The Terminal Wiener Index of Trees with Diameter or Maximum Degree*

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Abstract

The terminal Wiener index of a tree is the sum of distances for all pairs of pendent vertices, which recently arises in the study of phylogenetic tree reconstruction and the neighborhood of trees. This paper presents a sharp upper and lower bounds for the terminal Wiener index in terms of its order and diameter and characterizes all extremal trees which attain these bounds. In addition, we investigate the properties of extremal trees which attain the maximum terminal Wiener index among all trees of order n with fixed maximum degree.

Key words: Terminal Wiener index; Tree; Diameter; Maximum degree.

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1 Introduction

Many topological indices (molecular-structure descriptors) have been put forward in different studies, from biochemistry to pure mathematics. The Wiener index, which is one of the oldest and most widely used indices in quantitative structure-activity relationships, has been received great attention by mathematicians and chemists (for example, see [4, 6, 7, 18, 19]). Recently, some researchers considered terminal distance matrix [11, 13] and found that it was used in the mathematical modelling of proteins and genetic [11, 13, 14] and regarded it as a source of novel molecular-structure descriptors [13, 16]. Due to study on the terminal distance matrix and its chemical applications, Gutman, Furtula and Petrović [8] first proposed the concept of *terminal Wiener index*, which is defined as the sum of distances between all pairs of pendent vertices of trees. The terminal Wiener index is also arisen in the study of phylogenetic tree reconstruction and the neighborhood of trees [1, 12]. For more information on the terminal Wiener indices, the readers may refer to the recent papers [2, 3, 5, 9, 10, 15, 17, 20] and the references cited therein.

Let $T = (V(T), E(T))$ be a tree of order n with vertex set $V(T)$ and edge set $E(T)$. The distance between vertices v_i and v_j is the number of edges in the shortest path from v_i to v_j and denoted by $d_T(v_i, v_j)$ (or for short $d(v_i, v_j)$). Moreover, *terminal Wiener index* $TW(T)$ of a tree T can be expressed as

$$TW(T) = \sum_{\{v_i,v_j\}\subseteq L(T)} d_T(v_i, v_j), \tag{1}$$

where $L(T)$ is the set of pendent vertices in $V(T)$, i.e., the set of vertices with degree 1 in $V(T)$. Gutman et al. [8] gave a formula for the terminal Wiener index of trees

$$TW(T) = \sum_{e=uv\in E(T)} p_u(e|T)p_v(e|T), \tag{2}$$

where $p_u(e|T)$ and $p_v(e|T)$ denote the number of pendent vertices of two components of $T - e$ containing u and v, respectively. The rest of the paper is organized as follows. In Section 2, we present a sharp upper and lower bounds for terminal Wiener index of a tree in terms of the number of vertices and diameter and characterize all extremal trees which attain these bounds. In section 3, we investigate the properties of terminal Wiener index of a tree with fixed maximum degree.

2 Trees with fixed diameter

In this section, we only consider the terminal Wiener index of $n-$vertex trees with a fixed diameter d. Let $\mathcal{T}_{n,d}$ denote the set of all the trees of order n with fixed diameter d and let $\mathcal{T}_{n,d,l}$ denote the set of all the trees of order n with fixed diameter d and the number l of the pendent vertices. Clearly, $\mathcal{T}_{n,d}$ consists of only star $K_{1,n-1}$ for $d = 2$, and only path for $d = n - 1$. Moreover, $2 \le l \le n - d + 1$ with the left equality holding if and only if $d = n - 1$. A tree T is called *caterpillar* if the graph from T by deleting its all pendent vertices is a path. A tree is called *starlike tree of degree k* if there is only one vertex with degree $k \ge 3$. Gutman et al. [8] presented the following result.

Theorem 2.1 *[8] Let T be an $n-$vertex tree with the number $l \ge 3$ of pendent vertices. Then*

$$TW(T) \ge (n-1)(l-1) \tag{3}$$

with equality if and only if T is starlike of degree l.

In order to present the main result in this section, we need the following lemma.

Lemma 2.2 *Let T be an $n-$vertex tree with diameter d and the number l of the pendent vertices. Then*

$$\lceil \frac{n-1}{\lfloor \frac{d}{2} \rfloor} \rceil \le l \le n-d+1, \quad \text{if d is even;} \tag{4}$$

$$\lceil \frac{n-2}{\lfloor \frac{d}{2} \rfloor} \rceil \le l \le n-d+1, \quad \text{if d is odd.} \tag{5}$$

Proof. Let $P = v_0v_1\cdots v_d$ be a longest path since the diameter of T is d. For any vertex $u \in V(T)\backslash\{v_0,\cdots,v_d\}$, the distance between vertex u and the path P is at most $\lfloor \frac{d}{2} \rfloor$, i.e., $\text{dist}(u,P) = \min\{d(u,v) \mid v \in V(P)\} \le \lfloor \frac{d}{2} \rfloor$. Otherwise the diameter of T is larger than d. Since every vertex in $u \in V(T)\backslash\{v_0,\cdots,v_d\}$ lies on a path from some pendent vertex except $\{v_0,v_d\}$ to the path P, we have $\lfloor \frac{d}{2} \rfloor(l-2)+d+1 \ge n$. Therefore if d is even, then $\lfloor \frac{d}{2} \rfloor l \ge n-1$, i.e., $l \ge \lceil \frac{n-1}{\lfloor \frac{d}{2} \rfloor} \rceil$; if d is odd, then $\lfloor \frac{d}{2} \rfloor l \ge n-2$, i.e., $l \ge \lceil \frac{n-2}{\lfloor \frac{d}{2} \rfloor} \rceil$. So the assertion holds. ■

Now we are ready to present a sharp lower bound for the terminal Wiener index of $n-$vertex trees with fixed diameter d.

Theorem 2.3 *Let T be an $n-$vertex tree with fixed diameter d, i.e., $T \in \mathcal{T}_{n,d}$. Then* *where*

$$l_0 = \begin{cases} \lceil \frac{n-1}{\lfloor \frac{d}{2} \rfloor} \rceil, & \text{if } d \text{ is even,} \\ \lceil \frac{n-2}{\lfloor \frac{d}{2} \rfloor} \rceil, & \text{if } d \text{ is odd.} \end{cases}$$

Moreover, if $d \geq 3$, equality (6) holds if and only if T is starlike trees of degree l_0 and diameter d.

Proof. If $d = n - 1$, the assertion holds. Assume that $d \leq n - 2$. Let T^* be an n−vertex tree with diameter d such that

$$TW(T) \geq TW(T^*) \quad \text{for } T \in \mathcal{T}_{n,d}.$$

Denote by l the number of pendent vertices of T^*. By Lemma 2.2, $l \geq l_0 \geq 3$. On the other hand, $T^* \in \mathcal{T}_{n,d,l} \subseteq \mathcal{T}_{n,l}$. Hence by Theorem 2.1, we have $TW(T^*) \geq (n-1)(l-1)$ with equality if and only if T^* is starlike trees of degree l. Therefore

$$TW(T) \geq TW(T^*) \geq (n-1)(l-1) \geq (n-1)(l_0-1)$$

with equality if and only if T is starlike trees of degree l_0 with diameter d. ■

Remark For given an n and $d \leq n-2$, there always exists at least one n−vertex starlike tree T of degree l_0 with diameter d. For example, the n−vertex tree T is obtained from $l_0 - 2$ paths of length $\lfloor \frac{d}{2} \rfloor$ and 2 paths of length $\lceil \frac{d}{2} \rceil, n - \lfloor \frac{d}{2} \rfloor (l_0 - 2) - \lceil \frac{d}{2} \rceil - 1$, respectively, by identifying one end of their paths. Moreover, the following result can be easily obtained from the proof of Theorem 5 in [8].

Lemma 2.4 *[8] Let $g(x) = x(x-1) + (n-x-1)\lfloor \frac{x}{2} \rfloor \lceil \frac{x}{2} \rceil$ be positive integer function on x, where $n \geq 3$ is positive integer. Then $g(x)$ is strictly increasing with respect to $2 \leq x \leq \lfloor \frac{2n}{3} \rfloor + 2$; and strictly decreasing with respect to $\lfloor \frac{2n+1}{3} \rfloor + 2 \leq x \leq n-2$. Moreover,*

$$g(x) \leq \begin{cases} \frac{1}{27}(n^3 + 9n^2 + 9n - 27), & \text{if } 3 \mid n; \\ \frac{1}{27}(n^3 + 9n^2 + 6n - 16), & \text{if } 3 \mid (n-1); \\ \frac{1}{27}(n^3 + 9n^2 + 6n - 2), & \text{if } 3 \mid (n-2); \end{cases} \tag{7}$$

with equality holding if and only if

$$x = \begin{cases} \lfloor \frac{2n}{3} \rfloor + 2, & \text{if } 3 \mid n; \\ \lfloor \frac{2n}{3} \rfloor + 2 \text{ or } \lfloor \frac{2n+1}{3} \rfloor + 2, & \text{if } 3 \mid (n-1); \\ \lfloor \frac{2n}{3} \rfloor + 2, & \text{if } 3 \mid (n-2). \end{cases}$$

Theorem 2.5 *Let T be an $n-$vertex tree with diameter d, i.e., $T \in \mathcal{T}_{n,d}$. If $d \geq \lfloor \frac{n-2}{3} \rfloor$, then*

$$TW(T) \leq (n-d+1)(n-d) + (d-2)\lfloor \frac{n-d+1}{2} \rfloor \lceil \frac{n-d+1}{2} \rceil. \quad (8)$$

Moreover, if $n-d+1$ is even, then equality in (8) holds if and only if T is obtained from the path P_{d-1} of order $d-1$ by attaching to each of its terminal vertices $\frac{n-d+1}{2}$ new pendent vertices and this tree is unique. If $n-d+1$ is odd, then equality in (8) holds if and only if T is obtained from the path P_{d-1} of order $d-1$ by attaching to each of its terminal vertices $\lfloor \frac{n-d+1}{2} \rfloor$ new pendent vertices and by attaching one pendent vertex to some vertex of P_{d-1} and there are $\lfloor \frac{d}{2} \rfloor$ distinct trees.

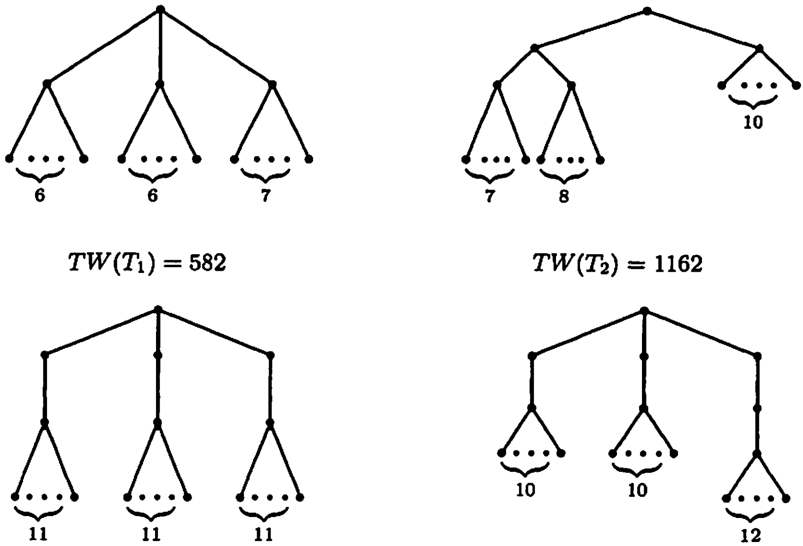
Proof. If $n = 3p$, let l be the number of pendent vertices of T. Then $l \leq n-d+1 \leq 3p-(p-1)+1 = 2p+2 = \lfloor \frac{2n}{3} \rfloor + 2$. By Theorem 4 in [8] and Lemma 2.4,

$$\begin{aligned} TW(T) &\leq l(l-1) + (n-1-l)\lfloor \frac{l}{2} \rfloor \lceil \frac{l}{2} \rceil \\ &\leq (n-d+1)(n-d) + (d-2)\lfloor \frac{n-d+1}{2} \rfloor \lceil \frac{n-d+1}{2} \rceil. \end{aligned}$$

If equality in (8) holds, then by Lemma 2.4, $l = n-d+1$. Moreover, by Theorem 4 in [8], all non-terminal edges $e = uv$, we have $p_u(e|T) = \lfloor \frac{n-d+1}{2} \rfloor$ and $p_v(e|T) = \lceil \frac{n-d+1}{2} \rceil$. Let $P_{d+1} = v_0 v_1 \cdots v_d$ be the longest path of T. Hence if $n-d+1$ is even, then for $e_1 = v_1 v_2$ and $e_{d-2} = v_{d-2} v_{d-1}$, we have $p_{v_1}(e_1|T) = \frac{n-d+1}{2}$ and $p_{v_{d-1}}(e_{d-2}|T) = \frac{n-d+1}{2}$. So T is obtained from the path P_{d-1} of order $d-1$ by attaching to each of its terminal vertices $\frac{n-d+1}{2}$ new pendent vertices and this tree is unique. If $n-d+1$ is odd, then $p_{v_1}(e_1|T) \geq \lfloor \frac{n-d+1}{2} \rfloor$ and $p_{v_{d-1}}(e_{d-2}|T) \geq \lfloor \frac{n-d+1}{2} \rfloor$. Hence T is obtained from the path P_{d-1} of order $d-1$ by attaching to each of its terminal vertices $\lfloor \frac{n-d+1}{2} \rfloor$ new pendent vertices and by attaching one pendent vertex to some vertex of P_{d-1} and there are $\lfloor \frac{d}{2} \rfloor$ distinct trees. Conversely, it is easy to show that the equality holds.

If $n = 3p+1$ and $n = 3p+2$, then by similar method, we can prove the assertion holds. ∎

Remark If $d = 2$ or $d = 3$, Theorem 2.5 is still true. But if $4 \leq d < \lfloor \frac{n-2}{3} \rfloor$, Theorem 2.5 is, in general, not true. With aid of computing calculation, trees T_1, T_2, T_3, T_4 (see Fig.1) have the largest terminal Wiener indices among all trees of order $n = 23$ with $d = 4$, $n = 30$ with $d = 5$, $n = 40$ with $d = 6$, and $n = 40$ with $d = 7$, respectively.



$TW(T_1) = 582$ $TW(T_2) = 1162$

$TW(T_3) = 2508$ $TW(T_4) = 2592$

Fig.1 T_1, T_2, T_3, T_4 have the maximum terminal Wiener index of trees in $\mathcal{T}_{23,4}, \mathcal{T}_{30,5}$, $\mathcal{T}_{40,6}$ and $\mathcal{T}_{40,7}$, respectively

3 Terminal Wiener index with fixed maximum degree

Let $\mathcal{T}_{n,\Delta}$ denote the set of all the trees of order n and with maximum degree Δ. If $\Delta = 2$, $\mathcal{T}_{n,2}$ consists of path P_n of order n, and $TW(P_n) = n - 1$. If $\Delta = n - 1$, then $\mathcal{T}_{n,n-1}$ consists of star $K_{1,n-1}$ and $TW(K_{1,n-1}) = (n-1)(n-2)$. By [3], the extremal trees having the minimum terminal Wiener index in $\mathcal{T}_{n,\Delta}$ are starlike trees. It is natural to ask which are extremal trees having the maximum terminal Wiener index. Through this section, assume that $3 \leq \Delta \leq n-2$. A tree T^* in $\mathcal{T}_{n,\Delta}$ is called *optimal* tree if $TW(T^*) \geq TW(T)$ for all $T \in \mathcal{T}_{n,\Delta}$. In this section, we discuss some properties of optimal trees. Schmuck, Wagner and Wang [15] proved the following result.

Theorem 3.1 *[15] Let $\mathcal{T}_\pi$ be the set of all trees with a given degree sequence $\pi = (d_1, d_2, \cdots, d_n)$ and $d_1 \geq d_2 \geq \cdots \geq d_k \geq 2 > d_{k+1} = \cdots = d_n = 1$. If $d_2 \geq 3$ and $TW(T^*) \geq TW(T)$ for any $T \in \mathcal{T}_\pi$, then T^* is an $n-$vertex caterpillar associated with $v_1, \cdots v_k$ vertices on the backbone of T^* in this order with $d(v_i) = x_i + 2$, $i = 1, \cdots k$, and*

$$TW(T^*) = (n-1)(n-k-1) + F(x_1, \cdots, x_k), \tag{9}$$

where

$$F(x_1,\cdots,x_k)=max\{F(y_1,\cdots,y_k)=\sum_{i=1}^{k-1}(\sum_{j=1}^{i}y_j)(\sum_{j=i+1}^{k}y_j):y_1\geq y_k\}$$

and the maximum is taken over all permutations $(y_1,\cdots,y_k)$ *of* $(d_1-2,\cdots,d_k-2)$.

It follows from the method of [15] and [21] that we are able to prove the following result.

Lemma 3.2 *Let* $w_1\geq w_2\geq\cdots\geq w_k\geq 0$ *be the integers with* $k\geq 5$ *and let*

$$F(x_1,\cdots,x_k)=max\{F(y_1,\cdots,y_k)=\sum_{i=1}^{k-1}(\sum_{j=1}^{i}y_j)(\sum_{j=i+1}^{k}y_j):y_1\geq y_k\},$$

where the maximum is taken over all permutations $(y_1,\cdots,y_k)$ *of* $(w_1,\cdots,w_k)$. *Then there exists a* $2\leq t\leq k-2$ *such that the following holds:*

$$x_1+x_2+\cdots+x_{t-1}\leq x_{t+2}+\cdots+x_k \tag{10}$$

and

$$x_1+x_2+\cdots+x_t>x_{t+3}+\cdots+x_k. \tag{11}$$

Further, if equation (10) is strict, then

$$x_1\geq x_2\geq\cdots\geq x_{t-1}\geq x_t\geq x_{t+1}\leq x_{t+2}\leq\cdots\leq x_k; \tag{12}$$

if equation (10) is equality, then

$$x_1\geq x_2\geq\cdots\geq x_{t-1}\geq x_t\geq x_{t+1}\leq x_{t+2}\leq\cdots\leq x_k \tag{13}$$

or

$$x_1\geq x_2\geq\cdots\geq x_{t-1}\geq x_t\leq x_{t+1}\leq x_{t+2}\leq\cdots\leq x_k. \tag{14}$$

Proof. By the definition of $F(x_1,\cdots,x_k)$, we get

$$\begin{aligned}0 &\leq F(x_1,\cdots,x_{i-1},x_i,x_{i+1},\cdots,x_k)-F(x_1,\cdots,x_{i-1},x_{i+1},x_i,\cdots,x_k)\\ &= (x_{i+1}-x_i)(\sum_{j=1}^{i-1}x_j-\sum_{j=i+2}^{k}x_j)\\ &= (x_{i+1}-x_i)f(i),\end{aligned}$$

where $f(i) = \sum_{j=1}^{i-1} x_j - \sum_{j=i+2}^{k} x_j$ for $1 \le i \le k-1$. Obviously, $f(1) < 0$, $f(2) \le 0$, $f(k-1) > 0$ and $f(i+1) \ge f(i)$ $(1 \le i \le k-1)$. Hence there exists a $2 \le t \le k-2$ such that $f(t) \le 0$, $f(t+1) > 0$, i.e (10) and (11) hold.

Furthermore, $f(1) \le f(2) \le \cdots \le f(t) \le 0 < f(t+1) \le f(t+2) \le \cdots \le f(k)$. If (10) is strict, i.e $f(t) < 0$, then

$$\sum_{j=1}^{i-1} x_j < \sum_{j=i+2}^{k} x_j \quad for \quad 1 \le i \le t,$$

$$\sum_{j=1}^{i-1} x_j > \sum_{j=i+2}^{k} x_j \quad for \quad t+1 \le i \le k-1.$$

Hence, we obtain

$$x_{i+1} - x_i \le 0 \quad for \quad 1 \le i \le t$$

and

$$x_{i+1} - x_i \ge 0 \quad for \quad t+1 \le i \le k-1,$$

which means

$$x_1 \ge x_2 \ge \cdots \ge x_t \ge x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

i.e (12) holds.

If (10) is equality, i.e $f(t) = 0$, then exists a $1 \le s < t$ such that $f(1) \le f(2) \le \cdots \le f(s) < f(s+1) = \cdots = f(t) = 0$. Then we have

$$x_1 \ge x_2 \ge \cdots \ge x_t \ge x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

or

$$x_1 \ge x_2 \ge \cdots \ge x_t \le x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

i.e (13) or (14) holds. This completes the proof. ■

Theorem 3.3 *Let $\pi = (d_1, d_2, \cdots, d_n)$ with $d_1 \ge \cdots \ge d_k \ge 2 \ge d_{k+1} = \cdots = d_l = 1$ and $d_2 \ge 3$, then if T^* is a maximum optimal tree in $\mathcal{T}_\pi$ with $F(x_1, \cdots, x_k)$ in equation (9), then there exists a $2 \le t \le k-2$ such that*

$$\sum_{i=1}^{t-1} x_i \le \sum_{i=t+2}^{k} x_i, \sum_{i=1}^{t} x_i > \sum_{i=t+3}^{k} x_i \tag{15}$$

and either

$$x_1 \ge x_2 \ge \cdots \ge x_t \ge x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

or

$$x_1 \ge x_2 \ge \cdots \ge x_t \le x_{t+1} \le x_{t+2} \le \cdots \le x_k.$$

Proof. It follows from Theorem 3.1 and Lemma 3.2 that the assertion holds. ■

Corollary 3.4 *Let $\mathcal{T}_{n,\Delta}$ denote the set of all the trees of order n and with maximum degree Δ. If $3 \le \Delta \le n-3$ and T^* is an optimal tree in $\mathcal{T}_{n,\Delta}$, then T^* is an $n-$caterpillar tree and $v_1, \cdots, v_k$ vertices on the backbone of T^* such that $d(v_i) = x_i + 2$ and there exists a $2 \le t \le k-2$ such that*

$$\sum_{i=1}^{t-1} x_i \le \sum_{i=t+2}^{k} x_i, \sum_{i=1}^{t} x_i > \sum_{i=t+3}^{k} x_i \tag{16}$$

and either

$$x_1 \ge x_2 \ge \cdots \ge x_t \ge x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

or

$$x_1 \ge x_2 \ge \cdots \ge x_t \le x_{t+1} \le x_{t+2} \le \cdots \le x_k$$

Proof. If $\Delta = n-2$, then it is easy to see that the assertion holds. If $\Delta \le n-3$, denote by $\pi = (d_1, \cdots, d_n)$ the degree sequence of T^* with $d_1 \ge \cdots \ge d_n$. If $d_2 = 2$, T^* is a starlike tree of degree Δ and $TW(T^*) = (n-1)(\Delta-1)$. The assertion holds. If $d_2 \ge 3$, by Theorems 3.1 and 3.3, the assertion also holds. ■

Lemma 3.5 *Let T^* be an optimal caterpillar with $v_1, \cdots v_k$ vertices on the backbone of T^* in the order and $d(v_i)$, $1 \le i \le k$ satisfying $d(v_1) \ge \cdots \ge d(v_t) \ge 3$ and $3 \le d(v_s) \le \cdots \le d(v_k)$, $t < s$. If $3 \le \Delta \le n-3$, $d(v_{t-1}) < \Delta$ and $d(v_s) < \Delta$, then $d(v_{t-2}) = d(v_{s+1}) = \Delta$, $d(v_t) = 3$ and $p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 = 0$.*

Proof. Let T_1 be a caterpillar from T^* by deleting one pendent edge at vertex v_t and adding one pendent edge at vertex v_{t-1}. Let T_2 be a caterpillar from T^* by deleting one pendent edge at vertex v_t and adding one pendent edge at vertex v_s. Then

$$TW(T^*) - TW(T_1) = p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 \ge 0 \tag{17}$$

and

$$\begin{aligned} TW(T^*) - TW(T_2) \ge (s-t)\{-2(d(v_t)-2) + 2 - (p_{v_{t-1}}(v_{t-1}v_t|T^*) \\ -p_{v_t}(v_{t-1}v_t|T^*) + 1)\} \ge 0 \end{aligned} \tag{18}$$

Hence by (17) and (18), $d(v_t) = 3$ and

$$p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 = 0. \tag{19}$$

Suppose that $d(v_{t-2}) < \Delta$. Then let T_3 be a caterpillar from T^* by deleting one pendent edge at vertex v_{t-1} and adding one pendent edge at vertex v_{t-2}. Hence by (19),

$$\begin{aligned} 0 &\leq TW(T^*) - TW(T_3) \\ &= -2(d(v_{t-1}) - 2) + p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 \\ &= -2(d(v_{t-1}) - 2) < 0, \end{aligned}$$

which is a contradiction. So $d(v_{t-2}) = \Delta$. Suppose that $d(v_{s+1}) < \Delta$. Then let T_4 be a caterpillar from T^* by deleting one pendent edge at vertex v_s and adding one pendent edge at vertex v_{s+1}. Hence

$$\begin{aligned} 0 &\leq TW(T^*) - TW(T_4) \\ &= -2((d(v_t) - 2) + \cdots + (d(v_s) - 2)) - (p_{v_{t-1}}(v_{t-1}v_t|T^*) \\ &\quad -p_{v_t}(v_{t-1}v_t|T^*) + 1) + 2 \\ &= -2((d(v_t) - 2) + \cdots + (d(v_s) - 2)) + 2 < 0, \end{aligned}$$

which is a contradiction. So $d(v_{s+1}) = \Delta$. ■

Lemma 3.6 *Let T^* be an optimal caterpillar with $v_1, \cdots v_k$ vertices on the backbone of T^* in the order and $d(v_i)$, $1 \leq i \leq k$ satisfying $d(v_1) \geq \cdots \geq d(v_t) \geq 3$ and $3 \leq d(v_s) \leq \cdots \leq d(v_k)$, $t < s$. If $3 \leq \Delta \leq n-3$, $d(v_{t-1}) < \Delta$, $d(v_s) = \Delta$ and $s > t+1$, then $d(v_{t-2}) = \Delta$, $d(v_t) = 3$ and $p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 = 0$.*

Proof. Let T_5 be a caterpillar from T^* by deleting one pendent edge at vertex v_t and adding one pendent edge at vertex v_{t-1} and Let T_6 be a caterpillar from T^* by deleting one pendent edge at vertex v_t and adding one pendent edge at vertex v_{t+1}. Then

$$TW(T^*) - TW(T_5) = p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 \geq 0 \tag{20}$$

and

$$\begin{aligned} TW(T^*) - TW(T_6) = -2(d(v_t) - 3) - (&p_{v_{t-1}}(v_{t-1}v_t|T^*) \\ &-p_{v_t}(v_{t-1}v_t|T^*) + 1) \geq 0. \end{aligned} \tag{21}$$

Hence by (20) and (21), we have $d(v_t) = 3$ and $p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t| T^*) + 1 = 0$. Suppose that $d(v_{t-2}) < \Delta$. Then let T_7 be a caterpillar from

T^* by deleting one pendent edge at vertex v_{t-1} and adding one pendent edge at vertex v_{t-2}. Hence

$$\begin{aligned} 0 &\le TW(T^*) - TW(T_7) \\ &= p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 - 2(d(v_{t-1}) - 2) \\ &= -2(d(v_{t-1}) - 2) < 0, \end{aligned}$$

which is a contradiction. So $d(v_{t-2}) = \Delta$. ■

Lemma 3.7 *Let T^* be an optimal caterpillar with $v_1, \cdots v_k$ vertices on the backbone of T^* in the order and $d(v_i)$, $1 \le i \le k$ satisfying $d(v_1) \ge \cdots d(v_t) \ge 3$ and $3 \le d(v_s) \le \cdots d(v_k)$, $t < s$. If $3 \le \Delta \le n-3$, $d(v_{t-1}) < \Delta$, $d(v_s) = \Delta$ and $s = t+1$, then $d(v_{t-3}) = \Delta$.*

Proof. If $d(v_{t-2}) = \Delta$, then $d(v_{t-3}) = \Delta$. Hence assume that $d(v_{t-2}) < \Delta$. let T_8 be a caterpillar from T^* by deleting one pendent edge at vertex v_{t-1} and adding one pendent edge at vertex v_{t-2} and let T_9 be a caterpillar from T^* by deleting one pendent edge at vertex v_{t-1} and adding one pendent edge at vertex v_t. Then

$$\begin{aligned} TW(T^*) - TW(T_8) = p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 \\ -2(d(v_{t-1}) - 2) \ge 0 \end{aligned} \tag{22}$$

and

$$TW(T^*) - TW(T_9) = -p_{v_{t-1}}(v_{t-1}v_t|T^*) + p_{v_t}(v_{t-1}v_t|T^*) + 1 \ge 0. \tag{23}$$

Hence by (22) and (23), we have $d(v_{t-1}) = 3$ and $p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) - 1 = 0$. Suppose that $d(v_{t-3}) < \Delta$. Then let T_{10} be a caterpillar from T^* by deleting one pendent edge at vertex v_{t-2} and adding one pendent edge at vertex v_{t-3}. Hence

$$\begin{aligned} 0 &\le TW(T^*) - TW(T_{10}) \\ &= p_{v_{t-1}}(v_{t-1}v_t|T^*) - p_{v_t}(v_{t-1}v_t|T^*) + 1 - 2(d(v_{t-2}) + d(v_{t-1}) - 4) \\ &= -2(d(v_{t-2}) - 2) < 0, \end{aligned}$$

which is a contradiction. Hence the assertion holds. ■

Theorem 3.8 *Let T^* be an optimal caterpillar with $v_1, \cdots v_k$ vertices on the backbone of T^* in the order and $d(v_i)$, $1 \le i \le k$ satisfying $d(v_1) \ge \cdots \ge d(v_t) \ge 3$ and $3 \le d(v_s) \le \cdots \le d(v_k)$, $t < s$. If $3 \le \Delta \le n-3$, then the following result holds.*

(1). If $d(v_{t-1}) < \Delta, d(v_s) < \Delta$, then $d(v_{t-2}) = d(v_{s+1}) = \Delta$.

(2). If $d(v_{t-1}) < \Delta, d(v_s) = \Delta$ *and* $s > t+1$, *then* $d(v_{t-2}) = \Delta$.

(3). If $d(v_{t-1}) < \Delta, d(v_s) = \Delta$ *and* $s = t+1$, *then* $d(v_{t-3}) = \Delta$.

(4). If $d(v_{t-1}) = \Delta, d(v_s) < \Delta$, $d(v_t) < \Delta$ *and* $d(v_{s+1}) < \Delta$, *then* $d(v_{s+2}) = \Delta$.

(5). If $d(v_{t-1}) = \Delta, d(v_s) < \Delta$, $d(v_t) = \Delta$ *and* $d(v_{s+1}) < \Delta$, *then* $d(v_{s+3}) = \Delta$.

Lemma 3.9 *Let* T *be a caterpillar with* $v_1, \cdots v_k$ *vertices on the backbone of* T *in the order and* $d(v_i)$, $1 \le i \le k, k \ge 3$. *If* $d(v_1) = \cdots d(v_t) = 3$, $d(v_s) = \cdots d(v_k) = 3$, *then*

$$TW(T) = \frac{(l-1)(l^2+7l-12)}{6} + (t+1)(l-(t+1))(n+2-2l), \quad (24)$$

where $l = n-k$ *is the number of the pendent vertices of* T.

Proof. $s - t = n + 3 - 2l$ and $l + k = n$. Moreover,

$$\begin{aligned} TW(T) &= l(l-1) + 2(l-2) + 3(l-3) + \cdots + t(l-t) \\ &\quad + (t+1)[l-(t+1)] + \cdots + (t+1)[l-(t+1)] \\ &\quad + (t+2)[l-(t+2)] + \cdots + (l-2)[l-(l-2)] \\ &= \frac{(l-1)(l^2+7l-12)}{6} + (t+1)[l-(t+1)](n+2-2l). \end{aligned}$$

■

Lemma 3.10 *Let* $g_1(x) = \frac{(x-1)(x^2+7x-12)}{6} + \frac{x^2}{4}(n+2-2x)$ *and* $g_2(x) = \frac{(x-1)(x^2+7x-12)}{6} + \frac{x^2-1}{4}(n+2-2x)$. *Then* $g_1(x)$ *and* $g_2(x)$ *are strictly increasing with respect to* x *in* $x \in (1, \frac{n+4}{2})$.

Proof. Note

$$g_1(x) = \frac{-4x^3 + (3n+18)x^2 - 38x + 24}{12},$$

$$g_1(x)' = \frac{1}{12}(-12x^2 + 2(3n+18)x - 38) > 0$$

for $x \in (1, \frac{n+4}{2})$. Hence $g_1(x)$ is strictly increasing with respect to x in $x \in (1, \frac{n+4}{2})$. Moreover,

$$g_2(x) = \frac{-4x^3 + (3n+18)x^2 - 32x - 3n + 18}{12}.$$

Then

$$g_2(x)' = \frac{1}{12}(-12x^2 + 2(3n+18)x - 32) > 0$$

for $x \in (1, \frac{n+4}{2})$. Hence $g_2(x)$ is strictly increasing with respect to x in $x \in (1, \frac{n+4}{2})$ ∎

Theorem 3.11 *Let T^* be an optimal tree in $\mathcal{T}_{n,3}$ with $n \geq 6$.*

(1).If $n = 4p$, then T^* is a caterpillar with $v_1, \cdots v_{2p-1}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, 2p-1$. In other words,

$$TW(T) \leq TW(T^*) = \frac{p(4p^2 + 18p - 4)}{3} \quad \text{for T} \in \mathcal{T}_{\text{n},3}$$

with equality if and only if T is a caterpillar with $v_1, \cdots v_{2p-1}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, 2p-1$.

(2). If $n = 4p+1$, then T^* is a caterpillar with $v_1, \cdots v_{2p}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, p, p+2, \cdots, 2p$. In other words,

$$TW(T) \leq TW(T^*) = \frac{p(4p^2 + 21p - 1)}{3} \quad \text{for T} \in \mathcal{T}_{\text{n},3}$$

with equality if and only if T is a caterpillar with $v_1, \cdots v_{2p}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, p, p+2, \cdots, 2p$.

(3). If $n = 4p+2$, then T^* is a caterpillar with $v_1, \cdots v_{2p}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, 2p$. In other words,

$$TW(T) \leq TW(T^*) = \frac{(2p+1)(2p^2 + 11p + 3)}{3} \quad \text{for T} \in \mathcal{T}_{\text{n},3}$$

with equality if and only if T is a caterpillar with $v_1, \cdots v_{2p}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, 2p$.

(4). If $n = 4p+3$, then T^* is a caterpillar with $v_1, \cdots v_{2p+1}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, p, p+2, \cdots, 2p+1$. In other words,

$$TW(T) \leq TW(T^*) = \frac{(2p+1)(2p^2 + 11p + 3)}{3} + (p+1)^2 \quad \text{for T} \in \mathcal{T}_{\text{n},3}$$

with equality if and only if T is a caterpillar with $v_1, \cdots v_{2p+1}$ vertices on the backbone of T in the order and $d(v_i) = 3$ for $i = 1, \cdots, p, p+2, \cdots, 2p+1$.

Proof. Let T^* be an $n-$vertex optimal tree in $\mathcal{T}_{n,3}$. By Corollary 3.4, T^* is an $n-$caterpillar with $v_1, \cdots, v_k$ vertices on the backbone with $d(v_1) \geq \cdots d(v_t) \geq 3$ and $3 \leq d(v_s) \leq \cdots d(v_k)$, $1 \leq t < s \leq k$. So, $d(v_i) = 3$, for $i = 1, \cdots, t$, and $i = s, \cdots, k$. Denote by l the number of pendent vertices of T^*. Then $l+k=n$ and $l \leq k+2$, which implies that $l \leq \frac{n+2}{2}$. By (24), we have

$$\begin{aligned} TW(T^*) &= \frac{(l-1)(l^2+7l-12)}{6} + (t+2)(l-(t+2))(n+2-2l) \\ &\leq \frac{(l-1)(l^2+7l-12)}{6} + \lfloor\frac{l}{2}\rfloor\lceil\frac{l}{2}\rceil(n+2-2l) \end{aligned}$$

If $n = 4p$, then by Lemma 3.10,

$$TW(T^*) \leq g_2(2p+1) = \frac{p(-8p^2+(3n+6)p+3n-4)}{3} = \frac{p(4p^2+18p-4)}{3}$$

Hence the assertion holds. If $n = 4p+1, 4p+2, 4p+3$, then by the same argument, the assertion holds. ■

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