

# The extremal values of the Wiener index of a tree with given degree sequence

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## Abstract

The Wiener index of a graph is the sum of the distances between all pairs of vertices, it has been one of the main descriptors that correlate a chemical compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In [M. Fischermann, A. Hoffmann, D. Rautenbach, L.A. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Discrete Appl. Math.* 122 (1–3) (2002) 127–137], the tree that minimizes the Wiener index among trees of given maximal degree is studied. We characterize trees that achieve the maximum and minimum Wiener index, given the number of vertices and the degree sequence.

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*Keywords:* Tree; Wiener index; Degree sequence

## 1. Terminology

All graphs in this paper will be finite, simple and undirected. A *tree*  $T = (V, E)$  is a connected, acyclic graph.  $V(T)$  denotes the vertex set of a tree  $T$ . We refer to vertices of degree 1 of  $T$  as *leaves*. The unique path connecting two vertices  $v, u$  in  $T$  will be denoted by  $P_T(v, u)$ . For a tree  $T$  and two vertices  $v, u$  of  $T$ , the *distance*  $d_T(v, u)$  between them is the number of edges on the path  $P_T(v, u)$ . For a vertex  $v$  of  $T$ , define the *distance of*  $v$  as  $g_T(v) = \sum_{u \in V(T)} d_T(v, u)$ . Then  $\sigma(T) = \frac{1}{2} \sum_{v \in V(T)} g_T(v)$  denotes the *Wiener index* of  $T$ .

For any vertex  $v \in V(T)$ , let  $d(v)$  denote the *degree* of  $v$ , i.e. the number of edges incident to  $v$ . The *degree sequence* of a tree is the sequence of the degrees (in descending order) of the non-leaf vertices.

We call a tree  $(T, r)$  *rooted at the vertex*  $r$  (or just  $T$  if it is clear what the root is) by specifying a vertex  $r \in V(T)$ . The *height* of a vertex  $v$  of a rooted tree  $T$  with root  $r$  is  $h_T(v) = d_T(r, v)$ , note that this concept is also referred to as the *depth* in many literatures.

For any two different vertices  $u, v$  in a rooted tree  $(T, r)$ , we say that  $v$  is a *successor* of  $u$  and  $u$  is an *ancestor* of  $v$  if  $P_T(r, u) \subset P_T(r, v)$ . Furthermore, if  $u$  and  $v$  are adjacent to each other and  $d_T(r, u) = d_T(r, v) - 1$ , we say that  $u$  is the *parent* of  $v$  and  $v$  is a *child* of  $u$ . Two vertices  $u, v$  are *siblings* of each other if they share the same parent. A subtree of a tree will often be described by its vertex set. For a vertex  $v$  in a rooted tree  $(T, r)$ , we use  $T(v)$  to denote the subtree induced by  $v$  and all its successors.

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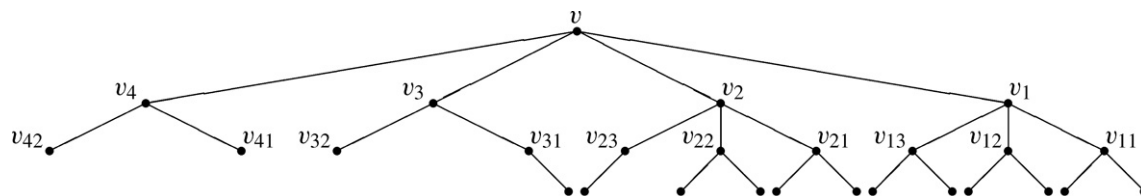


Fig. 1. A greedy tree.

## 2. Introduction

The structure of a chemical compound is usually modelled as a polygonal shape, which is often called the *molecular graph* of this compound. The biochemical community has been using topological indices to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics.

In 1947, Wiener [8] developed the Wiener Index. This concept has been one of the most widely used descriptors in the quantitative structure activity relationships, as the Wiener index has been shown to have a strong correlation with the chemical properties of the chemical compound.

Since the majority of the chemical applications of the Wiener index deal with chemical compounds that have acyclic organic molecules, whose molecular graphs are trees, the Wiener index of trees has been extensively studied over the past years, see [1] and the reference there for details.

It is well known that the Wiener index is maximized by the path and minimized by the star among general trees of the same size. Similar problems for more specific classes of trees seem to be more difficult. In [6], the Wiener index and the number of subtrees of binary trees are studied, a not yet understood relation between them is discussed for binary trees and trees in general. The correlation of various graph-theoretical indices including the Wiener index is studied in the recent work of Wagner [7].

To introduce our main results, we define the *greedy tree* (with a given degree sequence) as follows:

**Definition 2.1.** Suppose that the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following 'greedy algorithm':

- (i) Label the vertex with the largest degree as  $v$  (the root);
- (ii) Label the neighbors of  $v$  as  $v_1, v_2, \dots$ , assign the largest degrees available to them such that  $d(v_1) \geq d(v_2) \geq \dots$ ;
- (iii) Label the neighbors of  $v_1$  (except  $v$ ) as  $v_{11}, v_{12}, \dots$  such that they take all the largest degrees available and that  $d(v_{11}) \geq d(v_{12}) \geq \dots$ , then do the same for  $v_2, v_3, \dots$ ;
- (iv) Repeat (iii) for all the newly labelled vertices, always start with the neighbors of the labelled vertex with largest degree whose neighbors are not labelled yet.

Fig. 1 shows a greedy tree with degree sequence  $\{4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2\}$ .

From the definition of the greedy tree, we immediately get:

**Lemma 2.2.** A rooted tree  $T$  with a given degree sequence is a greedy tree if:

- (i) the root  $v$  has the largest degree;
- (ii) the heights of any two leaves differ by at most 1;
- (iii) for any two vertices  $u$  and  $w$ , if  $h_T(w) < h_T(u)$ , then  $d(w) \geq d(u)$ ;
- (iv) for any two vertices  $u$  and  $w$  of the same height,  $d(u) > d(w) \Rightarrow d(u') \geq d(w')$  for any successors  $u'$  of  $u$  and  $w'$  of  $w$  that are of the same height;
- (v) for any two vertices  $u$  and  $w$  of the same height,  $d(u) > d(w) \Rightarrow d(u') \geq d(w')$  and  $d(u'') \geq d(w'')$  for any siblings  $u'$  of  $u$  and  $w'$  of  $w$  or successors  $u''$  of  $u'$  and  $w''$  of  $w'$  of the same height.

We also define the *greedy caterpillar* as a tree  $T$  with given degree sequence  $\{d_1 \geq d_2 \geq \dots \geq d_k \geq 2\}$ , that is formed by attaching pendant edges to a path  $v_1 v_2 \dots v_k$  of length  $k - 1$  such that  $d(v_1) \geq d(v_k) \geq d(v_2) \geq d(v_{k-1}) \geq \dots \geq d(v_{\lfloor \frac{k}{2} \rfloor})$ . Fig. 2 shows a greedy caterpillar with degree sequence  $\{6, 5, 5, 5, 5, 5, 4, 3, 3\}$ .

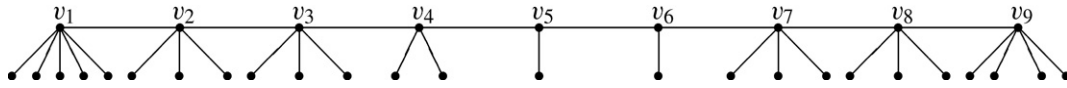


Fig. 2. A greedy caterpillar.

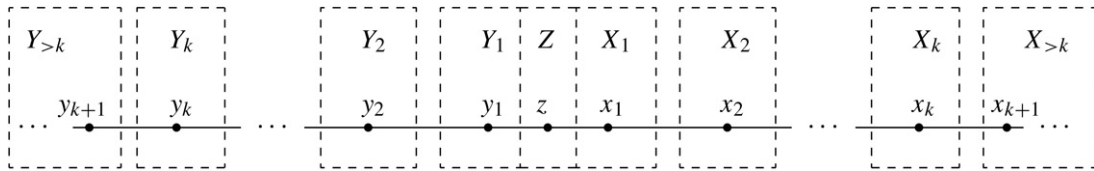


Fig. 3. The components resulted from a path with  $z$ .

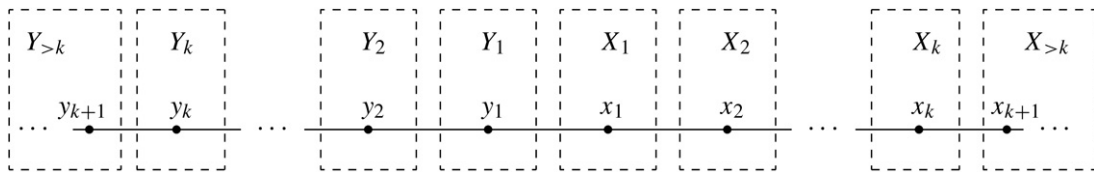


Fig. 4. The components resulted from a path without  $z$ .

In [2], the tree that minimizes the Wiener index among trees of given maximal degree is studied. However, the molecular graphs of the most practical interest have natural restrictions on their degrees corresponding to the valences of the atoms, therefore it is reasonable to consider a tree with a fixed degree sequence. In this note, we study the extremal values of the Wiener index of a tree with given degree sequence and characterize these trees. These trees are also shown to be the extremal trees with respect to *dominance order* by Fischermann, Rautenbach and Volkmann, for details see [3]. We will prove the following:

**Theorem 2.3.** *Given the degree sequence and the number of vertices, the greedy tree minimizes the Wiener index.*

**Theorem 2.4.** *Given the degree sequence and the number of vertices, the greedy caterpillar maximizes the Wiener index.*

In Section 3, a few lemmas are given regarding the structure of an extremal tree with given degree sequence, these results may be of interest on their own. We prove [Theorem 2.3](#) in Section 4 and [Theorem 2.4](#) in Section 5.

### 3. On the structure of an ‘optimal’ tree

For convenience, we will call a tree optimal if it minimizes the Wiener index among all trees with the same number of vertices and the same degree sequence.

Consider a path in an optimal tree, after the removal of the edges on this path, some connected components will remain. Take a vertex and label it as  $z$ , and label the vertices on its right as  $x_1, x_2, \dots$ , and the vertices on the left as  $y_1, y_2, \dots$ . Similarly, we can label the vertices on a path without  $z$ , simply take an edge and label the vertices on its right as  $x_1, x_2, \dots$ , and the vertices on the left as  $y_1, y_2, \dots$ .

Let  $X_i, Y_i$  or  $Z$  denote the component that contains the corresponding vertex. Let  $X_{>k}$  and  $Y_{>k}$  denote the trees induced by the vertices in  $V(X_{k+1}) \cup V(X_{k+2}) \cup \dots$  and  $V(Y_{k+1}) \cup V(Y_{k+2}) \cup \dots$  respectively (Figs. 3 and 4). Without loss of generality, assume that  $|V(X_1)| \geq |V(Y_1)|$ .

The next three lemmas hold for the path described above with (Fig. 3) or without (Fig. 4)  $z$ .

**Lemma 3.1.** *In the situation described above, if  $|V(X_i)| \geq |V(Y_i)|$  for  $i = 1, 2, \dots, k$ , then we can assume*

$$|V(X_{>k})| \geq |V(Y_{>k})| \tag{1}$$

*in an optimal tree.*

**Proof.** Suppose (for contradiction) that (1) does not hold. We will show that switching  $X_{>k}$  and  $Y_{>k}$  (after which (1) holds) will not increase the Wiener index.

First, for a path without  $z$ , note that in this operation, the lengths of the paths with both or neither end vertices in  $V(X_{>k}) \cup V(Y_{>k})$  do not change. Hence we only need to consider the sum of the lengths of the paths that contain exactly one end vertex in  $V(X_{>k}) \cup V(Y_{>k})$ .

For the distance between any vertex in  $X_i$  ( $i = 1, 2, \dots, k$ ) and any vertex in  $X_{>k}$ , this operation increases the distance by  $2i - 1$ , then the total amount increased is

$$\sum_{i=1}^k (2i - 1)|V(X_i)||V(X_{>k})|. \tag{2}$$

Similarly, for the distances between any vertex in  $Y_i$  ( $i = 1, 2, \dots, k$ ) and any vertex in  $X_{>k}$ , the total amount decreased is

$$\sum_{i=1}^k (2i - 1)|V(Y_i)||V(X_{>k})|. \tag{3}$$

For the distances between any vertex in  $Y_i$  ( $i = 1, 2, \dots, k$ ) and any vertex in  $Y_{>k}$ , the total amount increased is

$$\sum_{i=1}^k (2i - 1)|V(Y_i)||V(Y_{>k})|. \tag{4}$$

For the distances between any vertex in  $X_i$  ( $i = 1, 2, \dots, k$ ) and any vertex in  $Y_{>k}$ , the total amount decreased is

$$\sum_{i=1}^k (2i - 1)|V(X_i)||V(Y_{>k})|. \tag{5}$$

Now (2) + (4) - (3) - (5) yields the total change of the Wiener index via this operation

$$\begin{aligned} & \sum_{i=1}^k (2i - 1)(|V(X_i)||V(X_{>k})| + |V(Y_i)||V(Y_{>k})| - |V(Y_i)||V(X_{>k})| - |V(X_i)||V(Y_{>k})|) \\ &= \sum_{i=1}^k (2i - 1)(|V(X_i)| - |V(Y_i)|)(|V(X_{>k})| - |V(Y_{>k})|) \leq 0. \end{aligned}$$

For a path with  $z$ , note that the distance of a path with at least one end vertex in  $Z$  does not change during this operation. Similar to the first case, the total change of the Wiener index via this operation is

$$\sum_{i=1}^k (2i)(|V(X_i)| - |V(Y_i)|)(|V(X_{>k})| - |V(Y_{>k})|) \leq 0. \quad \square$$

**Lemma 3.2.** If  $|V(X_i)| \geq |V(Y_i)|$  for  $i = 1, 2, \dots, k - 1$  and  $|V(X_{>k})| \geq |V(Y_{>k})|$ , then we can assume

$$|V(X_k)| \geq |V(Y_k)| \tag{6}$$

in an optimal tree.

**Proof.** Suppose (for contradiction) that (6) does not hold, we will show that switching  $X_k$  and  $Y_k$  (after which (6) holds) will not increase the Wiener index.

Similar to the proof of Lemma 3.1, the total change of the Wiener index via this operation is

$$\begin{aligned} & \sum_{i=1}^{k-1} (2i - 1)(|V(X_i)| - |V(Y_i)|)(|V(X_k)| - |V(Y_k)|) \\ &+ (2k - 1)(|V(X_{>k})| - |V(Y_{>k})|)(|V(X_k)| - |V(Y_k)|) \leq 0 \end{aligned}$$

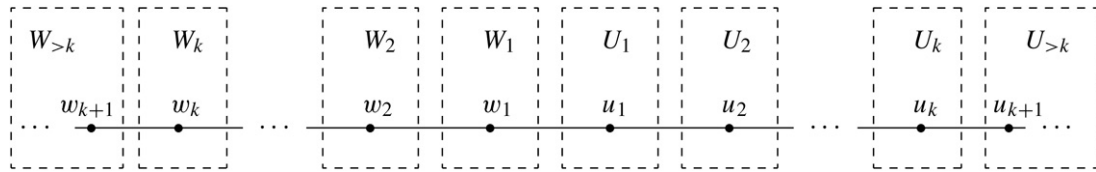


Fig. 5. The components resulted from a path.

for a path without  $z$  and

$$\sum_{i=1}^{k-1} (2i)(|V(X_i)| - |V(Y_i)|)(|V(X_k)| - |V(Y_k)|) + (2k)(|V(X_{>k})| - |V(Y_{>k})|)(|V(X_k)| - |V(Y_k)|) \leq 0$$

for a path with  $z$ .  $\square$

**Corollary 3.3.** *If  $|V(X_i)| \geq |V(Y_i)|$  for  $i = 1, 2, \dots, k - 1$  and  $|V(X_{>k-1})| \geq |V(Y_{>k-1})|$ , then we can assume  $d(x_k) \geq d(y_k)$  in an optimal tree.*

**Proof.** Suppose (for contradiction) that  $a = d(x_k) < d(y_k) = a + b$ . Removing  $x_k$  ( $y_k$ ) from  $X_k$  ( $Y_k$ ) will result in  $a$  ( $a + b$ ) components. Take any  $b$  components (let  $B$  be the set of vertices in these  $b$  components) from  $Y_k$  and attach them to  $x_k$ . After this operation we will have  $d(x_k) \geq d(y_k)$ , and the degree sequence of the tree is preserved.

We will show that this operation will not increase the Wiener index.

Similar to the previous proofs, the total change of the Wiener index in this operation is

$$\sum_{i=1}^{k-1} (2i - 1)(|V(Y_i)| - |V(X_i)|)|B| + (2k - 1)(|V(Y_{>k-1})| - |B| - |V(X_{>k-1})|)|B| \leq 0$$

for a path without  $z$  and

$$\sum_{i=1}^{k-1} (2i)(|V(Y_i)| - |V(X_i)|)|B| + (2k)(|V(Y_{>k-1})| - |B| - |V(X_{>k-1})|)|B| \leq 0$$

for a path with  $z$ .  $\square$

**Remark.** In Lemma 3.1, 3.2 and Corollary 3.3, if at least one strict inequality holds in the conditions, then the conclusion is forced and we can replace ‘can assume’ by ‘must have’ in the statement.

Now, for a maximal path in an optimal tree, we can label the vertices and components with vertices labelled as  $w_1, w_2, \dots$  and  $u_1, u_2, \dots$  and the components labelled as  $W_i$  and  $U_i$ , while  $U_1$  is the component with most vertices (Fig. 5) s.t. the following hold:

**Lemma 3.4.** *In an optimal tree, we can label the vertices such that*

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(U_m)| = |V(W_m)| = 1$$

if the path is of odd length  $(2m - 1)$ ; and

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(W_m)| = |V(U_{m+1})| = 1$$

if the path is of even length  $(2m)$ .

**Proof.** We only show the proof for a path of odd length, the other case is similar. First, we can assume that  $|V(U_1)| \geq |V(W_1)| \geq |V(U_2)|$  by symmetry. Now suppose that we have

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(W_{k-1})| \geq |V(U_k)| \tag{7}$$

for some  $k$ .

If equality holds in (7) except the last one, we can simply switch the label of  $U_i$  and  $W_i$  (if necessary) to guarantee that  $|V(U_k)| \geq |V(W_k)|$ . Otherwise, (7) implies that  $|V(U_{>k-1})| \geq |V(W_{>k-1})|$  by Lemma 3.1. If  $|V(W_k)| > |V(U_k)|$ , then

$$|V(U_{>k})| = |V(U_{>k-1})| - |V(U_k)| > |V(W_{>k-1})| - |V(W_k)| = |V(W_{>k})|.$$

Applying Lemma 3.2 to  $U_k$  and  $W_k$  (in the setting that  $x_i = u_i, y_i = w_i$  for  $i = 1, 2, \dots$ ) yields a contradiction. Thus we have

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(U_k)| \geq |V(W_k)|.$$

If all the equalities hold, we can switch the label of  $U_{i+1}$  and  $W_i$  for  $i \geq 1$  (if necessary) and guarantee that  $|V(W_k)| \geq |V(U_{k+1})|$ . Otherwise, apply Lemma 3.1 to  $U_{>k}$  and  $W_{>k-1}$  in the following setting:

$$Z = U_1, Y_i = U_{i+1}, X_i = W_i, z = u_1, y_i = u_{i+1}, x_i = w_i. \tag{8}$$

Then we have  $|V(X_i)| \geq |V(Y_i)|$  for  $i = 1, 2, \dots, k - 1$ , thus

$$|V(W_{>k-1})| = |V(X_{>k-1})| \geq |V(Y_{>k-1})| = |V(U_{>k})|$$

by Lemma 3.1. If  $|V(Y_k)| = |V(U_{k+1})| > |V(W_k)| = |V(X_k)|$ , then

$$|V(Y_{>k})| = |V(Y_{>k-1})| - |V(Y_k)| < |V(X_{>k-1})| - |V(X_k)| = |V(X_{>k})|.$$

Applying Lemma 3.2 to  $Y_k = U_{k+1}$  and  $X_k = W_k$  in setting (8) yields a contradiction. Thus we have

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(U_k)| \geq |V(W_k)| \geq |V(U_{k+1})|.$$

The lemma follows by induction.  $\square$

**Remark.** Lemma 3.4 can be shown in a much easier way by using an equivalent definition of the Wiener index, i.e.  $\sigma(T) = \sum_{uv \in E(T)} n(v)n(u)$ . Here  $n(v)$  ( $n(u)$ ) is the number of vertices in the component that contains  $v$  ( $u$ ) after removing  $uv$  from  $T$ . For the tree and path under consideration, we only need to consider the terms  $n(v)n(u)$  for the edges on the path. Then our result follows directly from a classic result of Hardy ([4], Theorem 371). We keep the combinatorial proof here to provide a better understanding of the whole idea.

**Lemma 3.5.** *In an optimal tree, for a path with labelling as in Lemma 3.4, we have*

$$d(u_1) \geq d(w_1) \geq d(u_2) \geq d(w_2) \geq \dots \geq d(u_m) = d(w_m) = 1$$

if the path is of odd length  $(2m - 1)$ ;

$$d(u_1) \geq d(w_1) \geq d(u_2) \geq d(w_2) \geq \dots \geq d(u_m) \geq d(w_m) = d(w_{m+1}) = 1$$

if the path is of even length  $(2m)$ .

**Proof.** We only show the proof for the path of odd length, the other case is similar.

First, we have

$$|V(U_1)| \geq |V(W_1)| \geq |V(U_2)| \geq |V(W_2)| \geq \dots \geq |V(U_m)| = |V(W_m)| = 1.$$

Now apply Corollary 3.3 to  $u_i, u_{i+1}$  for  $i = 1, 2, \dots, m - 1$  in the following setting:

$$y_1 = u_{i+1}, y_2 = u_{i+2}, \dots; \quad x_1 = u_i, x_2 = u_{i-1}, \dots, x_i = u_1, x_{i+1} = v_1, \dots$$

Then  $|V(X_{>1})| = \sum_{k=1}^m |V(W_k)| + \sum_{k=1}^{i-1} |V(U_k)| > \sum_{k=i+2}^m |V(U_k)| = |V(Y_{>1})|$ , implying that  $d(u_i) = d(x_1) \geq d(y_1) = d(u_{i+1})$ .

Thus we have

$$d(u_1) \geq d(u_2) \geq \dots \geq d(u_m).$$

Similarly, applying Corollary 3.3 to  $w_i, w_{i+1}$  for  $i = 1, 2, \dots, m - 1$  yields

$$d(w_1) \geq d(w_2) \geq \dots \geq d(w_m).$$

For  $u_i$  and  $w_i$ , if equality holds everywhere in Lemma 3.4, we can again switch the labels and have  $d(u_i) \geq d(w_i)$ . Otherwise, applying Corollary 3.3 to  $u_i, w_i$  (in the setting that  $x_i = u_i, y_i = w_i$  for  $i = 1, 2, \dots$ ) yields that  $d(u_i) \geq d(w_i)$  for  $i = 1, 2, \dots, m$ .

Similarly, applying Corollary 3.3 to  $w_i, u_{i+1}$  in the setting (8) yields that  $d(w_i) \geq d(u_{i+1})$  for  $i = 1, 2, \dots, m - 1$ . □

#### 4. Proof of Theorem 2.3

It has been shown that  $g_T(v)$  is minimized at one or two adjacent vertices on any path and hence in the whole tree (called the *centroid* of the tree), see [5,9] for details. From Lemmas 3.4 and 3.5, simple calculation shows:

On any path of an optimal tree labelled as in Lemmas 3.4 and 3.5,

$$\text{the minimal value of } g_T(v) \text{ is achieved at } u_1 \tag{9}$$

where  $d(u_1)$  and  $|V(U_1)|$  are maximum on the path.

There are two cases:

- (i) If there is only one vertex in the centroid, label it as  $v$ .
- (ii) If there are two vertices in the centroid, the two components (after the removal of the edge in between the two vertices in the centroid) contain the same number of vertices, simply choose either one as  $v$  and the other one as  $v_1$ .

We only show the first case, the second one is similar.

In an optimal tree  $T$ , consider  $T$  as rooted at  $v$ , we know  $v$  is of the largest degree immediately from (9) (hence (i) of Lemma 2.2 is satisfied).

Consider any path starting at a leaf  $u$ , passing  $v$ , ending at a leaf  $w$  whose only common ancestor with  $u$  is  $v$ . Apply Lemma 3.5 to this path such that  $u_1 = v$ , we must have  $|d_T(u, v) - d_T(w, v)| \leq 1$ , then the heights of any two leaves differ by at most 1 (hence (ii) of Lemma 2.2 is satisfied). Furthermore, it is also implied that

$$d(x) \geq d(y) \text{ for any two vertices such that } y \text{ is a successor of } x. \tag{10}$$

For a vertex  $x$  of height  $i$  and a vertex  $y$  of height  $j$  ( $i < j$ ), consider the following two cases:

- (a) if  $y$  is a successor of  $x$ , then we have  $d(x) \geq d(y)$  from (10);
- (b) otherwise, let  $u$  be the common ancestor of them that is on the path  $P_T(x, y)$ , apply Lemma 3.5 to the path that passes through  $y', y, u, x, x'$ , where  $y', x'$  are leaves that are successors (or equal to)  $y, x$  respectively. We must have  $u_1 = u$  by (9) and Lemma 3.4, then  $x = u_{k+1}, y = w_l$  or  $x = w_k, y = u_{l+1}$ , where  $k = i - h_T(u), l = j - h_T(u), k + 1 \leq l$ . Either way, Lemma 3.5 implies that  $d(x) \geq d(y)$ .

Hence (iii) of Lemma 2.2 is satisfied.

For two non-leaf vertices  $x$  and  $y$  of the same height  $i$  with  $d(x) > d(y)$ , let  $x'$  and  $y'$  (of the same height  $j$ ) be the successors of  $x$  and  $y$  respectively. Apply Lemma 3.5 to the longest path that passes through  $y', y, u, x, x'$ , where  $u$  is the common ancestor of  $x, y$  that is on the path  $P_T(x, y)$ . We must have  $u_1 = u$  by (9) and Lemma 3.4, then  $x = w_k, x' = w_l, y = u_{k+1}, y' = u_{l+1}$  as  $d(x) > d(y)$ , where  $k = i - h_T(u), l = j - h_T(u)$ . Thus implying that  $d(x') \geq d(y')$  (hence (iv) of Lemma 2.2 is satisfied).

Now let  $x_0$  ( $x'$ ) and  $y_0$  ( $y'$ ) be the parents (siblings) of  $x$  and  $y$  respectively, let  $x''$  and  $y''$  (of the same height  $j$ ) be successors of  $x'$  and  $y'$  respectively. The conclusion of (iv) implies

$$|V(T(x_0)/T(x''))| > |V(T(y_0)/T(y''))|. \tag{11}$$

Now consider the longest path that passes through  $y'', y', u, x', x''$ , where  $u$  is the common ancestor of  $x$  and  $y$  that is on the path  $P_T(x', y')$ . Apply Lemma 3.5, we must have  $u_1 = u$  by (9) and Lemma 3.4, then  $x' = w_k, x'' = w_l, y' = u_{k+1}, y'' = u_{l+1}$  by (11) and Lemma 3.4, where  $k = i - h_T(u), l = j - h_T(u)$ . Thus we have  $d(x') \geq d(y')$  and  $d(x'') \geq d(y'')$  (hence (v) of Lemma 2.2 is satisfied).

In conclusion, by Lemma 2.2, the optimal tree is the greedy tree.

#### 5. On Theorem 2.4

Similar to Lemma 3.4, we have the following for trees with given degree sequence that maximize the Wiener index (refer to Fig. 5), we leave the proof to the reader.

**Lemma 5.1.** *In a tree with a given number of vertices and degree sequence that maximizes the Wiener index, we can label the vertices on the path with  $U_1$  being the component consisting of the least vertices such that:*

$$|V(U_1)| \leq |V(W_1)| \leq |V(U_2)| \leq |V(W_2)| \leq \dots \leq |V(U_{m-1})| \leq |V(W_{m-1})|$$

if the path is of odd length  $(2m - 1)$ ; and

$$|V(U_1)| \leq |V(W_1)| \leq |V(U_2)| \leq |V(W_2)| \leq \dots \leq |V(W_{m-1})| \leq |V(U_m)|$$

if the path is of even length  $(2m)$ .

**Proof of Theorem 2.4.** Let  $T$  be the tree that maximizes the Wiener index with a given degree sequence. Consider the longest path, without loss of generality, let the path be  $w_m w_{m-1} \dots w_1 u_1 u_2 \dots u_m$  of odd length (the other case is similar).

First we show that every vertex not on the path is a leaf, otherwise, let  $x$  be a neighbor of  $w_i$  (the case for  $u_i$  is similar) that is not on the path and is not a leaf. Consider the longest path that contains  $w_m, w_i, x$ , i.e.  $w_m \dots w_i x x_1 \dots x_s y$  where  $y$  is a leaf.

Let  $W_i, U_i$  denote the components with respect to the path  $w_m w_{m-1} \dots w_1 u_1 u_2 \dots u_m$  as in Lemma 5.1. Let  $X_{w_m}, X_{w_{m-1}}, \dots, X_{w_i}, X_x, X_{x_1}, \dots, X_{x_s}$  denote the components resulting from removing the edges on the path  $w_m \dots w_i x x_1 \dots x_s y$ . Now consider the path  $w_m \dots w_i x x_1 \dots x_s y$ , we have

$$|V(X_{w_i})| \geq |V(U_{m-1})| \geq |V(W_i)| > |V(X_{x_s})|,$$

contradicting Lemma 5.1 (note that  $i \leq m - 2$ ). Thus, for every vertex on the path  $w_m w_{m-1} \dots w_1 u_1 u_2 \dots u_m$ , if it has any neighbor that is not on the path, they must be leaves. Applying Lemma 5.1 to the path  $w_m w_{m-1} \dots w_1 u_1 u_2 \dots u_m$  yields that  $T$  must be a greedy caterpillar.  $\square$

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