right)$ with $k \ge 2$. If T achieves the smallest reverse Wiener index for fixed n and k, then $s \le 2$, and $n_2 - n_1 = 1$ if $s = 2$.*

Proof. Suppose that there exist i and j with $1 \le i, j \le s$ such that $n_i - n_j \ge 2$ (which is obviously true if $s \ge 3$). Suppose without loss of generality that $v_{i'}$ has n_i pendant neighbors, one of which is denoted by u, and $v_{j'}$ has n_j pendant neighbors, where $1 \le i', j' \le k$. Let $T^* = T - uv_{i'} + uv_{j'}$. Then

$$\begin{aligned}
\Lambda(T) - \Lambda(T^*) &= W(T^*) - W(T) \\
&= n_i(n-n_i) + (n_j+2)(n-n_j-2) - \Big[(n_i+1)(n-n_i-1) + (n_j+1)(n-n_j-1)\Big] \\
&= 2(n_i - n_j - 1) > 0,
\end{aligned}$$

and thus $\Lambda(T) > \Lambda(T^*)$, a contradiction. The result follows. □

Now we use techniques from [27] to prove the following lemma.

Lemma 2.4. *For fixed n of the form* (1), *if* $T_{n,k}\left(n_1^{[b_1]}, n_2^{[b_2]}, \dots, n_s^{[b_s]}\right)$ *with* $k \ge 2$ *and* $s \le 2$ *where* $n_2 - n_1 = 1$ *if* $s = 2$ *achieves the smallest reverse Wiener index, then* $k = q$ *if* $r = 1, \dots, q$, $k \in \{q, q+1\}$ *if* $r = q+1$, *and* $k = q+1$ *if* $r = q+2, \dots, 2q+1$.

Proof. Let $T = T_{n,k}\left(n_1^{[b_1]}, n_2^{[b_2]}, \dots, n_s^{[b_s]}\right)$, where $s = 1, 2$, and $n_2 - n_1 = 1$ if $s = 2$, be a tree with the smallest reverse Wiener index for fixed n.

If $s = 1$, then $n_1 = \frac{n-1}{k} - 1$, $b_1 = k$, and thus

$$\Lambda(T) = 2n(n-1) - W(T) = n - 1 + \left(k + \left\lfloor \frac{n-1}{k} \right\rfloor\right)(n-1).$$

Suppose that $s = 2$. Then $n_1 = \left\lfloor \frac{n-1}{k} \right\rfloor - 1$, $n_2 = \left\lfloor \frac{n-1}{k} \right\rfloor$, $b_1 = \left\lfloor \frac{n-1}{k} \right\rfloor k - (n-k-1)$, $b_2 = n - 1 - \left\lfloor \frac{n-1}{k} \right\rfloor k$, and thus

$$\begin{aligned}
\Lambda(T) &= 2n(n-1) - W(T) \\
&= 3(n-1) + (n-2)k + \left(\left\lfloor \frac{n-1}{k} \right\rfloor k - n + k + 1\right) \cdot \left(\left\lfloor \frac{n-1}{k} \right\rfloor - 1\right)^2 + \left(n - 1 - \left\lfloor \frac{n-1}{k} \right\rfloor k\right) \cdot \left\lfloor \frac{n-1}{k} \right\rfloor^2 \\
&= 2(n-1) + (n-1)k - k\left\lfloor \frac{n-1}{k} \right\rfloor^2 + 2(n-1)\left\lfloor \frac{n-1}{k} \right\rfloor - k\left\lfloor \frac{n-1}{k} \right\rfloor \\
&= n - 1 + \left(k + \left\lfloor \frac{n-1}{k} \right\rfloor\right)(n-1) + \left(n - 1 - k\left\lfloor \frac{n-1}{k} \right\rfloor\right)\left(\left\lfloor \frac{n-1}{k} \right\rfloor + 1\right).
\end{aligned}$$

Note that $k + \left\lfloor \frac{n-1}{k} \right\rfloor \ge 4$ is an integer, and $\left(n - 1 - k\left\lfloor \frac{n-1}{k} \right\rfloor\right)\left(\left\lfloor \frac{n-1}{k} \right\rfloor + 1\right) = b_2(n_2+1) = n - 1 - b_1(n_1+1) < n - 1$. Since $\Lambda(T)$ is minimal, $k + \left\lfloor \frac{n-1}{k} \right\rfloor = \left\lfloor k + \frac{n-1}{k} \right\rfloor$ is minimal.

Note that the function $f(x) = x + \frac{n-1}{x}$ for $x > 0$ attains its minimum at $x = \sqrt{n-1}$. Then for $s \in \{1, 2\}$, $k + \left\lfloor \frac{n-1}{k} \right\rfloor$ is minimal if $k = \lfloor \sqrt{n-1} \rfloor$ or $k = \lceil \sqrt{n-1} \rceil$ (and perhaps for other values of k if $s = 2$). Since n may be written in the form of (1), we have $\lfloor \sqrt{n-1} \rfloor = q$, and $\lceil \sqrt{n-1} \rceil = q$ if $r = 1$ and $q + 1$ otherwise. Thus

$$k + \left\lfloor \frac{n-1}{k} \right\rfloor = \begin{cases} 2q & \text{if } r = 1, \dots, q, \\ 2q+1 & \text{if } r = q+1, \dots, 2q+1. \end{cases}$$

For fixed n, let $h_n(k) = \left(n - 1 - k\left\lfloor \frac{n-1}{k} \right\rfloor\right)\left(\left\lfloor \frac{n-1}{k} \right\rfloor + 1\right)$, which is minimal for integer k satisfying the above equality.

Case 1. $r = 1, \dots, q$. Let $k = q + t$ and $\left\lfloor \frac{n-1}{k} \right\rfloor = q - t$ for some $0 \le t \le q$. Then

$$h_n(k) = [q^2 + r - 1 - (q+t)(q-t)](q - t + 1) = -t[t^2 - (q+1)t + (r-1)] + rq + r - q - 1.$$

If $t \ge 1$, then $t^2 - (q+1)t + (r-1) = \left(t - \frac{q+1}{2}\right)^2 + (r-1) - \frac{(q+1)^2}{4} \le r - q - 1 < 0$, and thus $h_n(k) > rq + r - q - 1 = h_n(q)$, implying that $t = 0$, i.e., $k = q$.

Case 2. $r = q + 1$. Let $k = q + t$ and $\left\lfloor \frac{n-1}{k} \right\rfloor = q + 1 - t$ for some $0 \le t \le q + 1$. Then

$$h_n(k) = [q^2 + q + 1 - 1 - (q+t)(q+1-t)](q + 1 - t + 1) = -t[t^2 - (q+3)t + (q+2)].$$

If $t \ge 2$, then $t^2 - (q+3)t + (q+2) \le -q < 0$, and thus $h_n(k) > 0 = h_n(q) = h_n(q+1)$, implying that $t \in \{0, 1\}$, i.e., $k \in \{q, q+1\}$.

Case 3. $r = q + 2, \dots, 2q + 1$. Let $k = q + 1 + t$ and $\left\lfloor \frac{n-1}{k} \right\rfloor = q - t$ for some $0 \le t \le q$. Similarly as above, we have

$$h_n(k) = -t(t^2 - qt + r - 2q - 2) + (r - q - 1)(q + 1).$$

If $t \ge 1$, then $t^2 - qt + r - 2q - 2 \le r - 2q - 2 \le -1 < 0$, and thus $h_n(k) > (r - q - 1)(q + 1) = h_n(q + 1)$, implying that $t = 0$, i.e., $k = q + 1$.

The result follows from Cases 1–3. □

Let $\mathbb{T}_{n,d}$ be the set of n-vertex trees with diameter d, where $2 \le d \le n-1$.

Lemma 2.5. *Let T be a tree in $\mathbb{T}_{n,5}$ with the smallest reverse Wiener index. Then there exists $T^* \in \mathcal{CT}_n$ with diameter 4 such that $\Lambda(T^*) < \Lambda(T)$.*

Proof. Let T be a tree in $\mathbb{T}_{n,5}$ with the smallest reverse Wiener index. By Lemma 2.1, there exists no pendant neighbor for the centers of T. Let T^* be the tree obtained by contracting the edge connecting the centers u and v of T followed by attaching a pendant vertex to the new vertex resulting from identifying u and v. Then $T^* \in \mathbb{T}_{n,4}$ and its center has a pendant neighbor. It is easily seen that

$$\begin{aligned}\Lambda(T) - \Lambda(T^*) &= \frac{5}{2}n(n-1) - W(T) - (2n(n-1) - W(T^*)) \\ &= \frac{5}{2}n(n-1) - n_{T,1}(uv)n_{T,2}(uv) - 2n(n-1) + (n-1) \\ &\ge \frac{1}{2}(n-1)(n+2) - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil > 0,\end{aligned}$$

from which we get the desired result. □

For $2 \le d \le n-1$, let $f(n,d) = \min\{\Lambda(T) : T \in \mathbb{T}_{n,d}\}$, and let $\mathcal{T}_{n,d}$ be the set of trees in $\mathbb{T}_{n,d}$ with reverse Wiener index $f(n,d)$.

Obviously, $\mathbb{T}_{n,2} = \{S_n\}$, and $f(n,2) = \Lambda(S_n) = n-1$.

For $3 \le d \le n-1$, let $g(n,d) = \min\{\Lambda(T) : T \in \mathbb{T}_{n,d} \setminus \mathcal{T}_{n,d}\}$, and $\mathcal{T}'_{n,d}$ be the set of trees in $\mathbb{T}_{n,d}$ with reverse Wiener index $g(n,d)$.

For $2 \le a \le \lfloor \frac{n}{2} \rfloor$, let $D_{n,a}$ be the tree formed by adding an edge between the centers of the stars S_a and S_{n-a}.

Proposition 2.6. *For $n \ge 4$,*

$$f(n,3) = \frac{n^2}{2} + \frac{3n}{2} - 2 - \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil \text{ and } \mathcal{T}_{n,3} = \{D_{n,\lfloor \frac{n}{2} \rfloor}\}.$$

For $n \ge 6$,

$$g(n,3) = \frac{n^2}{2} + \frac{3n}{2} - 2 - \left(\left\lfloor \frac{n}{2} \right\rfloor - 1\right)\left(\left\lceil \frac{n}{2} \right\rceil + 1\right) \text{ and } \mathcal{T}'_{n,3} = \{D_{n,\lfloor \frac{n}{2} \rfloor - 1}\}.$$

Proof. Obviously, the trees in $\mathbb{T}_{n,3}$ are of the type $D_{n,a}$, where $2 \le a \le \lfloor \frac{n}{2} \rfloor$. For $2 \le a \le \lfloor \frac{n}{2} \rfloor$, we have

$$\begin{aligned}\Lambda(D_{n,a}) &= \frac{3}{2}n(n-1) - W(D_{n,a}) \\ &= \frac{3}{2}n(n-1) - [(n-1)(n-2) + a(n-a)] \\ &= \frac{n^2}{2} + \frac{3n}{2} - 2 - a(n-a),\end{aligned}$$

from which we know that, for fixed n, $\Lambda(D_{n,a})$ is decreasing for $2 \le a \le \lfloor \frac{n}{2} \rfloor$. The result follows. □

3. Trees with the second smallest reverse Wiener index

In this section, we determine the second smallest reverse Wiener index of n-vertex trees and characterize the trees achieving this value.

The following proposition is essentially equivalent to [27, Theorem 3]. However, we give a proof (on which part of the arguments following in Section 4 is based as well).

Proposition 3.1. *Let $n \geq 5$ be of the form* (1). *Then*

$$f(n,4) = \begin{cases} 2q^3 + q^2 + 3rq - 3q + 2r - 2 & \text{if } r = 1, \ldots, q, \\ 2q^3 + q^2 + 3rq - 4q + 3r - 3 & \text{if } r = q+1, \ldots, 2q+1, \end{cases}$$

$$\mathcal{T}_{n,4} = \begin{cases} \left\{T_{n,q}\left(q - 1^{[q]}\right)\right\} & \text{if } r = 1, \\ \left\{T_{n,q}\left(q - 1^{[q-r+1]}, q^{[r-1]}\right)\right\} & \text{if } r = 2, \ldots, q, \\ \left\{T_{n,q}\left(q^{[q]}\right), T_{n,q+1}\left(q - 1^{[q+1]}\right)\right\} & \text{if } r = q+1, \\ \left\{T_{n,q+1}\left(q - 1^{[2(q+1)-r]}, q^{[r-q-1]}\right)\right\} & \text{if } r = q+2, \ldots, 2q+1. \end{cases}$$

Proof. Let T be a tree with the smallest reverse Wiener index in $\mathbb{T}_{n,4}$. By Lemma 2.1, T must be written as $T = T_{n,k}\left(n_1^{[b_1]}, n_2^{[b_2]}, \ldots, n_s^{[b_s]}\right)$ with $k \geq 2$ and $\sum_{i=1}^{s} b_i n_i = n - k - 1$. By Lemma 2.3, $s \leq 2$. By Lemma 2.4, $k = q$ if $r = 1, \ldots, q$, $k \in \{q, q+1\}$ if $r = q+1$, and $k = q+1$ if $r = q+2, \ldots, 2q+1$.

Suppose that $k = q$. If $s = 1$, then $n = q^2 + r = 1 + k + n_1 k = 1 + q + n_1 q$, and thus $r - 1 = q(1 + n_1 - q)$, which implies that $r = 1, q+1, 2q+1$. If $s = 2$, then $n = q^2 + r = 1 + q + b_1 n_1 + b_2 n_2 = 1 + q + b_1 n_1 + b_2(n_1+1) = 1 + q + q n_1 + b_2$ where $1 \leq b_2 \leq q - 1$, and thus $r - b_2 - 1 = q(n_1 + 1 - q)$, which implies that $r = 2, \ldots, q, q+2, \ldots, 2q$, i.e., $r \neq 1, q+1, 2q+1$. In conclusion, if $k = q$, then $s = 1$ if and only if $r = 1, q+1, 2q+1$. Now suppose that $k = q+1$. If $s = 1$, then $n = q^2 + r = 1 + (q+1) + n_1(q+1)$, and thus $r = (q+1)(n_1 + 2 - q)$, which implies that $r = q+1$. If $s = 2$, then $n = q^2 + r = 1 + (q+1) + b_1 n_1 + b_2 n_2 = q + 2 + (q+1)n_1 + b_2$ where $1 \leq b_2 \leq q$, and thus $r - b_2 = (q+1)(n_1 + 2 - q)$, which implies that $r = 1, \ldots, q, q+2, \ldots, 2q+1$, i.e., $r \neq q+1$. In conclusion, if $k = q+1$, then $s = 1$ if and only if $r = q+1$.

Case 1. $r = 1$. Then $k = q$ and $s = 1$, and thus $T = T_{n,q}\left(q - 1^{[q]}\right)$ with $\Lambda(T) = 2q^3 + q^2$.

Case 2. $r = 2, \ldots, q$. Then $k = q$ and $s = 2$, and thus $n_1 = \left\lfloor \frac{q^2+r-1}{q} \right\rfloor - 1 = q - 1$, $n_2 = q$, $b_1 = q^2 - (q^2 + r - q - 1) = q - r + 1$ and $b_2 = r - 1$, i.e., $T = T_{n,q}\left(q - 1^{[q-r+1]}, q^{[r-1]}\right)$, where

$$\begin{aligned} \Lambda\left(T_{n,q}\left(q - 1^{[q-r+1]}, q^{[r-1]}\right)\right) &= 2n(n-1) - [(n-1)(n-1-q) + q(n-q)(q-r+1) \\ &\quad (q+1)(n-q-1) + (r-1)] \\ &= n^2 + n - nq^2 + nq - nr + q^3 + 2rq - 3q + r - 2 \\ &= 2q^3 + q^2 + 3rq - 3q + 2r - 2. \end{aligned}$$

Case 3. $r = q+1$. Then $k \in \{q, q+1\}$. By direct calculation, $\Lambda\left(T_{n,q}\left(q^{[q]}\right)\right) = \Lambda\left(T_{n,q+1}\left(q - 1^{[q+1]}\right)\right) = 2q^3 + 4q^2 + 2q$. Since $s = 1$, we have $T = T_{n,q}\left(q^{[q]}\right)$ or $T_{n,q+1}\left(q - 1^{[q+1]}\right)$.

Case 4. $r = q+2, \ldots, 2q+1$. Then $k = q+1$ and $s = 2$, and thus $n_1 = q - 1$, $n_2 = q$, $b_1 = 2(q+1) - r$ and $b_2 = r - q - 1$, i.e., $T_{n,q+1}\left(q - 1^{[2(q+1)-r]}, q^{[r-q-1]}\right)$, where

$$\begin{aligned} \Lambda\left(T_{n,q+1}\left(q - 1^{[2(q+1)-r]}, q^{[r-q-1]}\right)\right) &= 2n(n-1) - [(n-1)(n-2-q) + q(n-q)(2q+2-r) \\ &\quad +(q+1)(n-q-1)(r-q-1)] \\ &= n^2 + 2n - nq^2 + nq - nr + q^3 - q^2 + 2rq - 4q + r - 3 \\ &= 2q^3 + q^2 + 3rq - 4q + 3r - 3. \end{aligned}$$

The result follows from Cases 1–4. □

Now we are ready to give our main result in this section.

Theorem 3.2. *Among the trees in $\mathcal{T}_n$ with $n \geq 4$, $D_{n,\lfloor \frac{n}{2} \rfloor}$ for $n \leq 56$, $D_{57,28}$, $T_{57,7}\left(7^{[7]}\right)$ and $T_{57,8}\left(6^{[8]}\right)$ for $n = 57$, and the trees in $\mathcal{T}_{n,4}$ for $n \geq 58$ are the unique trees with the second smallest reverse Wiener index, which is equal to $\frac{n^2}{2} + \frac{3n}{2} - 2 - \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ for $n \leq 56$, 896 for $n = 57$, and $f(n,4)$ for $n \geq 58$, respectively, where $\mathcal{T}_{n,4}$ and $f(n,4)$ are given in Proposition 3.1.*

Proof. The case $n = 4$ is trivial. Suppose that $n \geq 5$. Let $T \in \mathcal{T}_n$. Let d be the diameter of T. If $d \geq 5$, then by Lemmas 2.1 and 2.2, we have

$$\begin{aligned} \Lambda(T) &\geq f(n,d) > f(n,4) > f(n,2) && \text{for even } d, \\ \Lambda(T) &\geq f(n,d) \geq f(n,5) > f(n,3) && \text{for odd } d. \end{aligned}$$

Thus the second smallest reverse Wiener index of the trees in $\mathcal{T}_n$ is equal to $\min\{f(n,3), f(n,4)\}$, and by Propositions 2.6 and 3.1, it is only achieved by $D_{n,\lfloor \frac{n}{2} \rfloor}$ or trees in $\mathcal{T}_{n,4}$, where, with n being of the form (1),

$$f(n,3) = \begin{cases} \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - \frac{7}{4} & \text{if } n \text{ is odd}, \\ \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - 2 & \text{if } n \text{ is even}, \end{cases}$$

and $f(n,4)$ is given in Proposition 3.1. If $n = 5, 6, \ldots, 56$, then it can be checked that $f(n,3) < f(n,4)$, and thus the result follows from Proposition 2.6. Suppose that $n \geq 57$.

Case 1. $r = 1, 2, \ldots, q$. Since $q^2 + q \geq 57$, we have $q \geq 8$. Note that $f(n,4) = 2q^3 + q^2 + 3rq - 3q + 2r - 2$. If n is odd, then since $\frac{1}{2}q^2 - 3q - \frac{1}{2} > 0$, we have

$$\begin{aligned} f(n,3) - f(n,4) &= \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - \frac{7}{4} - \left(2q^3 + q^2 + 3rq - 3q + 2r - 2\right) \\ &= \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 3q + \frac{1}{4} + \frac{1}{4}r^2 + \left(\frac{1}{2}q^2 - 3q - \frac{1}{2}\right)r \\ &\geq \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 3q + \frac{1}{4} + \frac{1}{4} + \left(\frac{1}{2}q^2 - 3q - \frac{1}{2}\right) \\ &= \frac{1}{4}q^4 - 2q^3 + q^2 = \frac{1}{4}q^2(q^2 - 8q + 4) \geq q^2 > 0, \end{aligned}$$

and if n is even, then

$$f(n,3) - f(n,4) \geq \frac{1}{4}q^4 - 2q^3 + q^2 - \frac{1}{4} \geq q^2 - \frac{1}{4} > 0.$$

Thus $f(n,3) > f(n,4)$.

Case 2. $r = q+1, q+2, \ldots, 2q+1$. Since $q^2+2q+1 \geq 57$, we have $q \geq 7$. Note that $f(n,4) = 2q^3+q^2+3rq-4q+3r-3$. Suppose first that n is odd. Since $\frac{1}{2}q^2 - 3q - \frac{3}{2} > 0$, we have

$$\begin{aligned} f(n,3) - f(n,4) &= \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - \frac{7}{4} - \left(2q^3 + q^2 + 3rq - 4q + 3r - 3\right) \\ &= \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 4q + \frac{5}{4} + \frac{1}{4}r^2 + \left(\frac{1}{2}q^2 - 3q - \frac{3}{2}\right)r \\ &\geq \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 4q + \frac{5}{4} + \frac{1}{4}(q+1)^2 + \left(\frac{1}{2}q^2 - 3q - \frac{3}{2}\right)(q+1) \\ &= \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{7}{4}q^2 \geq 0, \end{aligned}$$

and then $f(n,3) \geq f(n,4)$ with equality if and only if $q = 7$ and $r = q + 1 = 8$, i.e., $n = 57$. Now suppose that n is even. If $q = 7$, then $n = 58, 60, 62, 64$, and it is easily checked by the expressions for $f(n,3)$ and $f(n,4)$ that $f(n,3) > f(n,4)$. If $q \geq 8$, then

$$f(n,3) - f(n,4) \geq \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{7}{4}q^2 - \frac{1}{4} > 0,$$

and thus $f(n,3) > f(n,4)$.

Combining Cases 1 and 2, we have $f(n,3) > f(n,4)$ for $n \geq 58$ and $f(57,3) = f(57,4)$. The result for $n \geq 57$ follows from Propositions 2.6 and 3.1. □

4. Trees with the third smallest reverse Wiener index

In this section, we determine the third smallest reverse Wiener index of n-vertex trees and characterize the trees whose reverse Wiener indices achieve this value.

Proposition 4.1. *Let $n \geq 6$ be of the form* (1). *Then*

$$g(n,4) = \begin{cases} f(n,4)+1 & \text{if } r = q, q+2, \\ f(n,4)+2 & \text{if } r \neq q, q+2, \end{cases}$$

where $f(n,4)$ is given in Proposition 3.1, and

$$\mathcal{T}'_{n,4} = \begin{cases} \left\{T_{n,q}\left(q-2^{[1]}, q-1^{[q-r-1]}, q^{[r]}\right)\right\} & \text{if } r = 1,2, \\ \left\{T_{n,q}\left(q-1^{[q-1]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-4]}, q^{[3]}\right)\right\} & \text{if } r = 3, \\ \left\{T_{n,q}\left(q-1^{[q-r+2]}, q^{[r-3]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-r-1]}, q^{[r]}\right)\right\} & \text{if } r = 4,\dots,q-2, \\ \left\{T_{n,q+1}\left(q-2^{[2]}, q-1^{[q-1]}\right), T_{n,q}\left(q-1^{[3]}, q^{[q-4]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q^{[q-1]}\right)\right\} & \text{if } r = q-1, \\ \left\{T_{n,q+1}\left(q-2^{[1]}, q-1^{[q]}\right)\right\} & \text{if } r = q, \\ \left\{T_{n,q}\left(q-1^{[1]}, q^{[q-2]}, q+1^{[1]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-1]}, q^{[1]}\right)\right\} & \text{if } r = q+1, \\ \left\{T_{n,q}\left(q^{[q-1]}, q+1^{[1]}\right)\right\} & \text{if } r = q+2, \\ \left\{T_{n,q}\left(q^{[q-2]}, q+1^{[2]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[3]}\right), T_{n,q+1}\left(q-1^{[q]}, q+1^{[1]}\right)\right\} & \text{if } r = q+3, \\ \left\{T_{n,q+1}\left(q-2^{[1]}, q-1^{[2q-r]}, q^{[r-q]}\right), T_{n,q+1}\left(q-1^{[2q+3-r]}, q^{[r-q-3]}, q+1^{[1]}\right)\right\} & \text{if } r = q+4,\dots,2q-1, \\ \left\{T_{n,q+1}\left(q-2^{[1]}, q^{[q]}\right), T_{n,q+1}\left(q-1^{[3]}, q^{[q-3]}, q+1^{[1]}\right)\right\} & \text{if } r = 2q, \\ \left\{T_{n,q+1}\left(q-1^{[2]}, q^{[q-2]}, q+1^{[1]}\right)\right\} & \text{if } r = 2q+1. \end{cases}$$

Proof. By Proposition 3.1, the second smallest reverse Wiener index in $\mathbb{T}_{n,4}$ is precisely achieved by the smallest reverse Wiener index of trees in $\mathbb{T}_{n,4} \setminus \mathcal{T}_{n,4}$. Let T be a tree with the smallest reverse Wiener index in $\mathbb{T}_{n,4} \setminus \mathcal{T}_{n,4}$.

Case 1. $T \in \mathcal{CT}_n$. Then T may be written as $T = T_{n,k}\left(n_0; n_1^{[b_1]}, n_2^{[b_2]}, \dots, n_s^{[b_s]}\right)$. From the expression for $W(T)$ (given previous to Lemma 2.3), $\Lambda(T)$ is increasing with respect to n_0. Thus $n_0 = 1$, $k \geq 2$ and $\sum_{i=1}^{s} b_i n_i = n-k-2$, and by Lemma 2.3, we have $s \leq 2$, and $n_2 - n_1 = 1$ if $s = 2$. Using the same method in the proof of Lemma 2.4 to analyze $\Lambda\left(T_{n,k}\left(1; n_1^{[b_1]}, n_2^{[b_2]}, \dots, n_s^{[b_s]}\right)\right) = 4n-5+(n-2)k+\sum_{i=1}^{s} b_i n_i^2$, we have $k = q$ if $r = 1, \dots, q+1$, $k \in \{q, q+1\}$ if $r = q+2$, and $k = q+1$ if $r = q+3, \dots, 2q+1$. The rest of the proof is similar to the proof of Proposition 3.1.

If $r = 1$, then $T = T_{n,q}\left(1; q-2^{[1]}, q-1^{[q-1]}\right)$ with $\Lambda(T) = 2q^3+2q^2-2q+2$.

If $r = 2$, then $T = T_{n,q}\left(1; q-1^{[q]}\right)$ with $\Lambda(T) = 2q^3+2q^2+q+3$.

If $r = 3, \dots, q+1$, then $T = T_{n,q}\left(1; q-1^{[q-r+2]}, q^{[r-2]}\right)$ with $\Lambda(T) = 2q^3+2q^2+3rq-5q+3r-3$.

If $r = q+2$, then $T = T_{n,q}\left(1; q^{[q]}\right)$ with $\Lambda(T) = 2q^3+5q^2+4q+3$.

If $r = q+3, \dots, 2q+1$, then $T = T_{n,q+1}\left(1; q-1^{[2q-r+3]}, q^{[r-q-2]}\right)$ with $\Lambda(T) = 2q^3+2q^2+3rq-6q+4r-4$.

Case 2. $T \notin \mathcal{CT}_n$. Then T may be written as $T = T_{n,k}\left(n_1^{[b_1]}, n_2^{[b_2]}, \dots, n_s^{[b_s]}\right)$. Note that $T \notin \mathcal{T}_{n,4}$. There are two subcases.

Subcase 2.1. $s \leq 2$, and $n_2 - n_1 = 1$ if $s = 2$.

(i) $r = 1$. By the monotonicity of $f(x) = x + \frac{n-1}{x}$ in the proof of Lemma 2.4 and Proposition 3.1, we have $k \in \{q-1, q+1\}$. If $k = q-1$, then $T = T_{n,q-1}\left(q^{[q-2]}, q+1^{[1]}\right)$ with $\Lambda(T) = 2q^3+q^2+q+2$. If $k = q+1$, then $T = T_{n,q+1}\left(q-2^{[q]}, q-1^{[1]}\right)$ with $\Lambda(T) = 2q^3+q^2+q$. Thus $T = T_{n,q+1}\left(q-2^{[q]}, q-1^{[1]}\right)$.

(ii) $r = 2, \ldots, q$. Then $k \in \{q-1, q+1\}$. If $k = q-1$, then

$$T = \begin{cases} T_{n,q-1}\left(q^{[q-r-1]}, q+1^{[r]}\right) & \text{if } r = 2, \ldots, q-2, \\ T_{n,q-1}\left(q+1^{[q-1]}\right) & \text{if } r = q-1, \\ T_{n,q-1}\left(q+1^{[q-2]}, q+2^{[1]}\right) & \text{if } r = q, \end{cases}$$

where

$$\begin{aligned} \Lambda\left(T_{n,q-1}\left(q^{[q-r-1]}, q+1^{[r]}\right)\right) &= 2n(n-1) - [(n-1)(n-q) + (q+1)(n-q-1)(q-r-1) \\ &\quad +(q+2)(n-q-2)r] \\ &= n^2 - nq^2 + nq - nr + q^3 + q^2 + 2rq - 2q + 3r - 1 \\ &= 2q^3 + q^2 + 3rq - 2q + 3r - 1, \\ \Lambda\left(T_{n,q-1}\left(q+1^{[q-1]}\right)\right) &= 2q^3 + 4q^2 - 2q - 4, \\ \Lambda\left(T_{n,q-1}\left(q+1^{[q-2]}, q+2^{[1]}\right)\right) &= 2q^3 + 4q^2 + q + 1. \end{aligned}$$

If $k = q+1$, then $T = T_{n,q+1}\left(q-2^{[q-r+1]}, q-1^{[r]}\right)$, where

$$\begin{aligned} \Lambda\left(T_{n,q+1}\left(q-2^{[q-r+1]}, q-1^{[r]}\right)\right) &= 2n(n-1) - [(n-1)(n-2-q) \\ &\quad +(q-1)(n-q+1)(q-r+1) + q(n-q)r] \\ &= n^2 + 2n - nq^2 + nq - nr + q^3 - q^2 + 2rq - 2q - r - 1 \\ &= 2q^3 + q^2 + 3rq - 2q + r - 1. \end{aligned}$$

Thus $T = T_{n,q+1}\left(q-2^{[q-r+1]}, q-1^{[r]}\right)$ with $\Lambda(T) = 2q^3 + q^2 + 3rq - 2q + r - 1$.

(iii) $r = q+1$. Then $k \in \{q-1, q+2\}$. We have

$$T = \begin{cases} T_{n,q-1}\left(q+1^{[q-3]}, q+2^{[2]}\right) & \text{if } k = q-1, \\ T_{n,q+2}\left(q-2^{[q]}, q-1^{[2]}\right) & \text{if } t = q+2, \end{cases}$$

where $\Lambda\left(T_{n,q-1}\left(q+1^{[q-3]}, q+2^{[2]}\right)\right) = 2q^3 + 4q^2 + 4q + 6 > 2q^3 + 4q^2 + 4q = \Lambda\left(T_{n,q+2}\left(q-2^{[q]}, q-1^{[2]}\right)\right)$. Thus $T = T_{n,q+2}\left(q-2^{[q]}, q-1^{[2]}\right)$ with $\Lambda(T) = 2q^3 + 4q^2 + 4q$.

(iv) $r = q+2, \ldots, 2q$. Then $k \in \{q, q+2\}$. We have

$$T = \begin{cases} T_{n,q}\left(q^{[2q+1-r]}, q+1^{[r-q-1]}\right) & \text{if } k = q, \\ T_{n,q+2}\left(q-2^{[2q+1-r]}, q-1^{[r-q+1]}\right) & \text{if } k = q+2, \end{cases}$$

where

$$\begin{aligned} \Lambda\left(T_{n,q}\left(q^{[2q+1-r]}, q+1^{[r-q-1]}\right)\right) &= 2n(n-1) - [(n-1)(n-1-q) + (q+1)(n-q-1)(2q+1-r) \\ &\quad +(q+2)(n-q-2)(r-q-1)] \\ &= n^2 + n - nq^2 + nq - nr + q^3 + 2rq - 5q + 3r - 4 \\ &= 2q^3 + q^2 + 3rq - 5q + 4r - 4, \\ \Lambda\left(T_{n,q+2}\left(q-2^{[2q+1-r]}, q-1^{[r-q+1]}\right)\right) &= 2n(n-1) - [(n-1)(n-3-q) \\ &\quad +(q-1)(n-q+1)(2q+1-r) + q(n-q)(r-q-1)] \\ &= 2q^3 + q^2 + 3rq - q + 2r - 2 \\ &> \Lambda\left(T_{n,q}\left(q^{[2q+1-r]}, q+1^{[r-q-1]}\right)\right). \end{aligned}$$

Thus $T = T_{n,q}\left(q^{[2q+1-r]}, q+1^{[r-q-1]}\right)$ with $\Lambda(T) = 2q^3 + q^2 + 3rq - 5q + 4r - 4$.

(v) $r = 2q+1$. Then $k \in \{q, q+2\}$. If $k = q$, then $T = T_{n,q}\left(q+1^{[q]}\right)$, and if $k = q+2$, then $T = T_{n,q+2}\left(q-1^{[q+2]}\right)$, both with reverse Wiener index $2q^3 + 7q^2 + 6q$.

Subcase 2.2. There exist $1 \le i < j \le s$ such that $n_j - n_i \ge 2$. Let T^* be the tree constructed as in the proof of Lemma 2.3 from T. By the proof there, we have $\Lambda(T) = \Lambda(T^*) + 2(n_j - n_i - 1)$. Thus $\Lambda(T)$ is minimum if and only if $T^* \in \mathcal{T}_{n,4}$ and $n_j - n_i = 2$.

(i) $r = 1$. Then $T = T_{n,q}\left(q-2^{[1]}, q-1^{[q-2]}, q^{[1]}\right)$ with $\Lambda(T) = 2q^3 + q^2 + 2$.

(ii) $r = 2, \ldots, q$. Then $\Lambda(T)$ is at least the minimum of the reverse Wiener indices of

$$\begin{array}{rl}
T_{n,q}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[2]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-2]}, q+1^{[1]}\right) & \text{if } r = 2,\\
T_{n,q}\left(q-1^{[q-1]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-4]}, q^{[3]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[1]}, q+1^{[1]}\right) & \text{if } r = 3,\\
T_{n,q}\left(q-1^{[q-r+2]}, q^{[r-3]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-r-1]}, q^{[r]}\right), & \\
T_{n,q}\left(q-2^{[1]}, q-1^{[q-r]}, q^{[r-2]}, q+1^{[1]}\right) & \text{if } r = 4, \ldots, q-2,\\
T_{n,q}\left(q-1^{[3]}, q^{[q-4]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q^{[q-1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[1]}, q^{[q-3]}, q+1^{[1]}\right) & \text{if } r = q-1,\\
T_{n,q}\left(q-1^{[2]}, q^{[q-3]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q^{[q-2]}, q+1^{[1]}\right) & \text{if } r = q.
\end{array}$$

By comparing the reverse Wiener indices of these trees, we have

$$T = \begin{cases}
T_{n,q}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[2]}\right) & \text{if } r = 2,\\
T_{n,q}\left(q-1^{[q-1]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-4]}, q^{[3]}\right) & \text{if } r = 3,\\
T_{n,q}\left(q-1^{[q-r+2]}, q^{[r-3]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q-1^{[q-r-1]}, q^{[r]}\right) & \text{if } r = 4, \ldots, q-2,\\
T_{n,q}\left(q-1^{[3]}, q^{[q-4]}, q+1^{[1]}\right), T_{n,q}\left(q-2^{[1]}, q^{[q-1]}\right) & \text{if } r = q-1,\\
T_{n,q}\left(q-1^{[2]}, q^{[q-3]}, q+1^{[1]}\right) & \text{if } r = q
\end{cases}$$

with $\Lambda(T) = f(n,4) + 2$, where $f(n,4)$ is given in Proposition 3.1.

(iii) $r = q+1$. Then $T = T_{n,q}\left(q-1^{[1]}, q^{[q-2]}, q+1^{[1]}\right)$ or $T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-1]}, q^{[1]}\right)$, both with reverse Wiener index $2q^3 + 4q^2 + 2q + 2$.

(iv) $r = q+2, \ldots, 2q$. Then $\Lambda(T)$ is at least the minimum of the reverse Wiener indices of

$$\begin{array}{rl}
T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-2]}, q^{[2]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-1]}, q+1^{[1]}\right) & \text{if } r = q+2,\\
T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[3]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-2]}, q^{[1]}, q+1^{[1]}\right), & \\
T_{n,q+1}\left(q-1^{[q]}, q+1^{[1]}\right) & \text{if } r = q+3,\\
T_{n,q+1}\left(q-2^{[1]}, q-1^{[2q-r]}, q^{[r-q]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[2q+1-r]}, q^{[r-q-2]}, q+1^{[1]}\right), & \\
T_{n,q+1}\left(q-1^{[2q+3-r]}, q^{[r-q-3]}, q+1^{[1]}\right) & \text{if } r = q+4, \ldots, 2q-1,\\
T_{n,q+1}\left(q-2^{[1]}, q^{[q]}\right), T_{n,q+1}\left(q-2^{[1]}, q-1^{[1]}, q^{[q-2]}, q+1^{[1]}\right), & \\
T_{n,q+1}\left(q-1^{[3]}, q^{[q-3]}, q+1^{[1]}\right) & \text{if } r = 2q.
\end{array}$$

Thus

$$T = \begin{cases}
T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-2]}, q^{[2]}\right) & \text{if } r = q+2,\\
T_{n,q+1}\left(q-2^{[1]}, q-1^{[q-3]}, q^{[3]}\right), T_{n,q+1}\left(q-1^{[q]}, q+1^{[1]}\right) & \text{if } r = q+3,\\
T_{n,q+1}\left(q-2^{[1]}, q-1^{[2q-r]}, q^{[r-q]}\right), T_{n,q+1}\left(q-1^{[2q+3-r]}, q^{[r-q-3]}, q+1^{[1]}\right) & \text{if } r = q+4, \ldots, 2q-1,\\
T_{n,q+1}\left(q-2^{[1]}, q^{[q]}\right), T_{n,q+1}\left(q-1^{[3]}, q^{[q-3]}, q+1^{[1]}\right) & \text{if } r = 2q
\end{cases}$$

with $\Lambda(T) = f(n,4) + 2$, where $f(n,4)$ is given in Proposition 3.1.

(v) $r = 2q + 1$. Then $\Lambda(T) \geq \min\left\{\Lambda\left(T_{n,q+1}\left(q-2^{[1]}, q^{[q-1]}, q+1^{[1]}\right)\right), \Lambda\left(T_{n,q+1}\left(q-1^{[2]}, q^{[q-2]}, q+1^{[1]}\right)\right)\right\}$. By direct calculation, we have $T = T_{n,q+1}\left(q-1^{[2]}, q^{[q-2]}, q+1^{[1]}\right)$ with $\Lambda(T) = 2q^3 + 7q^2 + 5q + 2$.

By comparing the above cases, we have: if $r = 1$, then $\Lambda(T)$ is precisely the minimum of $2q^3+2q^2-2q+2$, $2q^3+q^2+q$ and $2q^3+q^2+2$; if $r = 2,\ldots,q-1$, then $\Lambda(T)$ is precisely the minimum of $2q^3+2q^2+3rq-5q+3r-3$, $2q^3+q^2+3rq-2q+r-1$ and $2q^3+q^2+3rq-3q+2r$; if $r = q$, then $\Lambda(T)$ is precisely the minimum of $2q^3+5q^2-2q-3$, $2q^3+4q^2-q-1$ and $2q^3+4q^2-q$; if $r = q+1$, then $\Lambda(T)$ is precisely the minimum of $2q^3+5q^2+q$, $2q^3+4q^2+4q$ and $2q^3+4q^2+2q+2$; if $r = q+2$, then $\Lambda(T)$ is precisely the minimum of $2q^3+5q^2+4q+3$, $2q^3+4q^2+5q+4$ and $2q^3+4q^2+5q+5$; if $r = q+3,\ldots,2q+1$, then $\Lambda(T)$ is precisely the minimum of $2q^3+2q^2+3rq-6q+4r-4$, $2q^3+q^2+3rq-5q+4r-4$ and $2q^3+q^2+3rq-4q+3r-1$. Now the result follows easily. □

Theorem 4.2. *Among the trees in $\mathcal{T}_n$ with $n \geq 5$, the trees in $\mathcal{T}'_{n,4}$ for $n = 5$ or $n \geq 58$, $D_{n,\lfloor \frac{n}{2}\rfloor-1}$ for $6 \leq n \leq 57$ are the unique trees with the third smallest reverse Wiener index, which is equal to 20 for $n = 5$, $\frac{n^2}{2}+\frac{3n}{2}-2-\left(\lfloor \frac{n}{2}\rfloor-1\right)\left(\lceil \frac{n}{2}\rceil+1\right)$ for $6 \leq n \leq 57$, and $g(n,4)$ for $n \geq 58$, where $\mathcal{T}'_{n,4}$ and $g(n,4)$ are given in Proposition 4.1.*

Proof. The case $n = 5$ is trivial. Suppose that $n \geq 6$. By Theorem 3.2, among the trees in $\mathcal{T}_n$ with $n \geq 6$, $D_{n,\lfloor \frac{n}{2}\rfloor}$ for $6 \leq n \leq 56$, $D_{57,28}$, $T_{57,7}\left(7^{[7]}\right)$ and $T_{57,8}\left(6^{[8]}\right)$ for $n = 57$, and the trees in $\mathcal{T}_{n,4}$ for $n \geq 58$ are the unique trees with the second smallest reverse Wiener index, which are equal to $f(n,3)$ for $n \leq 56$, $f(n,3) = f(n,4)$ for $n = 57$ and $f(n,4)$ for $n \geq 58$. By Proposition 4.1, and Lemmas 2.2 and 2.5, we have $f(n,d) > g(n,4)$ for $5 \leq d \leq n-1$. Thus the third smallest reverse Wiener index in $\mathcal{T}_n$ is equal to $\min\{g(n,3), f(n,4)\}$ for $6 \leq n \leq 56$, $\min\{g(n,3), g(n,4)\}$ for $n = 57$ and $\min\{f(n,3), g(n,4)\}$ for $n \geq 58$, and by Propositions 2.6 and 4.1, it is precisely achieved by graphs in $\mathcal{T}'_{n,3}$ and $\mathcal{T}_{n,4}$ for $6 \leq n \leq 56$, $\mathcal{T}'_{n,3}$ and $\mathcal{T}'_{n,4}$ for $n = 57$, and $\mathcal{T}_{n,3}$ and $\mathcal{T}'_{n,4}$ for $n \geq 58$.

Recall that the expressions for $f(n,3)$ and $g(n,3)$ are given in Proposition 2.6, while the expressions for $f(n,4)$ and $g(n,4)$ are given in Propositions 3.1 and 4.1, respectively. Let n be of the form (1). Recall that $f(n,3) \geq \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - 2$.

By direct checking, we have $g(n,3) < f(n,4)$ for $6 \leq n \leq 56$, and $g(57,3) < g(57,4)$. Thus the results for cases $n = 6,\ldots,57$ follow from Proposition 2.6. Suppose that $n \geq 58$.

Case 1. $r = 1,\ldots,q-1$. Then $q \geq 8$. Note that $\frac{1}{2}q^2 - 3q - \frac{1}{2} > 0$. We have

$$\begin{aligned} f(n,3) - g(n,4) &\geq \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - 2 - \left(2q^3 + q^2 + 3rq - 3q + 2r\right) \\ &= \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 3q - 2 + \frac{1}{4}r^2 + \left(\frac{1}{2}q^2 - 3q - \frac{1}{2}\right)r \\ &\geq \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 3q - 2 + \frac{1}{4} + \frac{1}{2}q^2 - 3q - \frac{1}{2} \\ &= \frac{1}{4}q^4 - 2q^3 + q^2 - \frac{9}{4} = \frac{1}{4}q^2(q^2 - 8q + 4) - \frac{9}{4} \geq q^2 - \frac{9}{4} > 0, \end{aligned}$$

and thus $f(n,3) > g(n,4)$.

Case 2. $r = q$. Then $q \geq 8$. We have

$$f(n,3) - g(n,4) \geq \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{9}{4}q^2 + \frac{5}{2}q - 1 = \frac{1}{4}q^2(q^2 - 6q - 9) + \frac{5}{2}q - 1 \geq \frac{7}{4}q^2 + \frac{5}{2}q - 1 > 0,$$

and thus $f(n,3) > g(n,4)$.

Case 3. $r = q+2$. Then $q \geq 7$. We have

$$f(n,3) - g(n,4) \geq \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{5}{4}q^2 - \frac{5}{2}q - 2 > 0,$$

and thus $f(n,3) > g(n,4)$.

Case 4. $r = q+1, q+3, \dots, 2q+1$. Note that $\frac{1}{2}q^2 - 3q - \frac{3}{2} > 0$. We have

$$\begin{aligned} f(n,3) - g(n,4) &\geq \frac{1}{4}q^4 + \frac{1}{2}rq^2 + \frac{3}{2}q^2 + \frac{1}{4}r^2 + \frac{3}{2}r - 2 - \left(2q^3 + q^2 + 3rq - 4q + 3r - 1\right) \\ &= \frac{1}{4}q^4 - 2q^3 + \frac{1}{2}q^2 + 4q - 1 + \frac{1}{4}r^2 + \left(\frac{1}{2}q^2 - 3q - \frac{3}{2}\right)r. \end{aligned}$$

If $r = q+1$, then $q \geq 8$, and thus $f(n,3) - g(n,4) \geq \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{7}{4}q^2 - \frac{9}{4} > 0$, while if $r = q+3, ..., 2q+1$, then $q \geq 7$, and thus $f(n,3) - g(n,4) \geq \frac{1}{4}q^4 - \frac{3}{2}q^3 - \frac{3}{4}q^2 - 5q - \frac{13}{4} > 0$. Thus $f(n,3) > g(n,4)$.

Combining Cases 1–4, we have $f(n,3) > g(n,4)$ for $n \geq 58$. Then the result follows from Proposition 2.6. □

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