Trees with extremal Wiener indices *

Sujuan Wang \textsuperscript{a}, Xiaofeng Guo \textsuperscript{b, a, †}

\textsuperscript{a} School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, P. R. China

\textsuperscript{b} College of Mathematics and System Sciences, Xinjiang University, Wulumuqi Xinjiang 830046, P. R. China

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Abstract

The Wiener index of a connected graph is the sum of distances for all pairs of vertices. In this paper, we consider the trees with order \(n\), diameter \(d\) or maximum degree \(\Delta\), and extremal Wiener indices. We obtain the tree with minimum Wiener index among all the trees of order \(n\) and with diameter \(d\), and the trees with minimum and maximum Wiener indices among all the caterpillar trees of order \(n\) and with diameter \(d\). We also obtain the tree with maximum Wiener index among all the trees of order \(n\) and with maximum degree \(\Delta\), and the trees with the second and the third maximum Wiener indices among all the trees of order \(n\), whose vertices are of degree 1 or \(\Delta\).

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† Corresponding author. \textit{E-mail:} xfguo@xmu.edu.cn
1 Introduction

The molecular-graph-based quantity $W$, introduced by Harold Wiener [1] in 1947, is nowadays known as the name Wiener index or Wiener number. For a connected graph $G$, let $V(G)$ denote the set of vertices and $E(G)$ the set of edges. Then the Wiener index of $G$, denoted by $W(G)$, is defined by

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v|G)$$ (1)

where $d(u, v|G)$ is the distance between vertices of $u$ and $v$ in $G$, and the summation goes over all pairs of vertices in $V(G)$.

Let $T$ be a tree and $e = uv$ an edge of $T$. Denote by $n_u(e|T)$ (resp. $n_v(e|T)$) the number of vertices of $T$ lying on one side of the edge $e$, closer to vertex $u$ (resp. $v$). Then the Wiener index of $T$ also satisfies the following relation [1]:

$$W(T) = \sum_{e=uv} n_u(e|T) \cdot n_v(e|T)$$ (2)

in which the summation goes over all edges of $T$.

There is a lot of mathematical and chemical literature on the Wiener index, especially on the Wiener index of trees. A survey of known results and open problems was given by Dobrynin et al. [2]. It is of great interest to identify the graphs with extremal Wiener indices for both chemical applications and mathematics, and many results have been obtained [3—11]. One of the most well known results is that [3,4] among all the trees of order $n$, the Wiener index is maximized by the path $P_n$ and minimized by the star $S_n$.

A maximal subtree of a tree $T$ containing a vertex $v$ as an end vertex will be called a branch of $T$ at $v$. A vertex of a tree $T$, having degree 3 or greater, is called a branching point of $T$. A tree $T$ is said to be a starlike tree if exactly one of its vertices has degree greater than two, viz. $T$ has exactly one branching point.

A rooted tree $T$ has one of its vertices, called the root, distinguished from the others.

A dendrimer of degree $\Delta$ on $n$ vertices, $D_{n,\Delta}$, is a tree with maximum degree $\Delta$ defined inductively as follows. The tree $D_{1,\Delta}$ consists of a single vertex labelled 1. The
tree $D_{n,\Delta}$ has vertex set \{1, 2, \ldots, n\} and is obtained by attaching a leaf $n$ to the smallest numbered vertex of $D_{n-1,\Delta}$, which has degree $< \Delta$.

The diameter of a graph is an important graph-theoretical parameter. Let $G(n,d)$ denote the set of all the connected graphs of order $n$ and with diameter $d$. Plesnik [11] obtained the graphs (may not be unique) with minimum Wiener index in $G(n,d)$ \((d \leq n-1)\). When $d < n-1$, they are cycle-containing graphs. Wagner [14] obtained the trees with maximum Wiener index among all the trees with $n$ edges and diameter $\leq 4$.

Let $T(n,\Delta)$ denote the set of all the trees of order $n$ and with maximum degree $\Delta$, and $T_{1,\Delta}(n)$ the set of all the trees of order $n$, whose vertices are of degree 1 or $\Delta$. Liu et al. [5] showed that the dendrimer $D_{n,\Delta}$ is the unique tree with minimum Wiener index in $T(n,\Delta)$. Later, by using different approaches, Fishermann et al. [6] and Jelen et al. [7] independently characterized the tree with minimum Wiener index among all the trees of order $n$ and with maximum degree $\leq \Delta$. In fact, it is also the dendrimer $D_{n,\Delta}$. Fishermann et al. [6] also showed that the tree $C_{\Delta}(n)$ is the unique tree with maximum Wiener index in $T(1,\Delta)(n)$.

Let $T^*(n,d)$ (resp. $C^*(n,d)$) denote the set of all the trees (resp. caterpillar trees) of order $n$ and with diameter $d$. Clearly, $C^*(n,d) \subseteq T^*(n,d)$.

In this paper, by using some tree transformations which strictly increase or decrease the Wiener index of trees, we obtain the tree with minimum Wiener index in $T^*(n,d)$ \((2 \leq d \leq n-1)\), the trees with minimum and maximum Wiener indices in $C^*(n,d)$, and additionally the tree with minimum Wiener index among all the trees of order $n$ and with diameter $\geq d$. And we also obtain the tree with maximum Wiener index in $T(n,\Delta)$, and the trees with the second and the third maximum Wiener indices in $T_{1,\Delta}(n)$.

The structures of the trees with maximum Wiener indices in $T^*(n,d)$ might be quite different according to different values of $n$ and $d$, and so we can’t characterize them in a general way. However, for some special values of $d$, $2 \leq d \leq 4$ or $n-3 \leq d \leq n-1$, the trees with maximum Wiener indices in $T^*(n,d)$ are also determined in this paper.
2 Wiener index versus diameter in trees

In this section, we will characterize the trees with extremal Wiener indices in $T^*(n, d)$ and in $C^*(n, d)$. In addition, we also obtain the trees with extremal Wiener indices among all the trees of order $n$ and with diameter at least $d$.

Figure 1: The trees $T_{n,d}$ and $T'_{n,d}$.

Let $n$ and $d$ be two integers satisfying $n > d \geq 2$. Let $T_{n,d}$ be the tree consisting of a path $P = v_0v_1 \ldots v_d$ together with $n - d - 1$ independent vertices all adjacent to $v_{[d/2]}$. When $d$ is odd, let $T'_{n,d}$ be the tree consisting of a path $P = v_0v_1 \ldots v_d$ together with $s$ independent vertices adjacent to $v_{[d/2]}$ and $t$ independent vertices adjacent to $v_{[d/2]}$, where $s \geq 0$, $t \geq 0$ and $s + t = n - d - 1$ (see figure 1). When $d$ is odd, $[d/2] + 1 = [d/2]$.

So if $s = 0$ or $t = 0$, then $T_{n,d} \cong T'_{n,d}$ ($d$ is odd).

The following theorem presents the tree with minimum Wiener index in $T^*(n, d)$.

**Theorem 2.1** If $T$ is a tree in $T^*(n, d)$ ($2 \leq d \leq n - 1$), then

$$W(T) \geq W(T_{n,d}).$$

The equality holds if and only if $T \cong T_{n,d}$.

In order to prove this conclusion, some preparations are needed.

**Lemma 2.2** [12] Let $T$ be a tree of order $n$ and $e = v_0v_1 \in E(T)$. Let $T_i$, $i=0,1$, be the components of $T - e$ containing $v_i$ with $|V(T_i)| = n_i$, and let $u_1, u_2, \ldots, u_t$ be pendant vertices of $T$, which is adjacent to $v_1$. Then, $W(T + \sum_{j=1}^{t}(-v_1u_j + v_0u_j)) - W(T) = t(n_1 - n_0 - t)$.

By lemma 2.2, the following is immediate.

**Lemma 2.3** Let $d \geq 3$ be an odd number. And let $T_{n,d}$ and $T'_{n,d}$ be the trees described as above. Then, $W(T'_{n,d}) \geq W(T_{n,d})$, with the equality if and only if $T'_{n,d} \cong T_{n,d}$.

Here, we need to use two tree transformations. The first one is the inner-moving transformation.

**Definition 2.4** Let $T_{11}$ be the tree consist of a path $u_0u_1u_2 \cdots u_t$ of length $t$ and rooted
Lemma 2.5 The inner-moving transformation decreases the Wiener index, viz.

\[ W(T_{11}) > W(T_{12}). \]

Proof. Set \( a_i = |V(X_i) \setminus u_i| \) \((l \leq i \leq t - 1)\). Then, \( a_l > 0 \) and \( a_i \geq 0 \) for \( l + 1 \leq i \leq t - 1 \). Using formula (2), we consider the difference \( W(T_{11}) - W(T_{12}) \). Comparing the structures of \( T_{11} \) and \( T_{12} \), we can get that \( n_u(e|T_{11}) \cdot n_v(e|T_{11}) = n_u(e|T_{12}) \cdot n_v(e|T_{12}) \) holds for every edge \( e = uv \) in \( E(T_{11}) \) and \( E(T_{12}) \), except that of \( e = u_tu_{t+1} \). Therefore,

\[
W(T_{11}) - W(T_{12}) = n_u(e|T_{11}) \cdot n_{u_{l+1}}(e|T_{11}) - n_u(e|T_{12}) \cdot n_{u_{l+1}}(e|T_{12}) \quad \text{(where } e = u_tu_{t+1})
\]

\[
= n_u(e|T_{11}) \cdot n_{u_{l+1}}(e|T_{11}) - (n_u(e|T_{11}) - a_l) \cdot (n_{u_{l+1}}(e|T_{11}) + a_l)
\]

\[
= a_l \cdot (n_{u_{l+1}}(e|T_{11}) - n_u(e|T_{11}) + a_l)
\]

Clearly, \( n_u(e|T_{11}) - a_l = l + 1 \). Noticing that \( a_i \geq 0 \) \((l + 1 \leq i \leq t - 1)\), we have \( n_{u_{l+1}}(e|T_{11}) \geq t - l \). So, \( n_{u_{l+1}}(e|T_{11}) - n_u(e|T_{11}) + a_l \geq (t - l) - (l + 1) = t - 2l - 1 \).

As \( 1 \leq l \leq [t/2] \leq t/2 - 1 \), we have \( l \leq t/2 - 1 \). Then, \( t - 2l - 1 \geq 1 > 0 \). And so \( n_{u_{l+1}}(e|T_{11}) - n_u(e|T_{11}) + a_l > 0 \). Note that \( a_l > 0 \). Therefore, \( W(T_{11}) > W(T_{12}) \).

The second tree transformation we need is the edge-growing transformation, which had been used by Dong and Guo [12] for ordering trees by their Wiener indices.

Definition 2.6 Let \( T_{21} \) be a tree of order \( n \) and \( T_{21} \neq S_n \). Let \( e = uv \) be a non-pendent edge of \( T_{21} \), and \( T_1 \) and \( T_2 \) be the two components of \( T_{21} - e \), \( u \in T_1 \), \( v \in T_2 \). \( T_{22} \) is the tree obtained from \( T_{21} \) in the following way:
(1) Contract the edge $e = uv$;
(2) Add a pendent edge to the vertex $u(= v)$;

The procedures (1) and (2) are called the \textit{edge-growing transformation} of $T_{21}$ (on edge $e$) or \textit{e.g.t.} of $T_{21}$ (on edge $e$) for short (see figure 3).

![Figure 3: The edge-growing transformation of the tree $T_{21}$.](image)

**Lemma 2.7** [12] The edge-growing transformation decreases the Wiener index, viz.

$$W(T_{21}) > W(T_{22}).$$

Now we come to the proof of Theorem 2.1.

**Proof of Theorem 2.1.** Let $T$ be a tree in $T^\ast(n, d)$, and let $P = v_0v_1\cdots v_d$ be a longest path in $T$. Clearly, $d_T(v_0) = d_T(v_d) = 1$. Let $X_i$ be the component of $T - E(P)$ containing $v_i$, $i = 1, 2, \cdots, d - 1$, which is a rooted tree with root $v_i$.

By e.g.t. for all the non-pendent edges of $T$ not on $P$, $T$ can be transformed to a caterpillar tree $T^\ast$ such that every rooted tree $X_i$ becomes a star (see figure 4). By lemma 2.7, $W(T) \geq W(T^\ast)$, with the equality if and only if $T \cong T^\ast$.

![Figure 4: A caterpillar tree in the proof of theorem 2.1.](image)

In addition, by i.m.t., $T^\ast$ can be transformed into either $T_{n,d}$ or $T'_{n,d}$ (if $d$ is odd). Now it follows from lemmas 2.3 and 2.5 that $W(T) \geq W(T^\ast) \geq W(T_{n,d})$, with the equality if and only if $T \cong T^\ast \cong T_{n,d}$.

**Corollary 2.8** If $T$ is a tree of order $n$ and with diameter at least $d$ ($2 \leq d < n$), then

$$W(T_{n,d}) \leq W(T) \leq W(P_n).$$

($\ast$)
The lower bound is realized if and only if \( T \cong T_{n,d} \) and the upper bound if and only if \( T \cong P_n \).

**Proof.** Note that the diameter of the path \( P_n \) is \( n - 1 \geq d \). As \( P_n \) maximizes the Wiener index among all the trees of order \( n \), the right-hand side inequality in (\(*) holds obviously.

Now we prove the left-hand side inequality in (\(*)). If \( T \) is a tree with diameter greater than \( d \), then \( T \) can be transformed into a tree (say \( T' \)) with diameter \( d \) by a number of e.g.t. By lemma 2.7, \( W(T) > W(T') \). So, we can conclude that if \( T \) minimizes the Wiener index among all the trees of order \( n \) and with diameter \( \geq d \), then \( T \) must be a tree of order \( n \) and with diameter \( d \). Then, the left-hand side inequality in (\*) follows from theorem 2.1. \( \blacksquare \)

Now, we consider the trees in \( C^*(n,d) \). Clearly, \( C^*(n,d) \subseteq T^*(n,d) \), and \( T_{n,d} \in C^*(n,d) \). The tree with minimum Wiener index in \( C^*(n,d) \) is also the tree \( T_{n,d} \). In addition, the tree with maximum Wiener index in \( C^*(n,d) \) can also be characterized.

Let \( L(n,l) \) (\( 2 \leq l \leq n - 1 \)) denote the set of all the trees of order \( n \) and with \( l \) pendant vertices. The following lemma gives the tree with maximum Wiener index in \( L(n,l) \), which was obtained by Shi [8] and later independently by Entringer [9].

**Lemma 2.9** [8,9] If \( T \) is a tree in \( L(n,l) \) (\( 2 \leq l \leq n - 1 \)), then
\[
W(T) \leq W(D(n,\lceil l/2 \rceil,\lfloor l/2 \rfloor)).
\]
The equality holds if and only if \( T \cong D(n,\lceil l/2 \rceil,\lfloor l/2 \rfloor) \).

The above lemma can be used to obtain the tree with maximum Wiener index in \( C^*(n,d) \).

**Theorem 2.10** If \( T \) is a tree in \( C^*(n,d) \) (\( 2 \leq d \leq n - 1 \)), then
\[
W(T_{n,d}) \leq W(T) \leq W(D(n,\lceil (n-d+1)/2 \rceil,\lfloor (n-d+1)/2 \rfloor)). \tag{\*}
\]
The lower bound is realized if and only if \( T \cong T_{n,d} \) and the upper bound if and only if \( T \cong D(n,\lceil (n-d+1)/2 \rceil,\lfloor (n-d+1)/2 \rfloor) \).

**Proof.** The left-hand side inequality in (\*) follows immediately from theorem 2.1.

Now we prove the right-hand side inequality in (\*). By lemma 2.9, \( D(n,\lceil (n-d+1)/2 \rceil,\lfloor (n-d+1)/2 \rfloor) \) is the unique tree with maximum Wiener index in \( L(n,n-d+1) \). It is not difficult to see that \( D(n,\lceil (n-d+1)/2 \rceil,\lfloor (n-d+1)/2 \rfloor) \in C^*(n,d) \subseteq L(n,n-d+1) \). So, \( D(n,\lceil (n-d+1)/2 \rceil,\lfloor (n-d+1)/2 \rfloor) \) is also the unique tree with maximum Wiener index in \( C^*(n,d) \). Thus, the right-hand side inequality in (\*) also holds. \( \blacksquare \)

Now we consider the trees with maximum Wiener index in \( T^*(n,d) \) (\( 2 \leq d \leq n - 1 \).
Here, the trees with maximum Wiener index in $T^*(n, d)$ are determined for $2 \leq d \leq 4$ or $n - 3 \leq d \leq n - 1$.

When the diameter $d = \bar{d} \in \{2, 3, n - 1, n - 2\}$, the trees in $T^*(n, \bar{d})$ are all caterpillar trees, viz. $T^*(n, \bar{d}) = C^*(n, \bar{d})$. Then, by theorem 2.10, the unique tree with maximum Wiener index in $T^*(n, \bar{d})$ is the tree $D(n, [(n - \bar{d} + 1)/2], [(n - \bar{d} + 1)/2])$.

When $d = 4$, the trees with maximum Wiener index in $T^*(n, 4)$ can be obtained from the result of Theorem 3 in Wagner [14]. But there is a little mistake in it (see the remark after Theorem 2.12). Here, we will restate the result as Theorem 2.12.

**Definition 2.11** [14] Let $(c_1, c_2, \ldots, c_t)$ be a partition of $n - 1$ ($n > 1$). A tree with diameter $\leq 4$ assigned to this partition is the tree

![Diagram of a tree]

where $v_1, v_2, \ldots, v_t$ have degrees $c_1, c_2, \ldots, c_t$ respectively. It has exactly $n - 1$ edges (viz. $n$ vertices). The tree itself is denoted by $S(c_1, c_2, \ldots, c_t)$.

Set $k = [\sqrt{n-1}]$ ($n > 1$). If $k^2 + k \geq n - 1$, set $T_m = S(\underbrace{k, \ldots, k}_{k^2+k-n+1}, \underbrace{k+1, \ldots, k+1}_{n-k^2-1})$. If $k^2 + k \leq n - 1$, set $T'_m = S(\underbrace{k, \ldots, k}_{k^2+2k-n+2}, \underbrace{k+1, \ldots, k+1}_{n-k^2-k-1})$. Notice that when $k^2 + k = n - 1$, $T_m$ and $T'_m$ are non-isomorphic trees with $W(T_m) = W(T'_m) = 2k^3(k + 1)$.

**Theorem 2.12** [14] Let $T$ be a tree with $n$ vertices and diameter $\leq 4$. Set $k = [\sqrt{n-1}]$.

1. If $k^2 + k > n - 1$, then $W(T) \leq W(T_m)$, with the equality if and only if $T \cong T_m$.
2. If $k^2 + k < n - 1$, then $W(T) \leq W(T'_m)$, with the equality if and only if $T \cong T'_m$.
3. If $k^2 + k = n - 1$, then $W(T) \leq W(T_m) = W(T'_m)$, with the equality if and only if $T \cong T_m$ or $T \cong T'_m$.

**Remark:** From the result of Theorem 3 in [14], we get that when $k^2 + k = n - 1$, the tree with maximum Wiener index among all the trees with $n$ vertices and diameter $\leq 4$ is the tree $T'_m$. But, in fact, when $k^2 + k = n - 1$, $T_m$ and $T'_m$ are both the trees with maximum Wiener index. In other words, Theorem 3 of [14] misses out the tree $T_m$ for the case when $k^2 + k = n - 1$.

It is not difficult to see that, if $n \geq 5$, $k = [\sqrt{n-1}] \geq 2$, and $T_m$ and $T'_m$ are trees with diameter 4. From theorem 2.12, we can conclude that the trees with maximum Wiener index in $T^*(n, 4)$ are either the tree $T_m$ if $k^2 + k > n - 1$, or the tree $T'_m$ if
$k^2 + k < n - 1$, or the trees $T_m$ and $T'_m$ if $k^2 + k = n - 1$.

For a tree $T$ in $T^*(n, n - 3)$ with diameter $d = n - 3 \geq 5$, let $P$ be a path of length $n - 3$ in $T$. Then, there are only two vertices in $T$, say $u$ and $v$, that are not on the path $P$. We partition the trees in $T^*(n, n - 3)$ into two classes: $C^*(n, n - 3)$ and $\overline{C}^*(n, n - 3) = T^*(n, n - 3) \setminus C^*(n, n - 3)$. Then any tree in $\overline{C}^*(n, n - 3)$ must be the tree $T_{n-3}^i$ (for some $2 \leq i \leq n - 5$) shown in figure 5.

Figure 5: The tree $T_{n-3}^i$ in $\overline{C}^*(n, n - 3)$.

By theorem 2.10, we know that the tree with maximum Wiener index in $C^*(n, n - 3)$ is the tree $D(n, 2, 2)$. By the inverse i.m.t., we can get that the tree with maximum Wiener index in $\overline{C}^*(n, n - 3)$ is the tree $T_{n-3}^2$ (isomorphic to $T_{n-3}^{n-5}$). Therefore, in order to obtained the tree with maximum Wiener index in $T^*(n, n - 3)$, we only need to compare $W(D(n, 2, 2))$ and $W(T_{n-3}^2)$. By formula (1) or (2), we have $W(D(n, 2, 2)) - W(T_{n-3}^2) = 2n - 14 > 0$ for $n - 3 \geq 5$, and so the tree with maximum Wiener index in $T^*(n, n - 3)$ ($n \geq 8$) is the tree $D(n, 2, 2)$.

Now, the trees with maximum Wiener indices in $T^*(n, d)$ ($2 \leq d \leq 4$ or $5 \leq n - 3 \leq d \leq n - 1$) have all been determined.

For the cases $5 \leq d \leq n - 4$, it is difficult to characterize the trees with maximum Wiener indices in $T^*(n, d)$. For a fixed value of $d$ and different values of $n$, the trees with maximum Wiener indices may have different structures. To illustrate this fact, we list the trees with maximum Wiener indices in $T^*(n, d)$ for some values of $n$ and $d$.

Let $T^i_{n,d}$ ($i = 1, 2, \ldots$) denote the trees with maximum Wiener indices in $T^*(n, d)$. Figure 6 shows the trees with maximum Wiener indices in $T^*(10, 5)$, $T^*(10, 6)$, $T^*(11, 5)$ and $T^*(11, 6)$, the Wiener indices of which are respectively as follows, $W(T^1_{10,5}) = W(T^2_{10,5}) = 127$, $W(T^1_{10,6}) = 139$, $W(T^1_{11,5}) = W(T^2_{11,5}) = 160$, $W(T^1_{11,6}) = W(T^2_{11,6}) = 176$.

From the above examples, it seems to be impossible to give a universal characterization for the trees with maximum Wiener indices in $T^*(n, d)$ for $5 \leq d \leq n - 4$. 
Figure 6: Some trees with maximum Wiener indices in $T^*(n, d)$, $5 \leq d \leq n - 4$.

3 Wiener index versus maximum degree in trees

In this section, we will characterize the tree with maximum Wiener index in $T(n, \Delta)$, and the trees with the second and the third maximum Wiener indices in $T_{1, \Delta}(n)$.

In order to obtain the tree with maximum Wiener index in $T(n, \Delta)$, we need the following tree transformation, which had been used by Gutman et al. [13].

![Figure 7: The lengthening transformation of the tree $T_{31}$.](image)

Let $T_{31}$ and $T_{32}$ be the trees depicted in figure 7, where $a$ and $b$ are two integers satisfying $b > a \geq 0$, and $R$ is a rooted tree with root $r$ and of order greater than 1. For convenience, we call the transformation $T_{31} \rightarrow T_{32}$ the lengthening transformation of $T_{31}$, or the l.t. of $T_{31}$ for short.

The following lemma is an immediate result of Theorem 2 in Gutman et al. [13].

**Lemma 3.1** [13] The lengthening transformation increases the Wiener index, viz.

$$W(T_{31}) < W(T_{32}).$$

**Theorem 3.2** If $T$ is a tree in $T(n, \Delta)$ ($\Delta \geq 3$), then

$$W(T) \leq W(D(n, \Delta - 1, 1))$$
The equality holds if and only if $T \cong D(n, \Delta - 1, 1)$.

**Proof.** As $T \in T(n, \Delta)$, there is at least one vertex, say $v$, such that $d_T(v) = \Delta$. Viz. there are $\Delta$ branches of $T$ at the vertex $v$. Suppose $T \not\cong D(n, \Delta - 1, 1)$. If $T$ is not a starlike tree, then there exist some branches of $T$ at $v$ that are not paths. Then, by repeatedly carrying out the l.t. on each of such branches, one can transform $T$ into a starlike tree (say $S^*$) with $v$ as the unique branching point. If $S^* \not\cong D(n, \Delta - 1, 1)$, then $S^*$ can be transformed into $D(n, \Delta - 1, 1)$ by a number of l.t. between different branches of $S^*$ at $v$. By lemma 3.1, $W(T) < W(D(n, \Delta - 1, 1))$. Thus, the result holds. ■

As referred above, Fishermann et al. [6] showed that the tree $C_\Delta(n)$ is the unique tree with maximum Wiener index in $T_{1,\Delta}(n)$. Now, we define a tree transformation that can be used to obtain the trees with the second and the third maximum Wiener indices in $T_{1,\Delta}(n)$.

**Definition 3.3** Let $\Delta, a, b$ be integers satisfying $\Delta \geq 3, b > a \geq 0$. And let $T_{41}$ be the tree depicted in figure 8, where $T_0$ is a rooted tree with root $r_0$ and $|V(T_0)| > \Delta - 1$. $T_{42}$ is the tree obtained from $T_{41}$ in the following way:

1) Delete all the edges $xx_i$ ($1 \leq i \leq \Delta - 1$);
2) Add all the edges $yx_i$ ($1 \leq i \leq \Delta - 1$).

The procedures (1) and (2) are called the $(\Delta - 1)$-regular-lengthening transformation of $T_{41}$ or $(\Delta - 1)$-r.l.t. of $T_{41}$ for short.

![Diagram](image)

Figure 8: The $(\Delta - 1)$-regular-lengthening transformation of the tree $T_{41}$.

**Lemma 3.4** The $(\Delta - 1)$-r.l.t. increases the Wiener index, viz.

$$W(T_{41}) < W(T_{42})$$

**Proof.** Let $E_1$ (resp. $E_2$) denote the set of all the pendent edges of $T_{41}$ (resp. $T_{42}$) not in $T_0$. Then, $|E_1| = |E_2| = (a + b)(\Delta - 2) + \Delta$. Set the paths $P_1^1 = u_1u_2 \cdots x$ and
$P_1^2 = r_0v_1 \cdots v_b$ in $T_{41}$. And set $P_2^1 = r_0u_1 \cdots u_a$ and $P_2^2 = v_1v_2 \cdots y$ in $T_{42}$. Comparing the structures of $T_{41}$ and $T_{42}$, we can get the following equalities:

\[
\sum_{e=uv \in E(T_0)} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv \in E(T_0)} n_u(e|T_{42}) \cdot n_v(e|T_{42});
\]

\[
\sum_{e=uv \in E_1} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv \in E_1} n_u(e|T_{42}) \cdot n_v(e|T_{42});
\]

\[
\sum_{e=uv \in E(P_1)} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv \in E(P_2)} n_u(e|T_{42}) \cdot n_v(e|T_{42});
\]

The edges not involved in the above equalities are the edges $r_0u_1$ in $T_{41}$ and $r_0v_1$ in $T_{42}$. Therefore, we have

\[
W(T_{42}) - W(T_{41}) = n_{r_0}(r_0v_1|T_{42}) \cdot n_{v_1}(r_0v_1|T_{42}) - n_{r_0}(r_0u_1|T_{41}) \cdot n_{u_1}(r_0u_1|T_{41})
\]

\[
= [b(\Delta - 1) + \Delta][n - b(\Delta - 1) - \Delta] - [a(\Delta - 1) + \Delta][n - a(\Delta - 1) - \Delta]
\]

\[
= (\Delta - 1)(b - a)[n - (a + b)(\Delta - 1) - 2\Delta]
\]

Note that $|V(T_0)| > \Delta - 1$. Let $T_{41}$ be the tree depicted in figure 9, where $d_0 = \frac{n - 2}{\Delta - 1} + 1$. Let $T_{42} \in T_{1,\Delta}(n)$ be the tree depicted in figure 9, where $d = d_0 - 1 = \frac{n - 2}{\Delta - 1} \geq 4$. The following theorem gives the tree with the second maximum Wiener index in $T_{1,\Delta}(n)$.

**Theorem 3.5** If $T$ is a tree in $T_{1,\Delta}(n) \setminus \{C_\Delta(n), T_\Delta(n)\}$ ($\Delta \geq 3, n \geq 4\Delta - 2$), then

\[
W(T) < W(T_\Delta(n)) < W(C_\Delta(n)).
\]
Proof. Note that $T \neq C_{\Delta}(n)$ and $T \neq T_{\Delta}(n)$. By a number of $(\Delta - 1)$-r.l.t., $T$ can be transformed into the tree $T_{\Delta}(n)$. By lemma 3.4, $W(T) < W(T_{\Delta}(n))$. Furthermore, $T_{\Delta}(n)$ can be transformed into $C_{\Delta}(n)$ by a step of $(\Delta - 1)$-r.l.t. So by lemma 3.4, $W(T_{\Delta}(n)) < W(C_{\Delta}(n))$. Therefore, the result holds.

Let $T'_{\Delta}(n), T''_{\Delta}(n) \in T_{1, \Delta}(n)$ be the trees depicted in figure 10, where $d = \frac{n-2}{\Delta-1} \geq 6$.

Theorem 3.6 If $T$ is a tree in $T_{1, \Delta}(n) \setminus \{C_{\Delta}(n), T_{\Delta}(n)\}$ $(\Delta \geq 3$, $n \geq 6\Delta - 4)$, then $W(T) \leq W(T'_{\Delta}(n))$. The equality holds if and only if $T \equiv T'_{\Delta}(n)$.

Figure 10: The trees $T'_{\Delta}(n)$ and $T''_{\Delta}(n)$ in $T_{1, \Delta}(n)$.

Proof. Note that $T \in T_{1, \Delta}(n) \setminus \{C_{\Delta}(n), T_{\Delta}(n)\}$. If $T \not\equiv T'_{\Delta}(n)$ and $T \not\equiv T''_{\Delta}(n)$, then $T$ can be transformed into $T'_{\Delta}(n)$ by a number of $(\Delta - 1)$-r.l.t. By lemma 3.4, $W(T) < W(T'_{\Delta}(n))$.

Let $P'$ (resp. $P''$) be the $(v_3 - v_{d-4})$-path in $T'_{\Delta}(n)$ (resp. $T''_{\Delta}(n)$), and let $E_1$ (resp. $E_2$) be the set of all the pendent edges of $T'_{\Delta}(n)$ (resp. $T''_{\Delta}(n)$). Clearly,
\[
\sum_{e=uv \in E(P')} n_u(e|T'_{\Delta}(n)) \cdot n_v(e|T'_{\Delta}(n)) = \sum_{e=uv \in E(P'')} n_u(e|T''_{\Delta}(n)) \cdot n_v(e|T''_{\Delta}(n)),
\]
\[
\sum_{e=uv \in E_1} n_u(e|T'_{\Delta}(n)) \cdot n_v(e|T'_{\Delta}(n)) = \sum_{e=uv \in E_2} n_u(e|T''_{\Delta}(n)) \cdot n_v(e|T''_{\Delta}(n)).
\]
Comparing the other edges in $T'_{\Delta}(n)$ and $T''_{\Delta}(n)$, we have that $W(T'_{\Delta}(n)) - W(T''_{\Delta}(n)) = 2(2\Delta - 1)[n-(2\Delta - 1)] - \Delta(n - \Delta) - (3\Delta - 2)[n-(3\Delta - 2)] = 2(\Delta - 1)^2 > 0$. So $W(T'_{\Delta}(n)) > W(T''_{\Delta}(n))$.

Thus, the result holds.

It becomes more and more complicated to determine the trees with the 4th, 5th, . . . , maximum Wiener indices in $T_{1, \Delta}(n)$. Other than the $(\Delta - 1)$-r.l.t., much discussion and comparison are also needed for determining the tree with the 4th maximum Wiener index in $T_{1, \Delta}(n)$. Here, we would not discuss it any more.
References


