

# The Wiener Index of Trees with Given Degree Sequences\*

Xiao-Dong Zhang<sup>†</sup> and Qi-Yuan Xiang

Department of Mathematics

Shanghai Jiao Tong University

800 Dongchuan road, Shanghai, 200240, P.R. China

Li-Qun Xu

Antai College of Economics and Management

Shanghai Jiao Tong University

800 Dongchuan road, Shanghai, 200240, P.R. China

Rong-Ying Pan

Suzhou Vocational University

Suzhou, Jiangsu, 210000, P.R. China

(Received January 10, 2008)

---

\*Supported by National Natural Science Foundation of China (No.10531070), National Basic Research Program of China 973 Program (No.2006CB805900), National Research Program of China 863 Program (No.2006AA11Z209) and the Natural Science Foundation of Shanghai (Grant No.06ZR14049).

<sup>†</sup>Correspondent author: Xiao-Dong Zhang (Email: xiaodong@sjtu.edu.cn)

### Abstract

The Wiener index is the sum of topological distances between all pairs of vertices in a connected graph such as represents the structural formula of a molecule. Firstly, we investigate some properties of the partially ordered set of all vectors associated with a tree with respect to majorization. Then these results are used to characterize the trees which minimize the Wiener index among all trees with a given degree sequence. Consequently, all extremal trees with the smallest Wiener index are obtained in the sets of all trees of order  $n$  with the maximum degree, the leaf number and the matching number respectively.

## 1 Introduction

*Molecular graphs* are usually used to describe molecules and molecular compounds. Topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure activity relationships of molecules and molecular compounds. Perhaps, one of the most widely known topological descriptors is the *Wiener index* which is named after chemist Wiener [21] who first considered it. Many chemical applications of the Wiener index deals with acyclic organic molecules, whose molecular graphs are trees. In the mathematical literature, the Wiener index seems to be the first studied by Entringer et al. [4]. For more information and background, the readers may refer to a recent and very comprehensive survey [3] and a book [19] which is dedicated to Harry Wiener on the Wiener index and the references therein. Let  $G = (V, E)$  be a simple connected graph with vertex set  $V(G) = \{v_1, \dots, v_n\}$  and edge set  $E(G)$ . Denote by  $d_G(v_i)$  (or for short  $d(v_i)$ ) the *degree* of vertex  $v_i$  of graph  $G$ . The *distance* between vertices  $v_i$  and  $v_j$  is the minimum number of edges between  $v_i$  and  $v_j$  and is 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

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

Since the Wiener index has been used to explain the variation in the physical and chemical properties of alkanes and correlate the pharmacological properties of

compounds with their structure, chemists are often interested in the Wiener index of certain trees which present molecular structures (for example, see [10], [9], [8], [3] and the references therein). For a saturated acyclic hydrocarbon which consists only of carbon atoms and hydrogen atoms, we may use a tree to describe it with each vertex representing a carbon atom. The vertex degree represents its *valency*. It is well known that there are many different molecules whose chemical formula are the same. For example, butane and isobutane are isomers with the same chemical formulas  $C_4H_{10}$ . It is natural to ask how many different molecules there are having the same chemical formula  $C_nH_{2n+2}$ . This problem was systematically addressed by Cayley by way of graph theoretical techniques. But then a natural question arise as to the relations of the Wiener indices among the different molecules with the same chemical formula, since molecular branching and molecular cyclicity are topological characteristics that are accounted for by the Wiener index (See [15] and [18]).

Entringer et al. [4] showed that among all trees of order  $n$  the star  $K_{1,n-1}$  and the path  $P_n$  have the minimum and maximum Wiener indices, respectively. Dankelmann [2] determined the maximum Wiener index in terms of the order and the independence number. Recently, Fischermann et al. [6] and Jelen et al. [13] 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  $\pi = (d_0, d_1, \dots, d_{n-1})$  is called *graphic* if there exists a simple connected graph having  $\pi$  as its vertex degree sequence. Ruch and Gutman [20] discussed the majorization partial ordering of potential degree sequences and the relation to being graphic. For more information, the reader may refer to [12] and [7]. For other terminology and notions, we follow [1]. These results and problems motivate us to propose the following problem:

**Problem 1.1** *For a given graphic degree sequence  $\pi$ , let*

$$\mathcal{G}(\pi) = \{G \mid G \text{ is connected with } \pi \text{ as its degree sequence}\}.$$

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

In this paper, we only consider a special case for the above problem, i.e., for a given degree sequence of some tree. One of the main results of this paper is as follows:

**Theorem 1.2** *For a given degree sequence of some tree, let*

$$\mathcal{T}(\pi) = \{T \mid T \text{ is a tree with } \pi \text{ as its degree sequence}\}.$$

*Then  $T^*(\pi)$  (or for short  $T^*$ , described in section 2) is a unique tree with the minimum Wiener index in  $\mathcal{T}(\pi)$ .*

The main Theorem 1.2 may be used to describe relations of the Wiener index among all different molecules with the same chemical formula so as to characterize variations amongst alkanes. For example, from Theorem 1.2, we may deduce the following result.

**Theorem 1.3** *Among all graphs representing molecules with the same chemical formula  $C_nH_{2n+2}$ , there is only one tree representing molecules with the minimum Wiener index and its structure is determined.*

Suppose that there are two molecules with the same chemical formula  $C_4H_{10}$ , if the Wiener index of one molecule is less than that of the other, then this molecule must be isobutane and the other is butane by Theorem 1.3, since there are two possible molecules with the same chemical formula  $C_4H_{10}$ .

The rest of the paper is organized as follows. In Section 2, a special tree  $T^*$  and the notation of a BFS-ordering are introduced. Moreover, some properties and preliminary results are presented. In Section 3, we investigate properties of a partially ordered set of all vectors associated with a tree. In Section 4, The above results are used to present a proof of Theorem 1.2 by establishing relations between the partially ordered set and the Wiener index. In Section 5, we derive some corollaries from the main results, which contain the main results of Fischermann et al. [6] and Jelen et al. [13]

## 2 Notation and preliminaries

In order to easily understand the construction of  $T^*$ , we first give an example to illustrate how to construct  $T^*$  before presenting the construction of  $T^*$  with  $n$  vertices. For example, for a given degree sequence  $\pi = (4, 4, 4, 3, 3, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1)$ ,  $T^*$  is the tree of order 18 (see Fig.1). There is a vertex  $v_{01}$  in layer 0 with  $d(v_{01}) = 4$ . Then  $v_{01}$  in layer 0 is adjacent to four vertices  $v_{11}, v_{12}, v_{13}, v_{14}$  in layer 1 whose degrees are 4, 4, 3, 3 respectively. Then  $v_{11}, v_{12}, v_{13}, v_{14}$  in layer 1 are adjacent to three, two and two vertices respectively in layer 2 from left to right. These vertices are denoted by  $v_{21}, v_{22}, \dots, v_{2,10}$  whose degrees are 3, 2, 1, 1, 1, 1, 1, 1, 1, 1 respectively. Then  $v_{21}, v_{22}$  are adjacent to two and one vertex respectively in layer 3. These vertices are denoted by  $v_{31}, v_{32}, v_{33}$  whose degrees are 1.

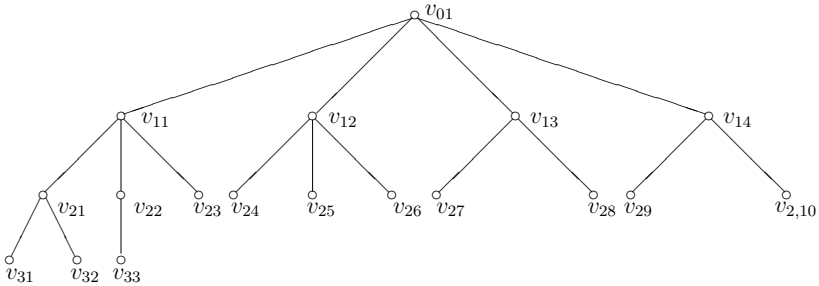


Figure 1

Generally, we may construct  $T^*$  with degree sequence  $\pi$ . Let  $\pi = (d_0, d_1, \dots, d_{n-1})$  with  $n \geq 3$  be a given nonincreasing degree sequence of some tree. Now we construct a special tree  $T^*$  with degree sequence  $\pi$  by using a "breadth-first" scheme, which considers the  $n$  vertices of  $T^*$  to be partitioned into a sequence of layers starting with the  $0^{th}$  layer consisting of a single vertex  $v_{01}$  of maximum degree. Then recursively develop the layers, with the  $1^{th}$  layer having  $d_0$  vertices each connected to  $v_{01}$ . Denote the number of vertices in the  $m^{th}$  layer by  $l_m$ , and the number in all layers preceding layer  $m$  by  $l_{<m}$ . Given  $l_m$  vertices in a layer  $m \geq 1$ , choose the degree of the  $i^{th}$

vertex  $v_{m,i}$  in this layer to be  $d_{i+l_{<m}}$  with all but 1 of its connections to be to vertices  $v_{m+1,k}$  in the next layer for  $k = j + \sum_{p=1}^{i-1} (d_{p+l_{<m}} - 1)$ , with  $j = 1$  to  $d_{i+l_{<m}} - 1$ . The number of vertices in this next layer then is  $l_{m+1} = \sum_{p=1}^{l_m} (d_{p+l_{<m}} - 1)$ , and the process is continued till all  $n$  vertices are accounted for.

Let  $T = (V, E)$  be a rooted tree with root  $r$ . Denote by  $\mathcal{T}_r(\pi)$  the set of all rooted trees with degree sequence  $\pi$ , i.e,

$$\mathcal{T}_r(\pi) = \{T \mid T \text{ is a rooted tree with } \pi \text{ as its degree sequence}\}.$$

The distance  $d(v, r)$  between  $v$  and the  $r$  is called the *height* of vertex  $v$  and denoted by  $h(v) = d(v, r)$ . For two vertices  $u$  and  $v$ , we say that  $u$  is a *successor* of  $v$  in a rooted tree  $T$ , if the path  $P(u, r)$  from vertex  $u$  to the rooted vertex  $r$  contains vertex  $v$ . Moreover, if  $u$  is a successor of  $v$  and  $u$  is adjacent to  $v$ , we say that  $u$  is a *child* of  $v$ , and that  $v$  is the *parent* of  $u$ . A *well-ordering* (*complete linear ordering*) of a set  $W$  is defined to be an ordering such that every set  $S \subseteq W$  there is a least element.

**Definition 2.1** Let  $T = (V, E)$  be a tree with root  $r$  and let  $(V, \trianglelefteq)$  be a well-ordering (or a complete linear ordering). The well-ordering  $\trianglelefteq$  of the vertex set  $V$  is called a *breadth-first search ordering* (*BFS-ordering* for short) if the following holds for all vertices  $u, v \in V$ :

- (1)  $u \trianglelefteq v$  implies  $h(u) \leq h(v)$ ;
- (2)  $u \trianglelefteq v$  implies  $d(u) \geq d(v)$ ;
- (3) if  $u_1$  is a child of  $u$  and  $v_1$  is a child of  $v$ ; and  $u \trianglelefteq v$ , then  $u_1 \trianglelefteq v_1$ .

We call trees that have a BFS-ordering of its vertices a *BFS-tree*.

All trees have an ordering which satisfy the conditions (1) and (3) by using a breadth-first search. But not all tree have a BFS-ordering. For example, the following tree  $T$  of order 17 with degree sequence  $\pi = (4, 4, 4, 3, 3, 3, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$  does not have a BFS-ordering (see Fig.2).

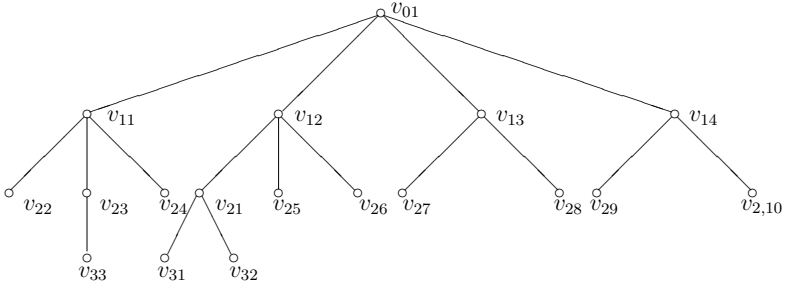


Figure 2

For properties of BFS-ordering, we have the following result from [22],

**Proposition 2.2** (Zhang [22]) *Let  $\pi$  be the degree sequence of some tree. Then there exists a unique tree  $T^*$  with degree sequence  $\pi$  having a BFS-ordering. In other words, any two trees with the same degree sequences and having a BFS-ordering are isomorphic.*

We recall the notion of majorization. For details, the readers are referred to the book of Marshall and Olkin [17].

Let  $x = (x_1, x_2, \dots, x_p)$  and  $y = (y_1, y_2, \dots, y_p)$  be two nonnegative integers. We arrange the entries of  $x$  and  $y$  in nondecreasing order  $x_{\uparrow} = (x_{[1]}, \dots, x_{[p]})$  and  $y_{\uparrow} = (y_{[1]}, \dots, y_{[p]})$ . If

$$\sum_{i=1}^k x_{[i]} \leq \sum_{i=1}^k y_{[i]}, \text{ for } k = 1, \dots, p,$$

$x$  is said to *weakly majorize*  $y$  and denoted  $y \preceq^w x$ . Further, if  $y \preceq^w x$  and

$$\sum_{i=1}^p x_{[i]} = \sum_{i=1}^p y_{[i]},$$

$x$  is said to *majorize*  $y$  and denoted by  $x \succeq y$  or  $y \preceq x$ . Moreover, if  $y \preceq^w x$  (resp.  $y \preceq x$ ) and  $x_{\uparrow} \neq y_{\uparrow}$ ,  $x$  is said to *strictly weakly majorize* (resp. *strictly majorize*)  $y$  and denoted by  $y \prec^w x$  (resp.  $y \prec x$ ). Here, we present two simple properties of majorization which will be used later.

**Proposition 2.3** *Let  $x = (x_1, \dots, x_k, y_1, \dots, y_l)$  and  $y = (x_1 + b, \dots, x_k + b, y_1 - b, \dots, y_l - b)$  be two nonnegative integer sequences with  $k \leq l$  and  $b > 0$ . If  $x_i \geq y_i$  for  $i = 1, \dots, k$ , then  $x \prec^w y$ .*

**Proposition 2.4** *If  $x \prec^w y$  and  $x' \preceq^w y'$ , then  $(x, x') \prec^w (y, y')$*

### 3 The partially ordered set

Let  $T = (V, E)$  be a rooted tree with root  $r$ . For each vertex  $u$ , let  $T(u)$  be the subtree of the rooted tree  $T$  induced by  $u$  and its all successors in  $T$ . In other words, if  $u$  is not the root  $r$  of tree  $T$  and  $v$  is the parent of  $u$ , then  $T(u)$  is the connected component of  $T$  obtained from  $T$  by deleting the edge  $uv$  such that the component does not contain the root  $r$ ; if  $u$  is the root  $r$ , then  $T(u)$  is the tree  $T$ . Let  $f_T(u) = |T(u)|$  be the number of vertices in  $T(u)$  and denote  $f(T) = (f_T(u), u \in V(T))$ . For a given degree sequence  $\pi$ , let

$$\Omega(\pi) = \{f(T), T \text{ is a rooted tree with degree sequence } \pi\}.$$

Clearly,  $\Omega(\pi)$  is a partially ordered set with respect to majorization. In this section, we discuss that any modification of a tree gives rise to a perturbation of its  $f(T)$ . Then we show that  $\Omega(\pi)$  has only one maximum element with respect to majorization.

**Lemma 3.1** *Let  $T \in \mathcal{T}_r(\pi)$ . Suppose that  $u$  and  $v$  are successors of  $w$  and there are two internal disjoint paths  $P(u, w) = (u, u_1, \dots, u_k, w)$  and  $P(v, w) = (v, v_1, \dots, v_l, w)$  with  $1 \leq k \leq l$  and  $f_T(u) < f_T(v)$ ,  $f_T(u_i) \geq f_T(v_i)$  for  $i = 1, \dots, k$ . Let  $T'$  be a tree with root  $r$  obtained from  $T$  by deleting the edges  $u_1u$  and  $v_1v$  and adding the edges  $u_1v$  and  $v_1u$ . Then  $T' \in \mathcal{T}_r(\pi)$  and  $f(T) \prec^w f(T')$ .*

**Proof.** Clearly,  $T$  and  $T'$  have the same degree sequence and  $T' \in \mathcal{T}_r(\pi)$ . Put  $b = f_T(v) - f_T(u) > 0$ . By the definition of  $f(T)$ , it is easy to see that  $f_{T'}(v_i) = f_T(v_i) - b$ ; for  $1 \leq i \leq l$ . Moreover,  $f_{T'}(u_i) = f_T(u_i) + b$ ; for  $1 \leq i \leq k$ . Hence by Proposition 2.3,  $(f_T(u_1), \dots, f_T(u_k), f_T(v_1), \dots, f_T(v_l)) \prec^w (f_{T'}(u_1), \dots, f_{T'}(u_k), f_{T'}(v_1), \dots, f_{T'}(v_l))$ . For any vertex  $y$  in  $V(T) \setminus \{u_1, \dots, u_k, v_1, \dots, v_l\}$ , we have  $f_{T'}(y) = f_T(y)$ . Therefore by Proposition 2.4,  $f(T) \prec^w f(T')$  ■



**Lemma 3.2** *Let  $T$  be a rooted tree with root  $r$ . Suppose that  $u$  and  $v$  are two successors of  $w$  such that there are two paths  $P(v, w) = (v, v_1, \dots, v_l, w)$  and  $P(u, w) = (u, w)$  with  $u \neq v_l$  and  $l \geq 1$ . If  $f_T(u) < f_T(v)$ , let  $T'$  be a rooted tree with root  $r$  obtained from  $T$  by deleting the two edges  $uw$  and  $vv_1$  and adding two edges  $uv_1$  and  $vw$ . Then  $T' \in \mathcal{T}_r(\pi)$  and*

$$f(T) \prec^w f(T').$$

**Proof.** It is easy to see that  $T' \in \mathcal{T}_r(\pi)$ . Let  $b = f_T(v) - f_T(u) > 0$ . Then  $f_{T'}(v_i) = f_T(v_i) - b$  for  $i = 1, \dots, l$ . Hence  $(f_T(v_1), \dots, f_T(v_l)) \prec^w (f_{T'}(v_1), \dots, f_{T'}(v_l))$ . Moreover,  $f_{T'}(y) = f_T(y)$  for  $y \in V \setminus \{v_1, \dots, v_l\}$ . Hence by Proposition 2.4, the assertion holds. ■

**Lemma 3.3**  *$T \in \mathcal{T}_r(\pi)$ . Suppose that  $u$  and  $v$  are two successors of  $w$  and there are two internal disjoint paths  $P(u, w) = (u, u_1, \dots, u_k, w)$  and  $P(v, w) = (v, v_1, \dots, v_l, w)$  with  $1 \leq k \leq l$  and  $f_T(u) \geq f_T(v)$ ,  $f_T(u_i) \geq f_T(v_i)$  for  $i = 1, \dots, k$ . If  $d_T(u) < d_T(v)$ , denote  $s = d_T(v) - d_T(u) > 0$ , and let  $T'$  be a tree with root  $r$  obtained from  $T$  by deleting the  $s$  edges  $vx_i$  and adding  $s$  edges  $ux_i, i = 1, \dots, s$ , where  $\{x_1, \dots, x_s\}$  are children of  $v$ . Then  $T' \in \mathcal{T}_r(\pi)$  and  $f(T) \prec^w f(T')$ .*

**Proof.** Since  $d_{T'}(u) = d_T(u)$  and  $d_{T'}(v) = d_T(v)$ , we have  $T' \in \mathcal{T}_r(\pi)$ . Let  $b = \sum_{i=1}^s f_T(x_i) > 0$ . By the definition of  $f(T)$ , it is easy to see that  $f_{T'}(v) = f_T(v) - b$ ,  $f_{T'}(v_i) = f_T(v_i) - b$ ; for  $i = 1, \dots, l$ . Moreover,  $f_{T'}(u) = f_T(u) + b$ ,  $f_{T'}(u_i) = f_T(u_i) + b$ ; for  $i = 1, \dots, k$ . Hence by Proposition 2.3, we have  $(f_T(u), f_T(u_1), \dots, f_T(u_k), f_T(v), f_T(v_1), \dots, f_T(v_l)) \prec^w (f_{T'}(u), f_{T'}(u_1), \dots, f_{T'}(u_k), f_{T'}(v), f_{T'}(v_1), \dots, f_{T'}(v_l))$ . For any vertex  $y$  in  $V(T) \setminus \{u, u_1, \dots, u_k, v, v_1, \dots, v_l\}$ , we have  $f_{T'}(y) = f_T(y)$ . Therefore by Proposition 2.4,  $f(T) \prec^w f(T')$ . ■

**Lemma 3.4** *Let  $T$  be a rooted tree with root  $r$ . Suppose that  $u$  and  $v$  are two successors of  $w$  such that there are two paths  $P(v, w) = (v, v_1, \dots, v_l, w)$  and  $P(u, w) = (u, w)$  with  $u \neq v_l$  and  $l \geq 1$ . If  $d_T(u) < d_T(v)$ , denote  $s = d_T(v) - d_T(u) > 0$ , and let  $T'$  be a tree with root  $r$  obtained from  $T$  by deleting the  $s$  edges  $vx_i$  and adding  $s$  edges  $ux_i, i = 1, \dots, s$ , where  $\{x_1, \dots, x_s\}$  are children of  $v$ . Then  $T' \in \mathcal{T}_r(\pi)$  and  $f(T) \prec^w f(T')$ .*

**Proof.** The proof of Lemma 3.4 is similar to that of Lemma 3.3 and is omitted. ■

**Lemma 3.5** *Let  $T \in \mathcal{T}_r(\pi)$ . Suppose that  $u$  is the parent of  $v$  and  $d_T(u) < d_T(v)$ . Denote  $s = d_T(v) - d_T(u) > 0$ , and let  $T'$  be a tree with root  $r$  obtained from  $T$  by deleting the  $s$  edges  $vx_i$  and adding  $s$  edges  $ux_i$ ,  $i = 1, \dots, s$ , where  $\{x_1, \dots, x_s\}$  are children of  $v$ . Then  $T' \in \mathcal{T}_r(\pi)$  and  $f(T) \prec^w f(T')$ .*

**Proof.** Clearly,  $T' \in \mathcal{T}_r(\pi)$ . Let  $b = \sum_{i=1}^s f_T(x_i) > 0$ . Then  $f_{T'}(v) = f_T(v) - b < f_T(v)$ , which implies  $f_T(v) \prec^w f_{T'}(v)$ . Moreover, for any  $y \neq v$ , we have  $f_{T'}(y) = f_T(y)$ . Hence by Proposition 2.4, the assertion holds. ■

Now we present the main result in this section which is interesting in its own right.

**Theorem 3.6** *Let  $T \in \mathcal{T}_r(\pi)$ . Then*

$$f(T) \preceq^w f(T^*)$$

*with equality if and only if  $T$  is isomorphic to  $T^*$ . In other words,  $\Omega(\pi)$  has only one maximum element which is  $T^*$  up to isomorphism.*

**Proof.** Clearly,  $\Omega(\pi) = \{f(T), T \in \mathcal{T}_r(\pi)\}$  is a partially ordered set with respect to  $\preceq^w$ . Let  $T$  be a rooted tree in  $\mathcal{T}_r(\pi)$  with  $f(T)$  being a maximal element in  $\{f(T), T \in \mathcal{T}_r(\pi)\}$ . We may assume that  $v_0 = r$  is the root of tree  $T$ . Put  $V_i = \{v : d(v, v_0) = i\}$  for  $i = 0, \dots, p+1$  such that  $V(T) = \bigcup_{i=0}^{p+1} V_i$ . Denote by  $|V_i| = s_i$  for  $i = 1, \dots, p+1$  and  $s_0 = 0$ . We now can relabel the vertices of  $V(T)$  by the recursion method. For  $V_0$ , relabel  $v_0$  by  $v_{01}$  which is the root of tree  $T$ . For  $V_1$ , which consists of all neighbors of vertices in  $V_0$  can be relabeled

$$v_{11}, \dots, v_{1,s_1},$$

which satisfy the following conditions:

$$f_T(v_{11}) \geq f_T(v_{12}) \geq \dots \geq f_T(v_{1,s_1})$$

and

$$f_T(v_{1i}) = f_T(v_{1j}) \text{ implies } d_T(v_{1i}) \geq d_T(v_{1j}) \text{ for } 1 \leq i < j \leq s_1.$$

Moreover,  $s_1 = d_T(v_{01})$ . Generally, we assume that all vertices of  $V_i$  are relabeled  $\{v_{i1}, \dots, v_{i,s_i}\}$  for  $i = 1, \dots, t$ . Now consider all vertices in  $V_{t+1}$ . Since  $T$  is tree, it is easy to see that

$$s_{t+1} = |V_{t+1}| = d_T(v_{t1}) + \dots + d_T(v_{t,s_t}) - s_t.$$

Hence for  $1 \leq r \leq s_t$ , all neighbors in  $V_{t+1}$  of  $v_{tr}$  are relabeled

$$v_{t+1, d_T(v_{t1}) + \dots + d_T(v_{t,r-1}) - (r-1) + 1}, \dots, v_{t+1, d_T(v_{t1}) + \dots + d_T(v_{t,r}) - r},$$

which satisfy the conditions:

$$f_T(v_{t+1,i}) \geq f_T(v_{t+1,j})$$

and

$$f_T(v_{t+1,i}) = f_T(v_{t+1,j}) \text{ implies } d_T(v_{t+1,i}) \geq d_T(v_{t+1,j})$$

for  $d_T(v_{t1}) + \dots + d_T(v_{t,r-1}) - (r-1) + 1 \leq i < j \leq d_T(v_{t1}) + \dots + d_T(v_{t,r}) - r$ . In this way, we relabeled all vertices of  $V(T) = \cup_{i=0}^{p+1} V_i$ . Therefore, we are able to define a well-ordering of vertices in  $V(T)$  as follows:

$$v_{ik} \leq v_{jl}, \text{ if } 0 \leq i < j \leq p+1 \text{ or } i = j \text{ and } 1 \leq k < l \leq s_i.$$

We have the following

**Claim:** This well-ordering is a BFS-ordering of tree  $T$ . In other words,  $T$  is isomorphic to  $T^*$  by Proposition 2.2.

**Proof. of Claim** From the construction of well-ordering, it only needs to show that the following assertion holds:

$$f_T(v_{01}) \geq f_T(v_{11}) \geq \dots \geq f_T(v_{1,s_1}) \geq f_T(v_{21}) \geq \dots \geq f_T(v_{2,s_2}) \geq \dots \geq f_T(v_{p+1,s_{p+1}})$$

and

$$d_T(v_{01}) = d_0, d_T(v_{11}) = d_{s_0+1}, \dots, d_T(v_{1,s_1}) = d_{s_0+s_1},$$

$$d_T(v_{21}) = d_{s_0+s_1+1}, \dots, d_T(v_{2,s_2}) = d_{s_0+s_1+s_2}, \dots,$$

$$d_T(v_{p+1,1}) = d_{s_0+\dots+s_{p+1}}, \dots, d_T(v_{p+1,s_{p+1}}) = d_{n-1}.$$

Therefore, we only need to show that

$$f_T(v_{h1}) \geq f_T(v_{h2}) \geq \cdots \geq f_T(v_{h,s_h}) \geq f_T(v_{h+1,1}) \quad (1)$$

and

$$d_T(v_{h1}) \geq d_T(v_{h2}) \geq \cdots \geq d_T(v_{h,s_h}) \geq d_T(v_{h+1,1}) \quad (2)$$

for  $h = 0, \dots, p + 1$ .

We show (1) and (2) by the induction on  $h$ . For  $h = 0$ , clearly, (1) holds since  $f_T(v_{01}) = n \geq f_T(v_{11})$ . By Lemma 3.5, (2) holds. Assume that (1) and (2) hold for  $h = t$ . We consider  $h = t + 1$  and using the contradiction method. Suppose that  $f_T(v_{t+1,i}) < f_T(v_{t+1,j})$  for  $1 \leq i < j \leq s_{t+1}$ . Then by the construction of vertex labeling, there exist two internal paths  $P(v_{t+1,i}, v_{t-k,i_{k+1}}) = \{v_{t+1,i}, v_{t,i_1}, \dots, v_{t-k+1,i_k}, v_{t-k,i_{k+1}}\}$  and  $P(v_{t+1,j}, v_{t-k,i_{k+1}}) = \{v_{t+1,j}, v_{t,j_1}, \dots, v_{t-k+1,j_k}, v_{t-k,i_{k+1}}\}$  with  $i_l \leq j_l$  for  $l = 1, \dots, k$ . Hence,  $f_T(v_{t-l+1,i_l}) \geq f_T(v_{t-l+1,j_l})$  by the induction hypothesis. Let  $T'$  be a tree with root  $v_{01}$  from  $T$  by adding the edges  $v_{t,i_1}v_{t+1,j}$  and  $v_{t,j_1}v_{t+1,i}$  and deleting the edges  $v_{t,i_1}v_{t+1,i}$  and  $v_{t,j_1}v_{t+1,j}$ . By Lemmas 3.1 and 3.2,  $T'$  is a rooted tree with the same degree sequence  $\pi$  and  $f(T) \prec^w f(T')$ . This contradicts  $T$  being a maximal element in  $\Omega(\pi)$ . So

$$f_T(v_{t+1,1}) \geq f_T(v_{t+1,2}) \geq \cdots \geq f_T(v_{t+1,s_{t+1}}).$$

Moreover, we will prove that  $f_T(v_{t+1,s_{t+1}}) \geq f_T(v_{t+2,1})$ . In fact, if  $f_T(v_{t+1,s_{t+1}}) < f_T(v_{t+2,1})$ , then by the induction prothesis and the construction of the vertex labeling, there are two paths  $P(v_{t+1,s_{t+1}}, v_{01}) = \{v_{t+1,s_{t+1}}, \dots, v_{1,s_1}, v_{01}\}$  and  $P(v_{t+2,1}, \dots, v_{11}, v_{01})$  such that  $f_T(v_{i,s_i}) \geq f_T(v_{i+1,1})$  for  $i = 1, \dots, t$ . Therefore, by Lemmas 3.1 and 3.2,  $f(T)$  is not a maximal element in  $\Omega(\pi)$ . It is a contradiction. Hence (1) holds for  $h = t + 1$ .

Suppose that  $d(v_{t+1,i}) < d(v_{t+1,j})$  for  $1 \leq i < j \leq s_{t+1}$ . Then by (1) and the construction of vertex labeling of tree  $T$ , we have  $f_T(v_{t+1,i}) \geq f_T(v_{t+1,j})$  and let  $b = d(v_{t+1,j}) - d(v_{t+1,i}) > 0$ . By the induction hypothesis, there are two internal disjoint paths  $P(v_{t+1,i}, v_{t-k,i_{k+1}}) = \{v_{t+1,i}, v_{t,i_1}, \dots, v_{t-k+1,i_k}, v_{t-k,i_{k+1}}\}$  and  $P(v_{t+1,j}, v_{t-k,i_{k+1}}) = \{v_{t+1,j}, v_{t,j_1}, \dots, v_{t-k+1,j_k}, v_{t-k,i_{k+1}}\}$  such that  $f_T(v_{t-h,i_l}) \geq f_T(v_{t-h,j_l})$  for  $l = 1, \dots, k$ .

Denote by  $s = d(v_{t+1,j}) - d(v_{t+1,i})$ . Let  $T'$  be a tree with root  $r$  obtained from  $T$  by deleting the  $s$  edges  $v_{t+1,j}x_l$  and adding edges  $v_{t+1,i}x_l$ ,  $l = 1, \dots, s$ , where  $\{x_1, \dots, x_s\}$  are children of  $v_{t+1,j}$ . Then by Lemmas 3.3 and 3.4, we have  $T' \in \mathcal{T}_r(\pi)$  and  $f(T) \prec^w f(T')$  which contradicts to  $f(T)$  being a maximal element in  $\Omega(\pi)$ . Therefore

$$d_T(v_{t+1,1}) \geq d_T(v_{t+1,2}) \geq \dots \geq d_T(v_{t+1,s_{t+1}}).$$

Similarly, we also show that  $d_T(v_{t+1,s_{t+1}}) \geq d_T(v_{t+2,1})$ . Hence (2) holds for  $h = t + 1$  also. Therefore by the induction method, (1) and (2) hold for  $h = 0, \dots, p + 1$ , which implies the claim holding. ■

Hence by Claim,  $T$  has a BFS-ordering. By Proposition 2.2,  $T$  is isomorphic to  $T^*$  and  $f(T) = f(T^*)$ . So  $T^*$  is only one tree in  $\mathcal{T}_r(\pi)$  up to isomorphism such that  $f(T^*)$  is only one maximum element in  $\Omega(\pi)$ . Then we complete the proof. ■

**Corollary 3.7** *Let  $T$  be a rooted tree in  $\mathcal{T}_r(\pi)$ . Then the following conditions are equivalent:*

- (1)  $T$  has a BFS-ordering;
- (2)  $f(T)_\dagger = f(T^*)_\dagger$ ;
- (3)  $T$  is isomorphic to  $T^*$ .

## 4 The minimum Wiener index in $\mathcal{T}(\pi)$

In order to prove our main results in this paper, we also need some notations and lemmas. For any vertex  $v$  of a tree  $T = (V, E)$ , denote by  $W_T(v) = \sum_{u \in V(T)} d_T(v, u)$  and which is called the *distance of the vertex  $v$* . A *centroid vertex* of  $T$  is defined to be such that its distance is no more than the distance of any other vertex in  $T$ . In other words,  $v$  is called a centroid of  $T$  if  $W_T(v) \leq W_T(u)$  for all  $u \neq v$ .

**Lemma 4.1** *Let  $r$  be both the root and a centroid of a rooted tree  $T$  of order  $n$  in  $\mathcal{T}_r(\pi)$ . Then for any vertex  $u$  other than  $r$ ,  $f_T(u) \leq \frac{n}{2}$ .*

**Proof.** Let  $v$  (which may be  $r$ ) be the parent of vertex  $u$ . Since  $r$  is a centroid of the tree  $T$ ,  $W_T(r) \leq W_T(u)$ . By Exercise 6.22 in [14],  $W_T(v) \leq W_T(u)$ . By the definition of  $W_T(u)$  and  $f_T(u)$ , we have

$$0 \leq W_T(u) - W_T(v) = (n - f_T(u)) - f_T(u).$$

Hence  $f_T(u) \leq \frac{n}{2}$ . ■

**Lemma 4.2** *Let  $r$  be both the root and a centroid of a rooted tree  $T$  of order  $n$  in  $\mathcal{T}_r(\pi)$ . Denote by  $\varphi(x) = t(n - t)$ . Then*

$$W(T) = \sum_{u \in V(T) - \{r\}} \varphi(f_T(u))$$

**Proof.** By [21] (see [3] also), it is easy to see that

$$W(T) = \sum_{e=uv \in E(T)} n_1(e)n_2(e),$$

where  $n_1(e)$  and  $n_2(e)$  are the number of the vertices of two connected components of  $T$  containing  $u$  and  $v$  respectively. Then  $n_1(e) + n_2(e) = n$ . Since for each edge  $e = uv \in E(T)$ , one vertex of  $\{u, v\}$  must be the parent of the other vertex, say  $v$  is the parent of  $u$ . Hence each edge  $e = uv \in E(T)$  we can see that there exists a 1-to-1 correspondence between the edge set  $E(T) = \{e = uv, v \text{ is the parent of } u\}$  and  $V(T) - \{r\}$ . Therefore for  $e = uv$  with  $v$  being the parent of  $u$ ,  $n_1(e) = f_T(u)$  and  $n_2(e) = n - f_T(u)$ . Then

$$W(T) = \sum_{e=uv \in E(T)} n_1(e)n_2(e) = \sum_{u \in V(T) - \{r\}} f_T(u)(n - f_T(u)) = \sum_{u \in V(T) - \{r\}} \varphi(f_T(u)).$$

■

The following Lemma from Proposition 4.B.2 in [17].

**Lemma 4.3** ([17]) *Let  $x = (x_1, \dots, x_n)$  and  $y = (y_1, \dots, y_n)$  be two nonnegative integer sequences. If  $x \preceq^w y$ , then  $\sum_{i=1}^n \phi(x_i) \geq \sum_{i=1}^n \phi(y_i)$  for all continuous increasing concave functions with equality if and only if  $x_{\uparrow} = y_{\uparrow}$ .*

**Theorem 4.4** *Let  $r$  be both the root and a centroid of a rooted tree  $T$  of order  $n$ . Let  $r'$  be both the root and a centroid of a tree  $T'$  of order  $n$ . If  $f(T) \preceq^w f(T')$ , then  $W(T) \geq W(T')$  with equality if and only if  $f(T)_{\uparrow} = f(T')_{\uparrow}$ .*

**Proof.** Clearly  $\varphi(t) = t(n-t)$  is continuous increasing concave functions for  $0 \leq t \leq \frac{n}{2}$ . By Lemma 4.1,  $f_T(u) \leq \frac{n}{2}$  for  $u \in V(T) - \{r\}$  and  $f_{T'}(u) \leq \frac{n}{2}$  for  $u \in V(T') - \{r'\}$ . Note that  $f_T(r) = f_{T'}(r') = n$ . Thus  $(f_T(u), u \in V(T) \setminus \{r\}) \preceq^w (f_{T'}(u'), u' \in V(T') \setminus \{r'\})$ . Hence the assertion follows from Lemmas 4.2 and 4.3. ■

Now we are ready to prove the main result in this paper.

**Proof. of Theorem 1.2.** Let  $T = (V, E)$  be any tree in  $\mathcal{T}(\pi)$  and let  $T$  be rooted at its a centroid  $r$ . By Theorem 3.6,  $f(T) \preceq^w f(T^*)$ . For the root  $r$  of  $T$  and the root  $v_{01}$  of  $T^*$ , we have  $f_T(r) = f_T(v_{01}) = n$ . Hence  $(f_T(u), u \in V(T) - \{r\}) \preceq^w (f_{T^*}(u), u \in V(T^*) - \{v_{01}\})$ . Moreover, it is easy to see that  $v_{01}$  is a centroid of  $T^*$ . Hence by Lemma 4.1,  $f_T(u) \leq \frac{n}{2}$  for  $u \in V(T) - \{r\}$  and  $f_{T^*}(u) \leq \frac{n}{2}$  for  $u \in V(T^*) - \{v_{01}\}$ . Clearly  $\varphi(t) = t(n-t)$  is continuous increasing concave functions for  $0 \leq t \leq \frac{n}{2}$ . By Lemmas 4.2 and 4.3, we have

$$W(T) = \sum_{u \in V(T) - \{r\}} \varphi(f_T(u)) \geq \sum_{u \in V(T^*) - \{v_{01}\}} \varphi(f_{T^*}(u)) = W(T^*)$$

with equality if and only if  $(f_T(u), u \in V(T) - \{r\})_{\uparrow} = (f_{T^*}(u), u \in V(T^*) - \{v_{01}\})_{\uparrow}$ . By Theorem 3.6,  $T$  must be isomorphic to  $T^*$ . ■

From the proof of Theorems 1.2 and 3.6, it is easy to see that we have the following

**Corollary 4.5** *For a given tree degree sequence  $\pi$ , A tree  $T$  has the minimum Wiener index in  $\mathcal{T}(\pi)$  if and only if  $T$  has a BFS-ordering. Moreover, the BFS-ordering is consistent with the vector  $f(T)$  of  $T$  with a centroid as the root in such a way that  $f_T(u) \geq f_T(v)$  implies  $u \preceq v$ .*

## 5 The minimum Wiener index in some classes of trees

Before we derive the minimum Wiener index in some classes of trees, we need the following result

**Proposition 5.1** *Let  $\pi = (d_0, \dots, d_{n-1})$  and  $\pi' = (d'_0, \dots, d'_{n-1})$  be two nonincreasing graphic degree sequences. If  $\pi \preceq \pi'$ , then there exists a series of graphic degree sequences  $\pi_1, \dots, \pi_k$  such that  $\pi \preceq \pi_1 \preceq \dots \preceq \pi_k \preceq \pi'$ , and only two components of  $\pi_i$  and  $\pi_{i+1}$  are different from 1.*

**Proof.** Since  $\pi \preceq \pi'$  and  $\pi \neq \pi'$ , we may assume that  $d_i = d'_i$  for  $i = 0, \dots, p - 1$ ;  $d_p < d'_p$ ;  $d_i \leq d'_i$  for  $i = p + 1, \dots, q - 1$  and  $d_q > d'_q$ , where  $0 \leq p < q \leq n - 1$ . Let  $\pi_1 = (d_0^{(1)}, \dots, d_{n-1}^{(1)})$  with  $d_i^{(1)} = d'_i$  for  $i \neq p, q$ ,  $d_p^{(1)} = d'_p - 1$  and  $d_q^{(1)} = d'_q + 1$ . Thus  $\pi \preceq \pi_1 \preceq \pi'$ . Moreover, there are only two components of  $\pi_1$  and  $\pi'$  which are different from 1. Observe that  $\min\{p, d'_p\} + \min\{q, d'_q\} - (\min\{p, d_p^{(1)}\} + \min\{q, d_q^{(1)}\}) \leq 0$  and  $\min\{q, d'_q\} - \min\{q, d_q^{(1)}\} \leq 0$ . By [5] (see also [1]),  $\pi'$  is graphic if and only if

$$\sum_{i=0}^k d'_i \leq k(k+1) + \sum_{k+1}^{n-1} \min\{k+1, d'_i\}, \text{ for } k = 0, \dots, n-1.$$

Hence it is easy to show that

$$\sum_{i=0}^k d_i^{(1)} \leq k(k+1) + \sum_{k+1}^{n-1} \min\{k+1, d_i^{(1)}\}, \text{ for } k = 0, \dots, n-1.$$

Then  $\pi_1$  is graphic degree sequence. By repeating the above procedures, the assertion holds. ■

**Lemma 5.2** *Let  $T$  be a rooted tree with root  $r$ . Suppose that  $u$  and  $v$  are successors of  $w$  and there are two internal disjoint paths  $P(u, w) = (u, u_1, \dots, u_k, w)$  and  $P(v, w) = (v, v_1, \dots, v_l, w)$  with  $0 \leq k \leq l$ . If  $d_T(u) \geq d_T(v) \geq 2$ ; and  $f_T(u) \geq f_T(v)$  and  $f_T(u_i) \geq f_T(v_i)$  for  $i = 1, \dots, k$ . Let  $x$  be a child of  $v$  and let  $T'$  be the root tree with root  $r$  obtained from  $T$  by deleting the edge  $vx$  and adding the edge  $ux$ .*



(1) Let  $\pi$  and  $\pi'$  be the degree sequences of  $T$  and  $T'$  respectively. Then  $\pi \preceq \pi'$  and only two components of  $\pi$  and  $\pi'$  are different from 1.

(2)  $f(T) \prec^w f(T')$ .

(3) If  $r$  is a centroid of  $T$  and  $T'$ , respectively, then  $W(T) > W(T')$ .

**Proof.** (1) Clearly  $d_{T'}(u) = d_T(u) + 1$ ,  $d_{T'}(v) = d_T(v) - 1$  and  $d_{T'}(y) = d_T(y)$  for any  $y \in V \setminus \{u, v\}$ . Since  $d_T(u) \geq d_T(v)$ , we have  $\pi \preceq \pi'$ . Moreover, only two components of  $\pi$  and  $\pi'$  are different from 1.

(2) Put  $b = f_T(x) > 0$ . By the definition, we have  $f_{T'}(u) = f_T(u) + b$ ,  $f_{T'}(u_i) = f_T(u_i) + b$  for  $i = 1, \dots, k$ ;  $f_{T'}(v) = f_T(v) - b$ , and  $f_{T'}(v_i) = f_T(v_i) - b$  for  $i = 1, \dots, l$ . Since  $f_T(u) \geq f_T(v)$  and  $f_T(u_i) \geq f_T(v_i)$  for  $i = 1, \dots, k$ , by Proposition 2.3, we have  $(f_T(u), f_T(u_1), \dots, f_T(u_k), f_T(v), f_T(v_1), \dots, f_T(v_l)) \prec^w (f_{T'}(u), f_{T'}(u_1), \dots, f_{T'}(u_k), f_{T'}(v), f_{T'}(v_1), \dots, f_{T'}(v_l))$ . On the other hand,  $f_T(y) = f_{T'}(y)$  for any  $y \in V(T) \setminus \{u, u_1, \dots, u_k, v, v_1, \dots, v_l\}$ . Hence by Proposition 2.4,  $f(T) \prec^w f(T')$ .

(3) It follows from (2) and Theorem 4.4. ■

**Theorem 5.3** Let  $\pi$  and  $\pi'$  be two tree degree sequences. Let  $T^*(\pi)$  and  $T^*(\pi')$  be two trees with the minimum Wiener indices in  $\mathcal{T}(\pi)$  and  $\mathcal{T}(\pi')$ , respectively. If  $\pi \preceq \pi'$ , then  $W(T^*(\pi)) \geq W(T^*(\pi'))$  with equality if and only if  $\pi = \pi'$ .

**Proof.** By Proposition 5.1, without loss of generality, we may assume that  $\pi \neq \pi'$  and  $\pi = (d_0, \dots, d_{n-1})$  and  $\pi' = (d'_0, \dots, d'_{n-1})$  with  $d_i = d'_i$  for  $i \neq p, q$ , and  $d_p = d'_p - 1$ ,  $d_q = d'_q + 1$ ,  $0 \leq p < q \leq n - 1$ . By Corollary 4.5, the BFS-ordering of a rooted  $T^*$  is consistent with the vector  $f(T^*(\pi))$  of  $T^*(\pi)$  in such a way that  $f_{T^*(\pi)}(u) > f_{T^*(\pi)}(v)$  implies  $u \triangleleft v$ . Hence we may assume that the vertices of  $T^*(\pi)$  are ordered  $\{v_0, \dots, v_{n-1}\}$  such that  $d(v_i) = d_i$  for  $i = 0, \dots, n - 1$  and  $f_{T^*(\pi)}(v_0) \geq f_{T^*(\pi)}(v_1) \geq \dots \geq f_{T^*(\pi)}(v_{n-1})$  with  $r$  being a root of  $T^*(\pi)$ . Moreover, since  $d_q = d'_q + 1 \geq 2$ , there exists a vertex  $v_k$  with  $k > q$  such that  $v_k v_q \in E(T^*(\pi))$  and  $v_k v_p \notin E(T^*(\pi))$ . Let  $T_1$  be a root tree obtained from  $T^*(\pi)$  by adding the edge  $v_k v_p$  and deleting the  $v_k v_q$ . Then the degree sequence of  $T_1$  is  $\pi'$  and  $T_1 \in \mathcal{T}_r(\pi')$ . From the construction of  $T^*(\pi)$ , it is easy to prove that  $T_1$  satisfies the condition of Lemma 5.2. Hence by (2) in Lemma 5.2, we have  $f(T^*(\pi)) \prec^w f(T_1)$ . By Theorem 3.6, we have  $f(T_1) \preceq^w$

$f(T^*(\pi'))$ . Since the root of tree  $T^*(\pi')$  is also an its centroid, we have  $f(T_1) \preceq^w f(T^*(\pi'))$ . Hence  $f(T^*(\pi)) \prec^w f(T^*(\pi'))$ . By Theorem 4.4,  $W(T^*(\pi)) \geq W(T^*(\pi'))$  with equality if and only if  $\pi = \pi'$ . ■

From Theorems 1.2 and 5.3, we may deduce extremal graphs with the minimum Wiener index in some class of graphs. For example, let  $\mathcal{T}_{n,s}^{(1)}$  be the set of all trees of order  $n$  with  $s$  leaves,  $\mathcal{T}_{n,\Delta}^{(2)}$  be the set of all trees of order  $n$  with the maximum degree  $\Delta$ ,  $\mathcal{T}_{n,\alpha}^{(3)}$  be the set of all trees of order  $n$  with the independence number  $\alpha$  and  $\mathcal{T}_{n,\beta}^{(4)}$  be the set of all trees of order  $n$  with the matching number  $\beta$ .

**Corollary 5.4** *Let  $\mathcal{T}_{n,s}^{(1)}$  be the set of all trees of order  $n$  with  $s$  leaves (i.e., pendent vertices). A tree  $T_1$  has the minimum Wiener index in  $\mathcal{T}_{n,s}^{(1)}$  if and only if  $T_1$  is a star with paths of almost the same length to each of its  $s$  leaves (in other words, let  $n - 1 = sq + t, 0 \leq t < s$  and  $T_1$  is obtained from  $t$  paths of order  $q + 2$  and  $s - t$  paths of order  $q + 1$  by identifying one end of the  $s$  paths).*

**Proof.** Let  $T_1$  be a tree in  $\mathcal{T}_{n,s}^{(1)}$  having the minimum Wiener index in  $\mathcal{T}_{n,s}^{(1)}$ . We assume that the nonincreasing degree sequence of  $T_1$  is  $\pi = (d_0, \dots, d_{n-1})$ . Thus  $d_{n-s-1} > 1$  and  $d_{n-s} = \dots = d_{n-1} = 1$ . Let  $T^*(\pi)$  have a BFS ordering in the set  $\mathcal{T}(\pi)$ . Then by Theorem 3.6, we have  $f(T_1) \preceq^w f(T^*(\pi))$ . Hence by Theorem 1.2,  $W(T_1) \geq W(T^*(\pi))$  with equality if and only if  $T_1$  is isomorphic to  $T^*(\pi)$ . Let  $T^*(\pi)$  have a BFS ordering tree with the degree sequence  $\pi' = (s, 2, \dots, 2, 1, \dots, 1)$ , where there are a number  $s$  of 1s in  $\pi'$ . By Proposition 2.2,  $T^*(\pi')$  is a star with paths of almost the same length to each of its  $s$  leaves. Moreover, it is easy to see that  $\pi \preceq^w \pi'$ . By Theorem 5.3, we have  $W(T^*(\pi)) \geq W(T^*(\pi'))$  with equality if and only if  $\pi = \pi'$ . Note that  $T^*(\pi') \in \mathcal{T}_{n,s}^{(1)}$ , then

$$W(T_1) \geq W(T^*(\pi)) \geq W(T^*(\pi)) \geq W(T^*(\pi')) \geq W(T_1).$$

Hence  $W(T_1) = W(T^*(\pi)) = W(T^*(\pi)) = W(T^*(\pi')) = W(T_1)$  and  $T_1$  is isomorphic to  $T^*(\pi')$ . ■

The following result has been proved by Fischermann et al. [6] and Jelen and Triesch [13] independently.

**Corollary 5.5** ([6], [13]) Let  $\mathcal{T}_{n,\Delta}^{(2)}$  be the set of all trees of order  $n$  with the maximum degree  $\Delta$ . A tree  $T_2$  has the minimum Wiener index in  $\mathcal{T}_{n,\Delta}^{(2)}$  with  $\Delta \geq 3$  if and only if  $T_2$  is  $T^*(\pi')$  in Theorem 1.2 with degree sequence  $\pi'$  which is as follows: Denote  $p = \lceil \log_{(\Delta-1)} \frac{n(\Delta-2)+2}{\Delta} \rceil - 1$  and  $n - \frac{\Delta(\Delta-1)^{p-2}}{\Delta-2} = (\Delta-1)r + q$  for  $0 \leq q < \Delta - 1$ . If  $q = 0$ , put  $\pi' = (\Delta, \dots, \Delta, 1, \dots, 1)$  with the number  $\frac{\Delta(\Delta-1)^{p-1}-2}{\Delta-2} + r$  of degree  $\Delta$ . If  $1 \leq q$ , put  $\pi' = (\Delta, \dots, \Delta, q, 1, \dots, 1)$  with the number  $\frac{\Delta(\Delta-1)^{p-1}-2}{\Delta-2} + r$  of degree  $\Delta$ .

**Proof.** Let  $T_2$  be a tree of order  $n$  with the maximum degree  $\Delta$  such that  $T_2$  has the minimum Wiener index in  $\mathcal{T}_{n,\Delta}^{(2)}$ . Then  $W(T) \geq W(T_2)$  for any tree  $T \in \mathcal{T}_{n,\Delta}^{(2)}$ . Denoted by  $\pi = (d_0, \dots, d_{n-1})$  the nonincreasing degree sequence of  $T_2$ . Let  $T^*(\pi)$  have a BFS-ordering in the set  $\mathcal{T}(\pi)$ . Then by Corollary 4.5,  $W(T_2) \geq W(T^*(\pi))$ . Assume that  $T^*(\pi')$  has  $p + 2$  layers. Then there is a vertex in layer 0 (i.e., root), there are exactly  $\Delta$  vertices in layer 1, there are exactly  $\Delta(\Delta - 1)$  vertices in layer 2,  $\dots$ , there are exactly  $\Delta(\Delta - 1)^{p-1}$  vertices in layer  $p$  and there are at most  $\Delta(\Delta - 1)^p$  vertices in layer  $p + 1$ . Hence

$$1 + \Delta + \Delta(\Delta - 1) + \dots + \Delta(\Delta - 1)^{p-1} < n \leq 1 + \Delta + \Delta(\Delta - 1) + \dots + \Delta(\Delta - 1)^p.$$

Thus

$$\frac{\Delta(\Delta - 1)^p - 2}{\Delta - 2} < n \leq \frac{\Delta(\Delta - 1)^{p+1} - 2}{\Delta - 2}.$$

Hence

$$p = \lceil \log_{(\Delta-1)} \frac{n(\Delta - 2) + 2}{\Delta} \rceil - 1$$

and there exist integers  $r$  and  $0 \leq q < \Delta - 1$  such that

$$n - \frac{\Delta(\Delta - 1)^p - 2}{\Delta - 2} = (\Delta - 1)r + q.$$

Therefore degrees of all vertices from layer 0 to layer  $p - 1$  are  $\Delta$  and there are  $r$  vertices in layer  $p$  with degree  $\Delta$ . Denote by  $m = \frac{\Delta(\Delta-1)^{p-1}-2}{\Delta-2} + r - 1$ . Then there are  $m + 1$  vertices with degree  $\Delta$  in  $T^*(\pi')$ . Hence the degree sequence of  $T^*(\pi') \in \mathcal{T}_{n,\Delta}$  is  $\pi' = (d'_0, \dots, d'_{n-1})$  with  $d'_0 = \dots = d'_m = \Delta$ ,  $d'_{m+1} = \dots = d'_{n-1} = 1$  for  $q = 0$ ; and is  $\pi' = (d'_0, \dots, d'_{n-1})$  with  $d'_0 = \dots = d'_m = \Delta$ ,  $d'_{m+1} = q$ ,  $d'_{m+2} = \dots = d'_{n-1} = 1$ .

Then  $W(T^*(\pi')) \geq W(T_2)$ . Further, it follows from  $d_0 \leq \Delta$  that  $\sum_{i=0}^k d_i \leq \sum_{i=0}^k d'_i$  for  $k = 0, \dots, m$ . Moreover, by  $d'_i = 1 \leq d_i$  for  $k = m+2, \dots, n-1$ , we have

$$\sum_{i=0}^k d_i = 2(n-1) - \sum_{i=k+1}^{n-1} d_i \leq 2(n-1) - \sum_{i=k+1}^{n-1} d'_i = \sum_{i=0}^k d'_i$$

for  $k = m+1, \dots, n-1$ . Thus  $\pi \preceq \pi'$ . Hence by Theorems 5.3,  $W(T(\pi)) \geq W(T^*(\pi'))$  with equality if and only if  $T = T^*$ . Therefore

$$W(T_2) \geq W(T^*(\pi)) \geq W(T^*(\pi')) \geq W(T_2).$$

So the assertion holds. ■

Dankelmann [2] presented a lower bound for the Wiener index of graphs in terms of the independence number and order. Here, we present a sharp lower bound for the Wiener index of trees in terms of the independence number and order.

**Corollary 5.6** *Let  $\mathcal{T}_{n,\alpha}^{(3)}$  be the set of all trees of order  $n$  with the independence number  $\alpha$ . A tree  $T_3$  has the minimum Wiener index in  $\mathcal{T}_{n,\alpha}^{(3)}$  if and only if  $T_3$  is  $T^*(\pi')$  in Theorem 1.2 with degree sequence  $\pi' = (\alpha, 2, \dots, 2, 1, \dots, 1)$  the numbers  $n - \alpha - 1$  of 2 and  $\alpha$  of 1 (i.e.,  $T_3$  is obtained from the star graph  $K_{1,\alpha}$  by adding a pendent edge to each of  $n - \alpha - 1$  pendent vertices of  $K_{1,\alpha}$ ).*

**Proof.** Let  $T_3$  have the minimum Wiener index in  $\mathcal{T}_{n,\alpha}^{(3)}$ . Denote by  $\pi = (d_0, \dots, d_{n-1})$  be the nonincreasing degree sequence of  $T_3$ . Then by Theorem 1.2,  $W(T_3) \geq W(T^*(\pi))$ . Let  $I$  be an independent set of  $T_3$  with the independence number  $\alpha$ . If there exists a pendent vertex  $u$  of degree 1 with  $u \notin I$ , then there exists a vertex  $v \in I$  with  $(u, v) \in E(T_3)$ . Hence  $I \cup \{u\} \setminus \{v\}$  is an independent set of  $T_3$  with the size  $\alpha$ . Therefore, there exists an independent set of  $T_3$  with size  $\alpha$  which contains all pendent vertices of  $T_3$ . Hence  $T_3$  has at most  $\alpha$  pendent vertices, which implies  $d_{n-\alpha-1} \geq 2$ . Hence it is easy to see that  $\pi \preceq \pi'$ . Therefore by Theorem 5.3, we have  $W(T^*(\pi)) \geq W(T^*(\pi'))$  with equality if and only if  $\pi = \pi'$ . By  $T^*(\pi') \in \mathcal{T}_{n,\alpha}^{(3)}$ , we have  $W(T^*(\pi')) \geq W(T_3)$ . Therefore

$$W(T_3) \geq W(T^*(\pi)) \geq W(T^*(\pi')) \geq W(T_3).$$

So the assertion holds. ■

**Corollary 5.7** Let  $\mathcal{T}_{n,\beta}^{(4)}$  be the set of all trees of order  $n$  with the matching number  $\beta$ . A tree  $T_4$  has the minimum Wiener index in  $\mathcal{T}_{n,\beta}^{(4)}$  if and only if  $T_4$  is  $T^*$  in Theorem 1.2 with degree sequence  $\pi^* = (n - \beta, 2, \dots, 2, 1, \dots, 1)$  and the number  $n - \beta$  of 1 (i.e.,  $T_4$  is obtained from the star graph  $K_{1,n-\beta}$  by adding a pendent edge to each of  $\beta - 1$  pendent vertices of  $K_{1,n-\beta}$ ).

**Proof.** The proof is similar to that of Corollary 5.6 and is omitted. ■

### Acknowledgements

The authors would like to thank the anonymous referees very much for valuable suggestions, corrections and comments which results in a great improvement of the original manuscript. In particular, one referee gives a clear and short construction of  $T^*$  and provides references [7], [12], [18], [19] and [20].

### References

- [1] J. A. Bondy and U. S. R. Murty, *Graph theory with applications*, Macmillan Press, New York, 1976.
- [2] P. Dankelmann, Average distance and independence number, *Discrete Appl. Math.* **51** (1994) 75–83.
- [3] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
- [4] R. C. Entringer, D. E. Jackson and D. A. Snyder, Distance in graphs, *Czechoslovak Math. J.* **26** (1976) 283–296.
- [5] P. Erdős and T. Gallai, Graphs with prescribed degrees of vertices (Hungarian) *Mat. Lapok* **11** (1960) 264–274.
- [6] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Szekely and L. Volkmann, Wiener index versus maximum degree in trees, *Discrete Appl. Math.* **122** (2002) 127–137.
- [7] M. Fischermann, D. Rautenbach and L. Volkmann, Extremal trees with respect to dominance order, *Ars Comb.* **76** (2005) 249–255.

- [8] I. Gutman, W. Linert, I. Lukovits and Ž Tomović, The multiplicative version of the Wiener index, *J. Chem. Inf. Comput. Sci.* **40** (2000) 113–116.
- [9] I. Gutman and J. H. Potgieter, Wiener index and intermolecular forces, *J. Serb. Chem. Soc.* **62** (1997) 185–192.
- [10] I. Gutman, Y. N. Yeh, S. L. Lee and J. C. Chen, Wiener numbers of dendrimers, *MATCH Commun. Math. Comput. Chem.* **30** (1994) 103–115.
- [11] H. Hosoya, Topological index, A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **4** (1971) 2332–2339.
- [12] D. J. Klein and D. Babiacutec, Partial orderings in chemistry, *J. Chem. Inf. Comput. Sci.* **37** (1997) 656–671.
- [13] F. Jelen and E. Triesch, Superdominance order and distance of trees with bounded maximum degree, *Discrete Appl. Math.* **125** (2003) 225–233.
- [14] L. Lovász, *Combinatorial Problems and Exercises*, 2nd Edition, North-Holland, Amsterdam, 1993.
- [15] I. Lukovits, General formulas for the Wiener index, *J. Chem. Inf. Comput. Sci.* **31** (1991) 503–507.
- [16] R. Merris, Laplacian matrices of graphs: a survey, *Linear Algebra Appl.* **197/198** (1994) 143–176.
- [17] A. W. Marshall and I. Olkin, *Inequalities: Theory of Majorization and Its Applications*, *Mathematics in Science and Engineering*, vol.143, Academic Press, New York, 1979.
- [18] O. E. Polansky and D. Bonchev, The Wiener number of graphs. I. general theory and changes due to some graph operations *MATCH Commun. Math. Comput. Chem.* **21** (1986) 133–186.
- [19] D. H. Rouvray and R. B. King, *Topology in Chemistry*, Horwood Pub., Chichester, 2002.
- [20] E. Ruch and I. Gutman, The branching extent of graphs, *J. Comb. Inf. Sys. Sci.* **4** (1979) 285–295.
- [21] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [22] X. D. Zhang, The Laplacian spectral radii of trees with degree sequences, *Discrete Math.* (2007) doi:10.1016/j.disc.2007.06.017.