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# Maximum Wiener Index of Trees with Given Degree Sequence*

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## Abstract

The Wiener index of a connected graph is the sum of topological distances between all pairs of vertices. Wang in [28] gave a mistaken result on the maximum Wiener index of trees with given degree sequence. In this paper we investigate the maximum Wiener index of trees with given degree sequences and the extremal trees which attain the maximum value.

## 1 Introduction

The Wiener index of a molecular graph, introduced by Wiener [30] in 1947, is one of the oldest and most widely used topological index in the quantitative structure property relationships. In the mathematical literature, the Wiener index seems to be first studied by Entringer et al. [6]. For more information and background, the

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readers may refer to a recent and very comprehensive survey [5] and a book [24], which is dedicated to Harry Wiener, on the Wiener index and the references therein. For some most recent research on the Wiener index see [1, 3, 15, 18, 27, 29, 31].

Through this paper, all graphs are finite, simple and undirected. Let $G = (V,\ E)$ be a simple connected graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G)$. Denote by $d_G(v_i)$ (or for short $d(v_i)$) the *degree* of vertex $v_i$. The *distance* between vertices $v_i$ and $v_j$ is the minimum number of edges between $v_i$ and $v_j$ and denoted by $d_G(v_i, v_j)$ (or for short $d(v_i, v_j)$). The *Wiener index* of a connected graph $G$ is defined as

$$W(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d(v_i, v_j)\ . \tag{1}$$

A *tree* is a connected and acyclic graph. A *caterpillar* is a tree in which a single path (called *Spine*) is incident to (or contains) every edge. For other terminology and notions, we follow from [2].

Entringer et al. [6] proved that the path $P_n$ and the star $K_{1,n-1}$ have the maximum and minimum Wiener indices, respectively, in the set consisting of all trees of order $n$. Dankelmann [4] obtained the all extremal graphs in the set of all connected graphs with given the order and the matching number which attained the maximum Wiener value. Moreover, Fischermann et al. [8] and Jelen et al. [16] independently determined all trees which have the minimum Wiener indices among all trees of order $n$ and maximum degree $\Delta$. A nonincreasing sequence of nonnegative integers $\pi = (d_1, d_2, \ldots, d_n)$ is called *graphic* if there exists a simple graph having $\pi$ as its vertex degree sequence. Hence it is natural to consider the following problem.

**Problem 1.1** *Let $\pi = (d_1, \ldots, d_n)$ be graphic degree sequence and*

$$\mathcal{G}_\pi = \{G:\ \text{the degree sequence of } G \text{ is } \pi\}\ .$$

*Find the upper (lower) bounds for the Wiener index of all graphs $G$ in $\mathcal{G}_\pi$ and characterize all extremal graphs which attain the upper (lower) bounds.*

Moreover, we call a graph *maximum (minimum) optimal* if it maximizes (minimizes) the Wiener index in $\mathcal{G}_\pi$. Recently, by the different techniques, Wang [28] and Zhang et al. [32] independently characterized the tree that minimizes the Wiener index among trees of given degree sequences. Moreover, they proved that the minimum optimal trees for a given tree degree sequence $\pi$ are unique. On the other hand, Wang in [28] also "*proved*" the only maximum optimal tree that maximizes the Wiener index among trees of given degree sequences. The result can be stated as follows:

**Theorem 1.2** *[28] Given the degree sequence and the number of vertices, the greedy caterpillar maximizes the Wiener index, where the greedy caterpillar with degree sequence $(d_1, \ldots, d_n)$ $(d_1 \geq d_2 \geq \cdots \geq d_k \geq 2 > d_{k+1} = 1)$ is formed by attaching pending edges to a path $v_1, v_2, \ldots, v_k$ of length $k-1$ such that*

$$d(v_1) \geq d(v_k) \geq d(v_2) \geq d(v_{k-1}) \geq \cdots \geq d(v_{\lceil \frac{k+1}{2} \rceil}) \ .$$

Unfortunately, this result is not correct. For example:

**Example 1.3** *Let $\pi = (13, 5, 5, 5, 4, 3, 1, \ldots, 1)$ be a degree sequence of tree with 31 vertices. Let $T_1$ and $T_2$ be two trees with degree sequences $\pi$ (see Fig.1).*

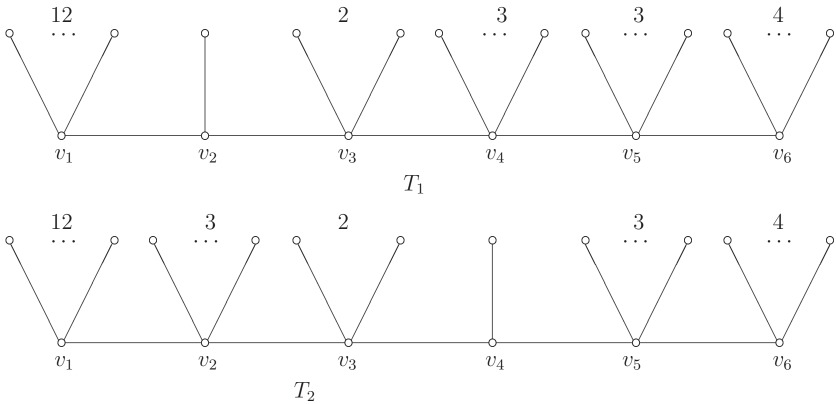


**Figure 1** $T_1$ **and** $T_2$

Clearly, $T_2$ is a greedy caterpillar and $T_1$ is not a greedy caterpillar. Moreover, they have the same degree sequences $\pi$ . By calculation, it is easy to see that

$$W(T_2) = 9870 < W(T_1) = 9886 \ .$$

Hence this example illustrates that Theorem 1.2 in [28] is not correct.

Motivated by Problem 1.1 and Example 1.3, we try to investigate the extremal trees which attain the maximum Wiener index among all trees with given degree sequences. The problem seems to be difficult. Because we find that the extremal tree depends on the values of components of degree sequences. The rest of the paper is organized as follows. In Section 2, we discuss some properties of the extremal tree with the maximum Wiener index and give an upper bound in terms of degree sequences. In Section 3, the extremal trees with the maximum Wiener index among given degree sequences $(d_1, \ldots, d_n)$, where $d_1 \geq \cdots \geq d_k \geq 2 > d_{k+1} = 1$ and $k \leq 6$ are characterized. Moreover, the extremal maximal trees are not unique.

# 2 Properties of extremal trees with the maximum Wiener index

Let $\mathcal{T}_\pi$ be the set of all trees with degree sequences $\pi = (d_1, d_2, \ldots, d_n)$ with $d_1 \geq d_2 \geq \cdots \geq d_n$. Shi in [26] proved that a maximum optimal tree must be a caterpillar.

**Lemma 2.1** *[26] Let $T^*$ be a maximum optimal tree in $\mathcal{T}_\pi$. Then $T^*$ is a caterpillar.*

From Lemma 2.1, we only need to consider all caterpillars with a degree sequence $\pi$. In order to study the structure of the maximum optimal trees, we present a formula for Wiener index of any caterpillar.

**Lemma 2.2** *Let $T$ be a caterpillar of order $n$ with the degree sequence $\pi = (d(v_1), \ldots, d(v_k), d(v_{k+1}), \ldots, d(v_n))$ (see Figure 2).*

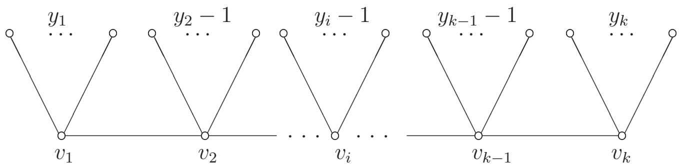


**Figure 2** $T$

*If* $d(v_i) = y_i + 1 \geq 2$ *for* $i = 1, \ldots, k$ *and* $d(v_{k+1}) = \cdots = d(v_n) = 1$ *, then*

$$W(T) = (n-1)^2 + F(y_1, \ldots, y_k), \tag{2}$$

*where*

$$F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) . \tag{3}$$

**Proof.** It is well known [14] that the formula (1) is equal to

$$W(T) = \sum_e n_1(e)\, n_2(e)$$

where $e = (u, v)$ is an edge of $T$, and $n_1(e)$ (resp. $n_2(e)$) is the number of vertices of the component of $T - e$ containing $u$ (resp. $v$). For $e_i = (v_i, v_{i+1}) \in E(T)$, the numbers of vertices of the two components of $T - e_i$ are $\sum_{j=1}^{i} d(v_j) - (i-1)$ and $\sum_{j=i+1}^{k} d(v_j) - (k-i-1)$ for $i = 1, \ldots, k-1$, respectively. Hence

$$\begin{aligned}
W(T) &= \sum_{e \in E(T)} n_1(e) n_2(e) \\
&= \sum_{e \text{ is pendent edge}} n_1(e) n_2(e) + \sum_{e \text{ is not pendent edge}} n_1(e) n_2(e) \\
&= (n-1)(n-k) + \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} d(v_j) - (i-1) \right) \left( \sum_{j=i+1}^{k} d(v_j) - (k-i-1) \right) \\
&= (n-1)(n-k) + \sum_{i=1}^{k-1} \left( 1 + \sum_{j=1}^{i} y_j \right) \left( 1 + \sum_{j=i+1}^{k} y_j \right) \\
&= (n-1)(n-k) + (k-1) \left( 1 + \sum_{j=1}^{k} y_j \right) + \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) \\
&= (n-1)^2 + F(y_1, \ldots, y_k),
\end{aligned}$$

where last equality is due to $\sum_{j=1}^{k} y_j = \sum_{j=1}^{k} d(v_j) - k = 2(n-1) - (n-k) - k = n-2$. This completes the proof. ■

**Remark** In this sequel, the caterpillar $T$ in Lemma 2.2 is denoted by $T(y_1, \ldots, y_k)$. Then degree sequence of $T(y_1, \ldots, y_k)$ is $(y_1 + 1, \ldots, y_k + 1, 1, \ldots, 1)$. The following theorem give a characterization of a maximum optimal tree.

**Theorem 2.3** *Let* $\pi = (d_1, \ldots, d_n)$ *with* $d_1 \geq \cdots \geq d_k \geq 2 \geq d_{k+1} = \cdots = d_n = 1$ . *Then* $T$ *is a maximum optimal tree in* $\mathcal{T}_\pi$ *if and only if* $T$ *is a caterpillar* $T(x_1, \ldots, x_k)$ *and* $(x_1, \ldots, x_k)$ *satisfies*

$$F(x_1, \ldots, x_k) = \max\left\{ F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) : \ y_1 \geq y_k \right\}, \qquad (4)$$

*where* $(y_1, \ldots, y_k)$ *is any permutation of* $(d_1 - 1, \ldots, d_k - 1)$ .

**Proof.** Necessity. Since $T$ is a maximum optimal tree in $\mathcal{T}_\pi$ , by Lemmas 2.1, $T$ must be a caterpillar and can be denoted by $T(z_1, \ldots, z_k)$ with $(z_1, \ldots, z_k)$ is the permutation of $(d_1 - 1, \ldots, d_k - 1)$ . Moreover, by Lemma 2.2, we have

$$W(T(z_1, \ldots, z_k)) = (n-1)^2 + F(z_1, \ldots, z_k).$$

For any permutation $(y_1, \ldots, y_k)$ of $(d_1 - 1, \ldots, d_k - 1)$ with $y_1 \geq y_k$ , there exists a caterpillar $T_1$ with the degree sequence $\pi$ such that

$$W(T_1) = (n-1)^2 + F(y_1, \ldots, y_k).$$

Because $T(z_1, \ldots, z_k)$ is a maximum optimal tree in $\mathcal{T}_\pi$ , we have

$$F(y_1, \ldots, y_k) = W(T_1) - (n-1)^2 \leq W(T(z_1, \ldots, z_k)) - (n-1)^2 = F(z_1, \ldots, z_k).$$

Sufficiency. If $T$ is a caterpillar $T(x_1, \ldots, x_k)$ and $(x_1, \ldots, x_k)$ satisfies

$$F(x_1, \ldots, x_k) = \max\left\{ F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) : y_1 \geq y_k \right\} \qquad (5)$$

where the maximum is taken over all permutations $(y_1, \ldots, y_k)$ of $(d_1 - 1, \ldots, d_k - 1)$ . Let $T_1$ be any tree with the degree sequence $\pi$ . By Lemma 2.1, there exists a caterpillar $T_2$ with the degree sequence $\pi$ such that $W(T_1) \leq W(T_2)$ . Then $T_2$ must be $T(y_1, \ldots, y_k)$ , where $(y_1, \ldots, y_k)$ is the permutation of $(d_1 - 1, \ldots, d_k - 1)$ . Hence

$$\begin{aligned} W(T_1) &\leq W(T_2) = (n-1)^2 + F(y_1, \ldots, y_k) \leq (n-1)^2 + F(x_1, \ldots, x_k) \\ &= W(T(x_1, \ldots, x_k)) . \end{aligned}$$

Therefore $T(x_1, \ldots, x_k)$ is a maximum optimal tree. This completes the proof. ■

Now we can present an upper bound for the Wiener index of any tree with given degree sequence $\pi$ in terms of degree sequences.

**Theorem 2.4** *Let $T$ be a tree with a given degree sequence $\pi = (d_1, \ldots, d_n)$, where $d_1 \geq \cdots \geq d_k > d_{k+1} = \cdots = d_n = 1$. Then*

$$W(T) \leq (n-1)^2 + \frac{k(k-1)}{4} \sum_{i=1}^{k} (d_i - 1)^2 \tag{6}$$

*with equality if and only if $k = 2$ and $d_1 = d_2$.*

**Proof.** Let $T(x_1, \ldots, x_k)$ be a caterpillar and $(x_1, \ldots, x_k)$ satisfy

$$F(x_1, \ldots, x_k) = \max\{F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) : y_1 \geq y_k\} \tag{7}$$

where $(y_1, \ldots, y_k)$ is any permutation of $(d_1 - 1, \ldots, d_k - 1)$. By Theorem 2.3, $W(T) \leq W(T(x_1, \ldots, x_k))$. Clearly,

$$F(x_1, \ldots, x_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} x_j \right) \left( \sum_{j=i+1}^{k} x_j \right) = \frac{1}{2}(x_1, \ldots, x_k) C (x_1, \ldots, x_k)^T$$

where

$$C = \begin{pmatrix} 0 & 1 & 2 & \cdots & k-2 & k-1 \\ 1 & 0 & 1 & \cdots & k-3 & k-2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ k-1 & k-2 & k-3 & \cdots & 1 & 0 \end{pmatrix}.$$

By Perron-Frobenius theorem (for example, see [13]), the largest eigenvalue $\lambda_1(C)$ of $C$ is at most $\frac{k(k-1)}{2}$ with equality if and only if $k = 2$. Hence by Rayleigh quotient,

$$(x_1, \ldots, x_k) C (x_1, \ldots, x_k)^T \leq \lambda_1(C) \sum_{i=1}^{k} x_i^2$$

with equality if and only if $(x_1, \ldots, x_k)^T$ is an eigenvector of $C$ corresponding to the eigenvalue $\lambda_1(C)$. Therefore,

$$F(x_1, \ldots, x_k) \leq \frac{k(k-1)}{4} \sum_{i=1}^{k} x_i^2$$

with equality if and only if $k = 2$ and $x_1 = x_2$. Hence

$$W(T) \leq (n-1)^2 + \frac{k(k-1)}{4} \sum_{i=1}^{k} {x_i}^2 \leq (n-1)^2 + \frac{k(k-1)}{4} \sum_{i=1}^{k} (d_i - 1)^2$$

with equality if and only if $k = 2$ and $d_1 = d_2$, since $(d(v_1), \ldots, d(v_k))$ is a permutation of $(d_1, \ldots, d_k)$. This completes the proof. $\blacksquare$

**Lemma 2.5** *Let $w_1 \geq w_2 \geq \cdots \geq w_k \geq 1$ be the positive integers with $k \geq 5$. Let*

$$F(z_1, \ldots, z_k) = \max \left\{ F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) : y_1 \geq y_k \right\}$$

*where $(y_1, \ldots, y_k)$ is any permutation of $(w_1, \ldots, w_k)$. Then there exists a $2 \leq t \leq k-2$ such that the following holds:*

$$z_1 + \cdots + z_{t-2} \leq z_{t+1} + \cdots + z_k \tag{8}$$

*and*

$$z_1 + \cdots + z_{t-1} > z_{t+2} + \cdots + z_k \ . \tag{9}$$

*Further, if equations (8) is strict, then*

$$z_1 \geq z_2 \geq \cdots \geq z_t, \qquad z_t \leq z_{t+1} \leq \cdots \leq z_k \ . \tag{10}$$

*If equations (8) becomes equality, then*

$$z_1 \geq z_2 \geq \cdots \geq z_t, \qquad z_t \leq z_{t+1} \leq \cdots \leq z_k \tag{11}$$

*or*

$$z_1 \geq z_2 \geq \cdots \geq z_{t-1}, \qquad z_{t-1} \leq z_t \leq \cdots \leq z_k \ . \tag{12}$$

**Proof.** Let

$$f(p) = \sum_{i=1}^{p-2} z_i - \sum_{i=p+1}^{k} z_i, \quad 2 \leq p \leq k-2 \ .$$

Clearly $f(2) < 0$, $f(k-1) > 0$ and

$$f(2) \leq f(3) \leq \cdots \leq f(k-1) \ .$$

Hence there exists a $2 \leq t \leq k-2$ such that $f(t) \leq 0$ and $f(t+1) > 0$. In other words, equations (8) and (9) hold. By the definition of $F(z_1, \ldots, z_k)$, we have for $1 \leq i \leq k-1$,

$$\begin{aligned} 0 &\leq F(z_1, \ldots, z_{i-1}, z_i, z_{i+1}, \ldots, z_k) - F(z_1, \ldots, z_{i-1}, z_{i+1}, z_i, \ldots, z_k) \\ &= (z_{i+1} - z_i) \left( \sum_{j=1}^{i-1} z_j - \sum_{j=i+2}^{k} z_j \right) \ . \end{aligned}$$

But for $1 \le i \le t-2$, by (8), we have $\sum_{j=1}^{i-1} z_j < \sum_{j=i+2}^{k} z_j$. Hence $z_1 \ge \cdots \ge z_{t-1}$. On the other hand, for $t \le i \le k-1$, by (9), we have $\sum_{j=1}^{i-1} z_j > \sum_{j=i+2}^{k} z_j$. Therefore $z_t \le z_{t+1} \cdots \le z_k$.

If (8) is strict, then $(z_1+\cdots+z_{t-2})-(z_{t+1}+\cdots+z_k) < 0$, which implies $z_{t-1} \ge z_t$. So (10) holds.

If (8) becomes equality, i.e., $z_1+\cdots+z_{t-2} = z_{t+1}+\cdots+z_k$, then it is easy to see that (11) or (12) holds. This completes the proof. ∎

**Corollary 2.6** *Let $w_1 \ge w_2 \ge \cdots \ge w_6 \ge 1$ be the positive integers. Let*

$$F(z_1,\ldots,z_6) = \max\left\{ F(y_1,\ldots,y_6) = \sum_{i=1}^{5}\left(\sum_{j=1}^{i} y_j\right)\left(\sum_{j=i+1}^{6} y_j\right) : \quad y_1 \ge y_6 \right\}$$

*where $(y_1,\ldots,y_6)$ is any permutation of $(w_1,\ldots,w_6)$. Then $(z_1,\ldots,z_6)$ is equal to one of the following five $(w_1,w_6,w_5,w_4,w_3,w_2)$, $(w_1,w_5,w_6,w_4,w_3,w_2)$, $(w_1,w_4,w_6,w_5,w_3,w_2)$, $(w_1,w_4,w_5,w_6,w_3,w_2)$, and $(w_1,w_3,w_6,w_5,w_4,w_2)$.*

**Proof.** By Lemma 2.5, there are just three cases:

**Case 1** $t=2$. Then by Lemma 2.5, $z_1 \ge z_2$ and $z_2 \le z_3 \le z_4 \le z_5 \le z_6$. Hence $(z_1,\ldots,z_6)$ must be $(w_1,w_6,w_5,w_4,w_3,w_2)$.

**Case 2** $t=3$. Then $z_1 \le z_4+z_5+z_6$ and $z_1+z_2 > z_5+z_6$. Moreover, $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$; or $z_1 \ge z_2$ and $z_2 \le z_3 \le z_4 \le z_5 \le z_6$. Therefore $(z_1,\ldots,z_6)$ must be one of $(w_1,w_6,w_5,w_4,w_3,w_2)$, $(w_1,w_5,w_6,w_4,w_3,w_2)$, $(w_1,w_4,w_6,w_5,w_3,w_2)$ and $(w_1,w_3,w_6,w_5,w_4,w_2)$.

**Case 3** $t=4$. Then $z_1+z_2 \le z_5+z_6$. Moreover, $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$; or $z_1 \ge z_2 \ge z_3 \ge z_4$ and $z_4 \le z_5 \le z_6$. Therefore, $(z_1,\ldots,z_6)$ must be one of $(w_1,w_4,w_6,w_5,w_3,w_2)$, $(w_1,w_5,w_6,w_4,w_3,w_2)$ and $(w_1,w_4,w_5,w_6,w_3,w_2)$. This completes the proof. ∎

**Theorem 2.7** *Let $\pi = (d_1,\ldots,d_n)$ be a tree degree sequence with $d_1 \ge d_2 \ge \cdots \ge d_k \ge 2$, $d_{k+1} = \cdots = d_n = 1$ and $k \ge 5$. If a caterpillar $T(x_1,\ldots,x_k)$ is a maximum optimal tree in $\mathcal{T}_\pi$ with $F(x_1,\ldots,x_k)$ in equation (2). Then there exists a $2 \le t \le k-2$*

*such that either*

$$\sum_{i=1}^{t-2} x_i \leq \sum_{i=t+1}^{k} x_i \quad \sum_{i=1}^{t-1} x_i > \sum_{t+2}^{k} x_i$$

*for* $x_1 \geq x_2 \geq \cdots \geq x_{t-1} \geq x_t, \quad x_t \leq x_{t+1} \leq \cdots \leq x_k$ *, or*

$$\sum_{i=1}^{t-2} x_i = \sum_{i=t+1}^{k} x_i, \quad \sum_{i=1}^{t-1} x_i > \sum_{t+2}^{k} x_i$$

*for* $x_1 \geq x_2 \geq \cdots \geq x_{t-1} \geq x_t, \quad x_t \leq x_{t+1} \leq \cdots \leq x_k$ *, or*

$$\sum_{i=1}^{t-2} x_i = \sum_{i=t+1}^{k} x_i, \quad \sum_{i=1}^{t-1} x_i > \sum_{t+2}^{k} x_i$$

*for* $x_1 \geq x_2 \geq \cdots \geq x_{t-1}, \quad x_{t-1} \leq x_t \leq \cdots \leq x_k$ *.*

**Proof.** It follows from Theorem 2.3 and Lemma 2.5 that the assertion holds. ■

# 3 The maximum optimal tree with many leaves

In this section, for a given degree sequence $\pi = (d_1, \ldots, d_n)$ with at least $n-6$ leaves, we give the maximum optimal trees with the maximum Wiener index in $\mathcal{T}_\pi$ . Moreover, the maximum optimal tree may be not unique.

**Theorem 3.1** *Let* $\pi = (d_1, \ldots, d_k, \ldots, d_n)$ *be tree degree sequence with* $n-k$ *leaves for* $2 \leq k \leq 4$*. Then the maximum optimal tree in* $\mathcal{T}_\pi$ *is the greedy caterpillar. In other words,*

*if* $k = 2$ *, then* $W(T) = (n-1)^2 + (d_1-1)(d_2-1)$ *, for* $T \in \mathcal{T}_\pi$*.*

*If* $k = 3$ *, then for any* $T \in \mathcal{T}_\pi$*,*

$$W(T) \leq (n-1)^2 + (d_1-1)(d_2+d_3-2) + (d_1+d_2-2)(d_3-1)$$

*with equality if and only if* $T$ *is the caterpillar* $T(d_1-1, d_3-1, d_2-1)$*.*

*If* $k = 4$*, then for any* $T \in \mathcal{T}_\pi$*,*

$$\begin{aligned} W(T) \;\leq\; & (n-1)^2 + (d_1-1)(d_2+d_3+d_4-3) \\ + \; & (d_1+d_2-2)(d_3+d_4-2) + (d_1+d_2+d_3-3)(d_4-1) \end{aligned}$$

*with equality if and only if* $T$ *is the caterpillar* $T(d_1-1, d_4-1, d_3-1, d_2-1)$ *.*

**Proof.** If $k=2$, it is obvious. If $k=3$, it is easy to see that $F(d_1-1,d_2-1,d_3-1) \leq F(d_1-1,d_3-1,d_2-1)$. By Theorem 2.3, the assertion holds.

If $k=4$, then by Theorem 2.3, let $T$ be a caterpillar $T(x_1,x_2,x_3,x_4)$ and

$$F(x_1,x_2,x_3,x_4) = \max\{F(y_1,y_2,y_3,y_4) : y_1 \geq y_4\},$$

where $(y_1,y_2,y_3,y_4)$ is any permutation of $(d_1-1,d_2-1,d_3-1,d_4-1)$. Because

$$F(x_1,x_2,x_3,x_4) - F(x_2,x_1,x_3,x_4) = (x_1-x_2)(x_3+x_4) \geq 0$$

and

$$F(x_1,x_2,x_3,x_4) - F(x_1,x_2,x_4,x_3) = (x_4-x_3)(x_1+x_2) \geq 0,$$

we have $x_1 \geq x_2$ and $x_4 \geq x_3$. So $(x_1,x_2,x_3,x_4) = (d_1-1,d_4-1,d_3-1,d_2-1)$. This completes the proof. ■

**Theorem 3.2** *Let $\pi = (d_1,\ldots,d_k,\ldots,d_n)$ be tree degree sequence with $n-5$ leaves.*

*(1). If $d_1 > d_2+d_3$, then the maximum optimal tree in $\mathcal{T}_\pi$ is the only caterpillar $T(d_1-1,d_5-1,d_4-1,d_3-1,d_2-1)$.*

*(2). If $d_1 = d_2+d_3$, then there are the exactly two maximum optimal trees in $\mathcal{T}_\pi$: one tree is the caterpillar $T(d_1-1,d_5-1,d_4-1,d_3-1,d_2-1)$; the other tree is the caterpillar $T(d_1-1,d_4-1,d_5-1,d_3-1,d_2-1)$.*

*(3). If $d_1 < d_2+d_3$, then the maximum optimal tree in $\mathcal{T}_\pi$ is the only caterpillar $T(d_1-1,d_4-1,d_5-1,d_3-1,d_2-1)$.*

**Proof.** By Theorem2.3, let $T(x_1,x_2,x_3,x_4,x_5)$ be a maximum optimal tree in $\mathcal{T}_\pi$. If $d_1 > d_2+d_3$, then by Theorem 2.7, it is easy to see that $t=2$, and $x_1 \geq x_2$ and $x_2 \leq x_3 \leq x_4 \leq x_5$. Hence $(x_1,x_2,x_3,x_4,x_5) = (d_1-1,d_5-1,d_4-1,d_3-1,d_2-1)$.

If $d_1 < d_2+d_3$, then by Theorem 2.7, it is easy to see that $x_1 \geq x_2 \geq x_3$ and $x_3 \leq x_4 \leq x_5$. Hence $(x_1,x_2,x_3,x_4,x_5) = (d_1-1,d_4-1,d_5-1,d_3-1,d_2-1)$ or $(d_1-1,d_3-1,d_5-1,d_4-1,d_2-1)$. But $W(T(d_1-1,d_4-1,d_5-1,d_3-1,d_2-1)) - W(T(d_1-1,d_3-1,d_5-1,d_4-1,d_2-1)) = 2(d_1-d_2)(d_3-d_4) \geq 0$ with equality if and only if $d_1=d_2$ or $d_3=d_4$. Hence the assertion (3) holds.

If $d_1 = d_2 + d_3$, then by Theorem 2.7, it is easy to see that either $x_1 \geq x_2$ and $x_2 \leq x_3 \leq x_4 \leq x_5$; or $x_1 \geq x_2 \geq x_3$ and $x_3 \leq x_4 \leq x_5$. Hence $(x_1, x_2, x_3, x_4, x_5) = (d_1 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$ or $(d_1 - 1, d_4 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$. Moreover, $F(d_1 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1) = F(d_1 - 1, d_4 - 1, d_5 - 1, d_3 - 1, d_2 - 1)$. Hence (2) holds. ■

**Lemma 3.3** *Let $w_1 \geq w_2 \geq \cdots \geq w_6 \geq 1$ be positive integers and*

$$F(y_1, \ldots, y_k) = \sum_{i=1}^{k-1} \left( \sum_{j=1}^{i} y_j \right) \left( \sum_{j=i+1}^{k} y_j \right) .$$

*Then*

$$\begin{aligned} & F(w_1, w_6, w_5, w_4, w_3, w_2) - F(w_1, w_5, w_6, w_4, w_3, w_2) \\ = \;& (w_1 - w_2 - w_3 - w_4)(w_5 - w_6) \end{aligned} \tag{13}$$

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \;& 2(w_1 - w_2 - w_3)(w_4 - w_5) \end{aligned} \tag{14}$$

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_4, w_5, w_6, w_3, w_2) \\ = \;& (w_1 + w_4 - w_2 - w_3)(w_5 - w_6) \end{aligned} \tag{15}$$

$$\begin{aligned} & F(w_1, w_4, w_5, w_6, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \;& (3w_3 - 3w_4 - w_5 + w_6)(w_1 - w_2) \; . \end{aligned} \tag{16}$$

**Proof.** By a simple calculation, it is easy to see that the assertion holds. ■

**Theorem 3.4** *Let $\pi = (d_1, \ldots, d_6, \ldots, d_n)$ be tree degree sequence with $n - 6$ leaves, i. e., $d_1 \geq \cdots \geq d_6 \geq 2$ and $d_7 = \cdots = d_n = 1$.*

*(1). If $d_1 > d_2 + d_3 + d_4 - 2$, then there is only one maximum optimal tree $T(d_1 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$ in $\mathcal{T}_\pi$.*

*(2). If $d_1 = d_2 + d_3 + d_4 - 2$, then there are exactly two maximum optimal trees in $\mathcal{T}_\pi$: one maximum optimal tree is $T(d_1 - 1, d_6 - 1, d_5 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$; the other maximum optimal tree is $T(d_1 - 1, d_5 - 1, d_6 - 1, d_4 - 1, d_3 - 1, d_2 - 1)$.*

*(3). $d_2+d_3-1<d_1<d_2+d_3+d_4-2$, then there is only one maximum optimal tree $T(d_1-1, d_5-1, d_6-1, d_4-1, d_3-1, d_2-1)$ in $\mathcal{T}_\pi$.*

*(4). If $d_2+d_3-1=d_1$, then there are exactly two maximum optimal trees in $\mathcal{T}_\pi$: one maximum optimal tree is $T(d_1-1, d_5-1, d_6-1, d_4-1, d_3-1, d_2-1)$; the other maximum optimal tree is $T(d_1-1, d_4-1, d_6-1, d_5-1, d_3-1, d_2-1)$.*

*(5). If $\max\{d_2+d_3-d_4,\ d_2+\frac{1}{3}(d_5-d_6)\}<d_1<d_2+d_3-1$, then there is only one maximum optimal tree $T(d_1-1, d_4-1, d_6-1, d_5-1, d_3-1, d_2-1)$ in $\mathcal{T}_\pi$.*

*(6). If $d_1=d_2+d_3-w_4>d_2+\frac{1}{3}(d_5-d_6)$, then there are exactly two maximum optimal trees in $\mathcal{T}_\pi$: one maximum optimal tree is $T(d_1-1, d_4-1, d_6-1, d_5-1, d_3-1, d_2-1)$; the other maximum optimal tree is $T(d_1-1, d_4-1, d_5-1, d_6-1, d_3-1, d_2-1)$.*

*(7). If $d_1=d_2+\frac{1}{3}(d_5-d_6)>d_2+d_3-d_4$, then there are exactly two maximum optimal trees in $\mathcal{T}_\pi$: one maximum optimal tree is $T(d_1-1, d_4-1, d_6-1, d_5-1, d_3-1, d_2-1)$; the other maximum optimal tree is $T(d_1-1, d_3-1, d_6-1, d_5-1, d_4-1, d_2-1)$.*

*(8). If $d_1=d_2+d_3-d_4=d_2+\frac{1}{3}(d_5-d_6)$, then there are exactly three maximum optimal trees in $\mathcal{T}_\pi$: they are $T(d_1-1, d_4-1, d_6-1, d_5-1, d_3-1, d_2-1)$; $T(d_1-1, d_4-1, d_5-1, d_6-1, d_3-1, d_2-1)$ and $T(d_1-1, d_3-1, d_6-1, d_5-1, d_4-1, d_2-1)$.*

*(9). If $d_2+\frac{1}{3}(d_5-d_6)\le d_1<d_2+d_3-d_4$, or $d_1\le d_2+\frac{1}{3}(d_5-d_6)<d_2+d_3-d_4$, then there is only one maximum optimal tree $T(d_1-1, d_4-1, d_5-1, d_6-1, d_3-1, d_2-1)$ in $\mathcal{T}_\pi$.*

*(10). If $d_2+d_3-d_4\le d_1<d_2+\frac{1}{3}(d_5-d_6)$; or $d_1\le d_2+d_3-d_4<d_2+\frac{1}{3}(d_5-d_6)$, then there is only one maximum optimal tree $T(d_1-1, d_3-1, d_6-1, d_5-1, d_4-1, d_2-1)$ in $\mathcal{T}_\pi$.*

*(11). If $d_1<d_2+\frac{1}{3}(d_5-d_6)=d_2+d_3-d_4$, then there are exactly two maximum optimal trees in $\mathcal{T}_\pi$: one maximum optimal tree is $T(d_1-1, d_3-1, d_6-1, d_5-1, d_4-1, d_2-1)$; the other maximum optimal tree is $T(d_1-1, d_4-1, d_5-1, d_6-1, d_3-1, d_2-1)$.*

**Proof.** The proof is referred to appendix since it is technique. ■

**Remark**. From Theorem 3.4, we can see that the maximum optimal trees depend on the values of all components of the tree degree sequences and not unique, while the minimum optimal tree is unique for a given tree degree sequence. Moreover, Theorem 3.4 explains that it seems to be difficult for characterize all the maximum optimal trees for a given tree degree sequence.

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# Appendix: Proof of Theorem 3.4

**Lemma 3.5** *Let $w_1 \geq w_2 \geq \cdots \geq w_6 \geq 1$ be positive integers. If*

$$F(z_1, \ldots, z_6) = \max\{F(y_1, \ldots, y_6) : y_1 \geq y_6\}$$

*where $(y_1, \ldots, y_6)$ is any permutation of $(w_1, \ldots, w_6)$, then the following statement holds.*

*(1). If $w_1 > w_2 + w_3 + w_4$, then $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_6, w_5, w_4, w_3, w_2)$.*

*(2). If $w_1 = w_2 + w_3 + w_4$, then $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_6, w_5, w_4, w_3, w_2)$ or $(w_1, w_5, w_6, w_4, w_3, w_2)$.*

*(3). If $w_2 + w_3 < w_1 < w_2 + w_3 + w_4$, then $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$.*

*(4). If $w_2 + w_3 = w_1$, then $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$ or $(w_1, w_4, w_6, w_5, w_3, w_2)$.*

*(5). If $\max\{w_2 + w_3 - w_4, w_2 + \frac{1}{3}(w_5 - w_6)\} < w_1 < w_2 + w_3$, then $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$.*

*(6). If* $w_1 = w_2 + w_3 - w_4 > w_2 + \frac{1}{3}(w_5 - w_6)$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ *or* $(w_1, w_4, w_5, w_6, w_3, w_2)$.

*(7). If* $w_1 = w_2 + \frac{1}{3}(w_5 - w_6) > w_2 + w_3 - w_4$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ *or* $(w_1, w_3, w_6, w_5, w_4, w_2)$.

*(8). If* $w_1 = w_2 + w_3 - w_4 = w_2 + \frac{1}{3}(w_5 - w_6)$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$, *or* $(w_1, w_4, w_5, w_6, w_3, w_2)$ *or* $(w_1, w_3, w_6, w_5, w_4, w_2)$.

*(9). If* $w_2 + \frac{1}{3}(w_5 - w_6) \le w_1 < w_2 + w_3 - w_4$, *or* $w_1 \le w_2 + \frac{1}{3}(w_5 - w_6) < w_2 + w_3 - w_4$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_5, w_6, w_3, w_2)$.

*(10). If* $w_2 + w_3 - w_4 \le w_1 < w_2 + \frac{1}{3}(w_5 - w_6)$; *or* $w_1 \le w_2 + w_3 - w_4 < w_2 + \frac{1}{3}(w_5 - w_6)$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_3, w_6, w_5, w_4, w_2)$.

*(11). If* $w_1 < w_2 + \frac{1}{3}(w_5 - w_6) = w_2 + w_3 - w_4$, *then* $(z_1, z_2, z_3, z_4, z_5, z_6) = (w_1, w_4, w_5, w_6, w_3, w_2)$ *or* $(w_1, w_3, w_6, w_5, w_4, w_2)$.

**Proof.** (1). $w_1 > w_2 + w_3 + w_4$. By (8) and (9) in Lemma 2.5, we have $t = 2$ and $(z_1, \ldots, z_6) = (w_1, w_6, w_5, w_4, w_3, w_2)$.

(2). $w_1 = w_2 + w_3 + w_4$. By (8) and (9) in Lemma 2.5, we have $t = 3$. By (11) and (12). we consider the following two cases. If $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$, then by corollary 2.6 and $w_1 = w_2 + w_3 + w_4$, we have $(z_1, \ldots, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$. If $z_1 \ge z_2$ and $z_2 \le z_3 \le z_4 \le z_5 \le z_6$, then $(z_1, \ldots, z_6) = (w_1, w_6, w_5, w_4, w_3, w_2)$. Hence (2) holds.

(3). $w_2 + w_3 < w_1 < w_2 + w_3 + w_4$. We consider the following four cases:

**Case 1:** $w_2 + w_3 + w_5 < w_1 < w_2 + w_3 + w_4$. By (8) and (9) in Lemma 2.5, we have $t = 3$ and $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$. Hence by Corollary 2.6, $(z_1, \ldots, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$.

**Case 2:** $w_2 + w_3 + w_5 = w_1 < w_2 + w_3 + w_4$. Similarly,

$$(z_1, \ldots, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2) .$$

**Case 3:** $w_2 + w_4 + w_5 < w_1 < w_2 + w_3 + w_5$ and $w_1 > w_2 + w_3$. By (8) and (9) in Lemma 2.5, we have $t = 3$. Further $(z_1, \ldots, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$ or $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$. But by Lemma 3.3, we have

$$F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) = 2(w_1 - w_2 - w_3)(w_4 - w_5).$$

Hence $(z_1,\dots,z_6)=(w_1,w_5,w_6,w_4,w_3,w_2)$.

**Case 4:** $w_2+w_3<w_1\le w_2+w_4+w_5$. By (8) and (9) in Lemma 2.5, we have $t=3$. Further $(z_1,\dots,z_6)=(w_1,w_3,w_6,w_5,w_4,w_2)$, or $(w_1,w_4,w_6,w_5,w_3,w_2)$, or $(w_1,w_5,w_6,w_4,w_3,w_2)$. But by Lemma 3.3, we have

$$\begin{aligned}&F(w_1,w_3,w_6,w_5,w_4,w_2)-F(w_1,w_2,w_6,w_5,w_4,w_3)\\=\;&2(w_2-w_3)(2w_1-w_4+w_6)\ge 0\end{aligned}$$

$$\begin{aligned}&F(w_1,w_4,w_6,w_5,w_3,w_2)-F(w_1,w_3,w_6,w_5,w_4,w_2)\\=\;&(w_3-w_4)(3w_1-3w_2-w_5+w_6)\ge 0\end{aligned}$$

$$\begin{aligned}&F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)\\=\;&2(w_1-w_2-w_3)(w_4-w_5)\ .\end{aligned}$$

Hence $(z_1,\dots,z_6)=(w_1,w_5,w_6,w_4,w_3,w_2)$.

(4). $w_2+w_3=w_1$. From the proof of (3), it is easy to see that $(z_1,\dots,z_6)=(w_1,w_5,w_6,w_4,w_3,w_2)$ or $(w_1,w_4,w_6,w_5,w_3,w_2)$, because $F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)=0$. Therefore (4) holds.

(5). $\max\{w_2+w_3-w_4,w_2+\frac{1}{3}(w_5-w_6)\}<w_1<w_2+w_3$. We consider the four cases.

**Case 1:** $w_1>w_2+w_4+w_5$ and $w_1>w_2+w_3-w_5$. By (8) and (9) in Lemma 2.5, we have $z_1\ge z_2\ge z_3$ and $z_3\le z_4\le z_5\le z_6$. Then $(z_1,\dots,z_6)=(w_1,w_5,w_6,w_4,w_3,w_2)$ or $(w_1,w_4,w_6,w_5,w_3,w_2)$. But

$$\begin{aligned}&F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)\\=\;&2(w_4-w_5)(w_1-w_2-w_3)\le 0\end{aligned}$$

with equality if and only if $w_4=w_5$. Therefore $(z_1,\dots,z_6)=(w_1,w_4,w_6,w_5,w_3,w_2)$.

**Case 2:** $w_1>w_2+w_4+w_5$ and $w_1\le w_2+w_3-w_5$. By (8) and (9) in Lemma 2.5, we have $z_1\ge z_2\ge z_3$ and $z_3\le z_4\le z_5\le z_6$. Then $(z_1,\dots,z_6)=(w_1,w_5,w_6,w_4,w_3,w_2)$ or $(w_1,w_4,w_6,w_5,w_3,w_2)$. But by Lemma 3.3, we have

$$\begin{aligned}&F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)\\=\;&2(w_4-w_5)(w_1-w_2-w_3)\le 0\end{aligned}$$

with equality if and only if $w_4 = w_5$ . Therefore $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ .

**Case 3:** $w_1 \le w_2+w_4+w_5$ and $w_1 > w_2+w_3-w_5$ . By (8) and (9) in Lemma 2.5, we have $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$ . Then $(z_1, \ldots, z_6) = (w_1, w_5, w_6, w_4, w_3, w_2)$ , or $(w_1, w_4, w_6, w_5, w_3, w_2)$ , or $(w_1, w_3, w_6, w_5, w_4, w_2)$ . But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \; & 2(w_4 - w_5)(w_1 - w_2 - w_3) \le 0 \end{aligned}$$

with equality if and only if $w_4 = w_5$ . Moreover,

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (w_3 - w_4)(3w_1 - 3w_2 - w_5 + w_6) \ge 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$ . Therefore $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ .

**Case 4:** $w_1 \le w_2+w_4+w_5$ and $w_1 \le w_2+w_3-w_5$ . By (8) and (9) in Lemma 2.5, we have $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$ . Then $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ , or $(w_1, w_3, w_6, w_5, w_4, w_2)$ . But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (w_3 - w_4)(3w_1 - 3w_2 - w_5 + w_6) \ge 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$ . Therefore $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$ .

(6). $w_1 = w_2 + w_3 - w_4 > w_2 + \frac{1}{3}(w_5 - w_6)$ . By (8) and (9) in Lemma 2.5, we have $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$; or $z_1 \ge z_2 \ge z_3 \ge z_4$ and $z_4 \le z_5 \le z_6$ . Then $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$; or $(w_1, w_3, w_6, w_5, w_4, w_2)$; or$(w_1, w_5, w_6, w_4, w_3, w_2)$; or $(w_1, w_4, w_5, w_6, w_3, w_2)$ . But

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (w_3 - w_4)(3w_1 - 3w_2 - w_5 + w_6) \ge 0 \end{aligned}$$

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \; & 2(w_1 - w_2 - w_3)(w_4 - w_5) \le 0 \end{aligned}$$

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_4, w_5, w_6, w_3, w_2) \\ = \; & (w_1 + w_4 - w_2 - w_3)(w_5 - w_6) = 0 \ . \end{aligned}$$

Therefore $(z_1,\ldots,z_6)=(w_1,w_4,w_6,w_5,w_3,w_2)$ or $(w_1,w_4,w_5,w_6,w_3,w_2)$.

(7) $w_1=w_2+\frac{1}{3}(w_5-w_6)>w_2+w_3-w_4$. By (8) and (9) in Lemma 2.5, we have $z_1\geq z_2\geq z_3$ and $z_3\leq z_4\leq z_5\leq z_6$. Then $(z_1,\ldots,z_6)=(w_1,w_4,w_6,w_5,w_3,w_2)$; or $(w_1,w_3,w_6,w_5,w_4,w_2)$; or $(w_1,w_5,w_6,w_4,w_3,w_2)$. But by Lemma 3.3, we have

$$\begin{aligned}&F(w_1,w_4,w_6,w_5,w_3,w_2)-F(w_1,w_3,w_6,w_5,w_4,w_2)\\ =\;&(w_3-w_4)(3w_1-3w_2-w_5+w_6)=0\end{aligned}$$

and

$$\begin{aligned}&F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)\\ =\;&2(w_1-w_2-w_3)(w_4-w_5)\leq 0\,.\end{aligned}$$

Hence $(z_1,\ldots,z_6)=(w_1,w_4,w_6,w_5,w_3,w_2)$ or $(w_1,w_3,w_6,w_5,w_4,w_2)$.

(8). $w_1=w_2+w_3-w_4=w_2+\frac{1}{3}(w_5-w_6)$. It follows from (6) and (7) that (8) holds.

(9). Assume that $w_2+\frac{1}{3}(w_5-w_6)\leq w_1<w_2+w_3-w_4$. Then we have to consider the following two cases:

**Case 1:** $w_1>w_2+w_4+w_5$. By (8) and (9) in Lemma 2.5, we have $z_1\geq z_2\geq z_3$ and $z_3\leq z_4\leq z_5\leq z_6$; or $z_1\geq z_2\geq z_3\geq z_4$ and $z_4\leq z_5\leq z_6$. Hence $(z_1,\ldots,z_6)=(w_1,w_4,w_6,w_5,w_3,w_2)$, $(w_1,w_4,w_5,w_6,w_3,w_2)$, or $(w_1,w_5,w_6,w_4,w_3,w_2)$. By Lemma 3.3, we have

$$\begin{aligned}&F(w_1,w_5,w_6,w_4,w_3,w_2)-F(w_1,w_4,w_6,w_5,w_3,w_2)\\ =\;&2(w_1-w_2-w_3)(w_4-w_5)\leq 0\end{aligned}$$

with equality if and only if $w_4=w_5$, and

$$\begin{aligned}&F(w_1,w_4,w_6,w_5,w_3,w_2)-F(w_1,w_4,w_5,w_6,w_3,w_2)\\ =\;&2(w_1+w_4-w_2-w_3)(w_5-w_6)\leq 0\end{aligned}$$

with equality if and only if $w_5=w_6$. Therefore $(z_1,\ldots,z_6)=(w_1,w_4,w_5,w_6,w_3,w_2)$.

**Case 2:** $w_1\leq w_2+w_4+w_5$. By (8) and (9) in Lemma 2.5, we have $z_1\geq z_2\geq z_3$ and $z_3\leq z_4\leq z_5\leq z_6$; or $z_1\geq z_2\geq z_3\geq z_4$ and $z_4\leq z_5\leq z_6$. Hence $(z_1,\ldots,z_6)=$

$(w_1, w_4, w_6, w_5, w_3, w_2)$ or $(w_1, w_3, w_6, w_5, w_4, w_2)$ or $(w_1, w_4, w_5, w_6, w_3, w_2)$ or $(w_1, w_5, w_6, w_4, w_3, w_2)$. But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \quad & (3w_1 - 3w_2 - w_5 + w_6)(w_3 - w_4) \le 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$,

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_5, w_6, w_4, w_3, w_2) \\ = \quad & 2(-w_1 + w_2 + w_3)(w_4 - w_5) \ge 0 \end{aligned}$$

and

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_4, w_5, w_6, w_3, w_2) \\ = \quad & (w_1 + w_4 - w_2 - w_3)(w_5 - w_6) \ge 0 \end{aligned}$$

with equality if and only if $w_5 = w_6$. Therefore $(z_1, \ldots, z_6) = (w_1, w_4, w_5, w_6, w_3, w_2)$.

Assume that $w_1 \le w_2 + \frac{1}{3}(w_5 - w_6) < w_2 + w_3 - w_4$. By (8) and (9) in Lemma 2.5, we have $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$; or $z_1 \ge z_2 \ge z_3 \le z_4$ and $z_4 \le z_5 \le z_6$. Hence, $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$; or $(w_1, w_3, w_6, w_5, w_4, w_2)$; or $(w_1, w_5, w_6, w_4, w_3, w_2)$; or $(w_1, w_4, w_5, w_6, w_3, w_2)$. But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \quad & (3w_1 - 3w_2 - w_5 + w_6)(w_3 - w_4) \le 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$;

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \quad & 2(w_1 - w_2 - w_3)(w_4 - w_5) \le 0 \end{aligned}$$

$$\begin{aligned} & F(w_1, w_4, w_5, w_6, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \quad & (3w_3 - 3w_4 - w_5 + w_6)(w_1 - w_2) \ge 0 \end{aligned}$$

with equality if and only if $w_1 = w_2$. Therefore $(z_1, \ldots, z_6) = (w_1, w_4, w_5, w_6, w_3, w_2)$.

(10). Assume that $w_2 + w_3 - w_4 \le w_1 < w_2 + \frac{1}{3}(w_5 - w_6)$. By (8) and (9) in Lemma 2.5, we have $z_1 \ge z_2 \ge z_3$ and $z_3 \le z_4 \le z_5 \le z_6$; or $z_1 \ge z_2 \ge z_3 \le z_4$ and

$z_4 \leq z_5 \leq z_6$. Hence, $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$; or $(w_1, w_3, w_6, w_5, w_4, w_2)$; or $(w_1, w_5, w_6, w_4, w_3, w_2)$; or $(w_1, w_4, w_5, w_6, w_3, w_2)$. But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (3w_1 - 3w_2 - w_5 + w_6)(w_3 - w_4) \leq 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$,

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \; & 2(w_1 - w_2 - w_3)(w_4 - w_5) \leq 0 \end{aligned}$$

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_4, w_5, w_6, w_3, w_2) \\ = \; & (w_1 + w_4 - w_2 - w_3)(w_5 - w_6) \geq 0 \end{aligned}$$

with equality if and only if $w_5 = w_6$. Therefore $(z_1, \ldots, z_6) = (w_1, w_3, w_6, w_5, w_4, w_2)$.

Assume that $w_1 \leq w_2 + w_3 - w_4 < w_2 + \frac{1}{3}(w_5 - w_6)$. By (8) and (9) in Lemma 2.5, we have $z_1 \geq z_2 \geq z_3$ and $z_3 \leq z_4 \leq z_5 \leq z_6$; or $z_1 \geq z_2 \geq z_3 \leq z_4$ and $z_4 \leq z_5 \leq z_6$. Hence, $(z_1, \ldots, z_6) = (w_1, w_4, w_6, w_5, w_3, w_2)$; or $(w_1, w_3, w_6, w_5, w_4, w_2)$; or $(w_1, w_5, w_6, w_4, w_3, w_2)$; or $(w_1, w_4, w_5, w_6, w_3, w_2)$. But by Lemma 3.3, we have

$$\begin{aligned} & F(w_1, w_4, w_6, w_5, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (3w_1 - 3w_2 - w_5 + w_6)(w_3 - w_4) \leq 0 \end{aligned}$$

with equality if and only if $w_3 = w_4$,

$$\begin{aligned} & F(w_1, w_5, w_6, w_4, w_3, w_2) - F(w_1, w_4, w_6, w_5, w_3, w_2) \\ = \; & 2(w_1 - w_2 - w_3)(w_4 - w_5) \leq 0 \end{aligned}$$

and

$$\begin{aligned} & F(w_1, w_4, w_5, w_6, w_3, w_2) - F(w_1, w_3, w_6, w_5, w_4, w_2) \\ = \; & (3w_3 - 3w_4 - w_5 + w_6)(w_1 - w_2) \leq 0 \end{aligned}$$

with equality if and only if $w_1 = w_2$. Therefore $(z_1, \ldots, z_6) = (w_1, w_3, w_6, w_5, w_4, w_2)$.

(11). $w_1 < w_2 + w_3 - w_4 = w_2 + \frac{1}{3}(w_5 - w_6)$. It follows from (9) and (10) that (11) holds. ■

**Proof.** of Theorem 3.4. It follows from Theorem 2.3 and Lemma 3.5 that the assertion holds. ■