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# SPARSE TREES WITH A GIVEN DEGREE SEQUENCE

by

AO SHEN

(Under the Direction of Hua Wang)

## ABSTRACT

In this thesis, we consider the properties of sparse trees, and summarize a collection of trees under some constraints (i.e given degree sequence, given number of leaves, given maximum degree sequence  $\Delta$ , etc.) which have maximum Wiener index and minimum number of subtrees at the same time. The Wiener index is one of the most important topological indices in chemical graph theory. The Steiner  $k$ -Wiener index can be regarded as the generalization of the Wiener index, when  $k = 2$ , the Steiner Wiener index is the same as Wiener index. The Steiner  $k$ -Wiener index of a tree  $T$  is the summation of all sizes of subtrees which contain any  $k$ -subset of vertex set  $V(T)$ . In the case of sparse trees with given degree sequence, we provide computational results which may shed some light on the extremal tree with maximum Steiner Wiener index.

**INDEX WORDS:** Wiener index, Number of subtrees, Steiner Wiener index, Degree sequence

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SPARSE TREES WITH A GIVEN DEGREE SEQUENCE

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## SPARSE TREES WITH A GIVEN DEGREE SEQUENCE

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## DEDICATION

When I first decided to step into this field of study, I received doubts from almost everyone around me. Friends and Family insisted that I would not succeed because my background in Mathematics was lacking. Only my advisor, Dr. Wang, had faith in me and guided me through each barrier along the way. Thank you, Dr. Wang, for never giving up on me, even when I wanted to give up on myself. I can never express the depth of my gratitude for your patience and your devotion to your students. You have been a great mentor, and I hold our relationship as student and teacher in the highest esteem. Your tutelage will certainly benefit me in my future life adventures.

I still thank everyone who doubted me on my choices, because you fueled my tank when I needed to keep running, and helped me turned my weakness to advantage.

I want to dedicate this thesis to you all. Without you guys, this dissertation would be impossible.

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In memory of Rev. Northrip, I believe you have been watching me accomplish this in heaven. Even though your physical body has passed away, your love will be everlasting.

Last but not least, for all the friends and people around me, all your advice and kindly support will always be remembered by me. I will carry on this positive energy to be better with what I do.

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## LIST OF SYMBOLS

A symbol table can be created in various ways. Here are a few:

Tabular environment:

$\mathbb{R}$	Real Numbers
$\mathbb{C}$	Real Numbers
$\mathbb{Z}$	Integers
$\mathbb{N}$	Natural Numbers
$\mathbb{N}_0$	Natural Numbers including 0
$L_p(\mathbb{R})$	$p$ -integrable functions over $\mathbb{R}$
$L(X, Y)$	Linear maps from $X$ to $Y$
$\text{rank}(T)$	Rank of a linear map

Multicols environment:

$\mathbb{R}$  Real Numbers

$\mathbb{N}_0$  Natural Numbers including 0

$\mathbb{C}$  Real Numbers

$L_p(\mathbb{R})$   $p$ -integrable functions over  $\mathbb{R}$

$\mathbb{Z}$  Integers

$L(X, Y)$  Linear maps from  $X$  to  $Y$

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Itemize environment:

- $\mathbb{R}$  Real Numbers

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- $L_p(\mathbb{R})$   $p$ -integrable functions over  $\mathbb{R}$
- $L(X, Y)$  Linear maps from  $X$  to  $Y$
- $\text{rank}(T)$  Rank of a linear map

# CHAPTER 1

## INTRODUCTION

### 1.1 GRAPH TERMINOLOGIES

In this thesis, we only consider simple graphs with no loops and no multi-edges. Let  $G = (V(G), E(G))$  denote a graph with vertex set  $V(G)$  and edge set  $E(G)$ . Then, let  $|V(G)|$  ( $|E(G)|$ , respectively) be the number of vertex set  $V(G)$  (edge set  $E(G)$ , respectively). A tree is a connected acyclic (no cycles) graph. It is easily verified that a connected graph  $G$  on  $n$  vertices is a tree if and only if  $|E(G)| = n - 1$ . Keeping in line with terminologies in [2], let  $T$  be a tree. For a vertex  $x$  of  $T$ , the neighborhood of  $x$  is the set of all vertices which are adjacent to  $x$  and denoted by  $N_T(x)$ . The degree of  $x$  is denoted by  $deg(x)$ , and  $deg(x) = |N_T(x)|$ . A pendant vertex is a vertex of degree 1, and is also called a leaf. A branch vertex is a vertex of degree  $\geq 3$ . A chemical tree is a tree wherein no vertex has degree more than 4.

The degree sequence is the non-increasing sequence of vertex degrees, which is corresponding to the valences of atoms in a molecular graph.

The distance between two vertices  $x$  and  $y$  is denoted by  $d_T(x, y)$  or  $d(x, y)$  which is the number of edges between two vertices  $x$  and  $y$  in  $T$ . The unique path connecting two vertices  $x$  and  $y$  in  $T$  is denoted by  $P_T(x, y)$ . We will use  $T - x$  or  $T - xy$  to denote the graph obtained from  $T$  by deleting the vertex  $x \in V(T)$  or the edge  $xy \in E(T)$ .

A tree  $(T, r)$  is said to be rooted at  $r$  by specifying some  $r \in V(T)$ . For any two distinct vertices  $v, u$  in a rooted tree  $(T, r)$ , if  $P_T(r, u) \subset P_T(r, v)$ , then we say that  $v$  is a successor of  $u$ . If  $u$  and  $v$  are adjacent and  $d_T(r, u) = d_T(r, v) - 1$ , we say that  $u$  is a parent of  $v$  and  $v$  is a child of  $u$ . If  $v$  is any vertex of a rooted tree  $(T, r)$ , let  $T(v)$  denote the subtree induced by  $v$ , which contains  $v$  and all of its successors in  $T$ .

Given the plethora of definitions, we provide an example to illustrate each of these

important concepts.

With given vertex degrees, the greedy tree is achieved through 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  $\deg(v_{11}) \geq \deg(v_{12}) \geq \dots$ ;
- 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  $\deg(v_{11}) \geq \deg(v_{12}) \geq \dots$ , then do the same for  $v_2, v_3, \dots$ ;
- iv Repeat (iii) for all the newly labeled vertices. Always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

A greedy tree with degree sequence

$$(4, 4, 4, 3, 3, 3, 3, 3, 3, 3, 2, 2, 1, \dots, 1).$$

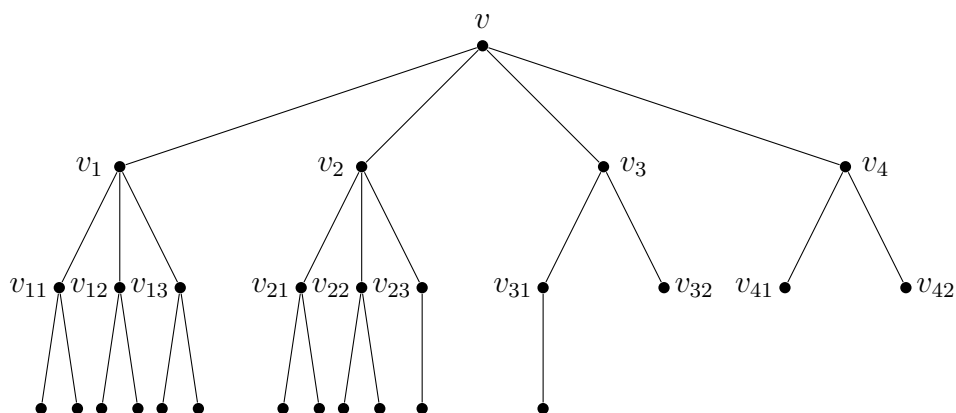


Figure 1.1: A greedy tree  $T$

In Figure 1.1,  $T$  is a chemical tree. There are three vertices  $v, v_1, v_2$  having degree 4, vertices  $v_3, v_4, v_{11}, v_{12}, v_{13}, v_{21}, v_{22}$  have degree 3, and they are all branch vertices. The

degree sequence is the non-increasing sequence of degrees of all vertices. The distance between vertices  $v_{11}$  and  $v_{21}$  is 4, and the unique path connecting vertices  $v_{11}$  and  $v_{21}$  is  $P_T(v_{11}, v_{21}) : v_{11}, v_1, v, v_2, v_{21}$  (see Figure 1.2).

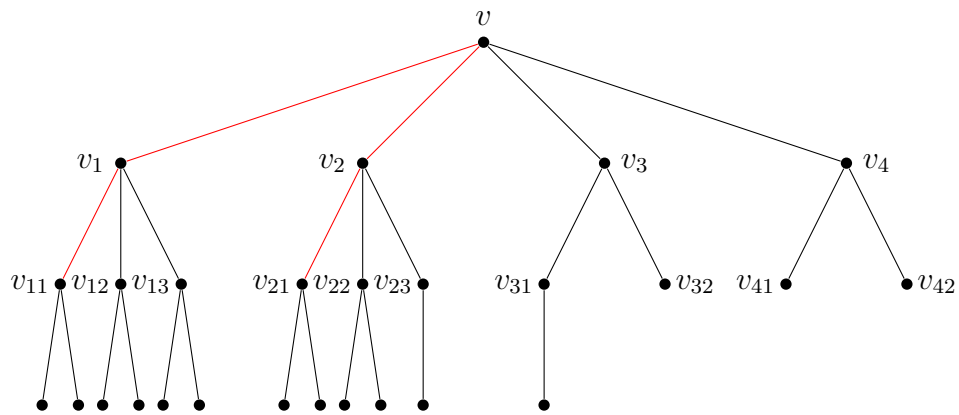


Figure 1.2: A greedy tree and the distance

Let  $v$  be the root of  $T$ , for vertices  $v_2$  and  $v_{21}$  in this rooted tree  $(T, r)$ , it is easy to see that  $P_T(v, v_2) \subset P_T(v, v_{21})$ , so  $v_{21}$  is a successor of  $v_2$ , similarly,  $v_{22}, v_{23}$  are successors of  $v_2$ , too. Furthermore,  $v_2$  and  $v_{21}$  are adjacent and  $d_T(v, v_2) = d_T(v, v_{21}) - 1$ , therefore,  $v_2$  is a parent of  $v_{21}$  and  $v_{21}$  is a child of  $v_2$ . The subtree induced by  $v_2$ ,  $T(v_2)$ , is the subtree which is induced by  $v_2$  and all its successors in  $T$  (see Figure 1.3)

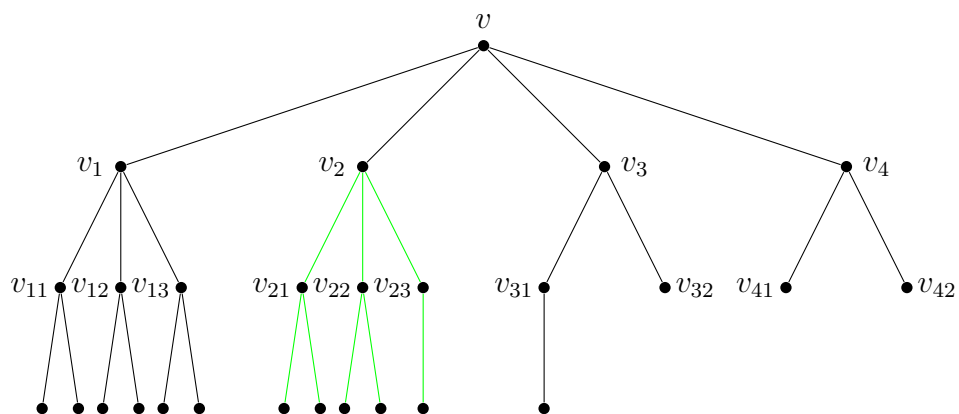


Figure 1.3: A greedy tree and the subtree

## 1.2 WIENER INDEX AND THE NUMBER OF SUBTREES

In 1947, Harry Wiener [21, 22] realized that there exist correlations between the boiling points of paraffins and their molecular structure. He introduced the first chemical index, which is called the Wiener index, and he show that the Wiener index of organic compounds is closely related to its structure The Wiener index is defined as the sum of distances between all pairs of vertices:

$$W(G) = \sum_{u,v \in V(G)} d(u,v).$$

In the past years, the Wiener index has been investigated in many aspects and many papers are published (see [8, 12, 13, 18, 19, 20]).

The Steiner distance is closely related to the Wiener index. For a subset  $S$  of  $V(T)$  of size  $k$ , the Steiner distance of  $S$ , denoted  $d(S)$  is the minimum size of a connected subgraph of  $T$  whose vertex set contains  $S$ . In the case where  $k = 2$ , the Steiner distance of  $S = u, v$ , is exactly the distance between  $u$  and  $v$ . The Steiner  $k$ -Wiener index of  $G$ , denoted  $SW_k(G)$ , which was first introduced by Li, Mao, and Gutman, is defined by

$$SW_k(G) = \sum_{S \subseteq V(G), |S|=k} d(S).$$

It appears to the Steiner  $k$ - Wiener index  $SW_k(G)$  was studied by Dankelmann [3, 4] under the term average Steiner Wiener index. Recently, the Steiner Wiener index has received more and more attention. (see [10, 11])

Here we give an example to show how to compute  $SW_k(G)$ . For the graph in Figure 1.4, when  $k = 4$ , we first present all subsets of order 4 of the set of vertices  $V(G) = \{v_1, v_2, v_3, v_4, v_5, v_6\}$ , then we compute the Steiner distance  $d(S)$ . After summing up all possible subsets  $S$  of order 4, we will obtain  $SW_4(G)$ .

- $S_1 = \{v_1, v_2, v_3, v_4\}, d(S_1) = 3;$
- $S_2 = \{v_1, v_2, v_3, v_5\}, d(S_2) = 3;$



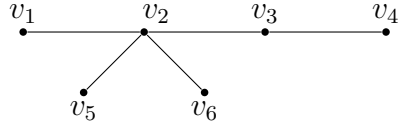


Figure 1.4: An example to show how to compute  $SW_4(G)$

- $S_3 = \{v_1, v_2, v_3, v_6\}, d(S_3) = 3;$
- $S_4 = \{v_1, v_2, v_4, v_5\}, d(S_4) = 4;$
- $S_5 = \{v_1, v_2, v_4, v_6\}, d(S_5) = 4;$
- $S_6 = \{v_1, v_2, v_5, v_6\}, d(S_6) = 3;$
- $S_7 = \{v_2, v_3, v_4, v_5\}, d(S_7) = 3;$
- $S_8 = \{v_2, v_3, v_4, v_6\}, d(S_8) = 3;$
- $S_9 = \{v_2, v_3, v_5, v_6\}, d(S_9) = 3;$
- $S_{10} = \{v_2, v_4, v_5, v_6\}, d(S_{10}) = 4;$
- $S_{11} = \{v_3, v_4, v_5, v_6\}, d(S_{11}) = 4;$
- $S_{12} = \{v_1, v_4, v_5, v_6\}, d(S_{12}) = 5;$
- $S_{13} = \{v_1, v_3, v_4, v_5\}, d(S_{13}) = 4;$
- $S_{14} = \{v_1, v_3, v_4, v_6\}, d(S_{14}) = 4;$
- $S_{15} = \{v_1, v_3, v_5, v_6\}, d(S_{15}) = 4;$

Then we sum up all values  $d(S_1), \dots, d(S_{15}),$

$$SW_4(G) = d(S_1) + \dots + d(S_{15}) = 3 \times 7 + 4 \times 7 + 5 = 54.$$

Székely and Wang [15] first studied the number of subtrees of some trees. For a tree  $T$  and a vertex  $v$  of  $T$ , let  $F_T(v)$  be the number of subtrees of  $T$  that contain  $v$ . Let  $F(T)$  denote the number of non-empty subtrees of  $T$ . Numerical evidence suggests that there exists some negative correlation between the Wiener index and the number of subtrees in trees: extremal trees with minimum Wiener index also maximizes the number of subtrees and vice versa. Many papers with regard to the number of subtrees have been published, see for example [1, 14, 16, 17, 28].

CHAPTER 2  
SURVEY OF SPARSE TREES

In this chapter we explore sparse trees that maximize the Wiener index and minimize the number of subtrees in various classes of trees.

2.1 WIENER INDEX

First, it is well known that the Wiener index is maximized by a path in general trees.

**Theorem 2.1.** [5] *Amongst all trees with a given order  $n$ , the path maximizes the Wiener index.*

A binary tree is a tree  $T$  such that every vertex of  $T$  has degree 1 or 3. A path is obviously not a binary tree. Among binary trees of given order we have the following.

**Theorem 2.2.** [7] *Amongst binary trees with  $n$  leaves, the Wiener index is maximized by some binary caterpillar.*

Along the same line, we are sometimes interested in trees with a given maximum degree.

Suppose maximum degree  $\Delta \geq 2$ . Let  $T_{n,\Delta}$  be the tree obtained from path  $P_{n-\Delta+1}$  by attaching  $\Delta - 1$  pendant edges to one of the pendant vertices of  $P_{n-\Delta+1}$ .

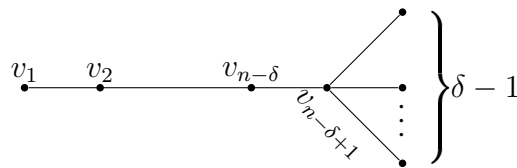


Figure 2.1:  $T_{n,\Delta}$

**Theorem 2.3.** [7] *Let  $\Delta$  be a positive integer more than two, and let  $T$  be a tree with  $n$  vertices, which has the maximum degree at least  $\Delta$ . Then the Wiener index is maximized by  $T_{n,\Delta}$ , with equality if and only if  $T = T_{n,\Delta}$ .*

Corresponding to the maximum degree constraint is the diameter. It has been of interest to study extremal structures, sparse trees in particular, in trees with a given diameter.

The dumbbell  $D(n, a, b)$  consists of the path  $P_{n-a-b}$  together with  $a$  pendant edges attached to one pendant vertex of  $P_{n-a-b}$  and  $b$  pendant edges attached to the other pendant vertex. See Figure 2.2.

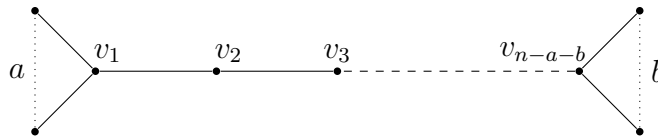


Figure 2.2: The dumbbell  $D(n, a, b)$

**Theorem 2.4.** [6, 13] *Let  $T$  be a tree on  $n$  vertices with  $k$  pendant vertices,  $D(n, \lfloor \frac{k+1}{2} \rfloor, \lfloor \frac{k}{2} \rfloor)$  maximizes the Wiener index.*

## 2.2 THE NUMBER OF SUBTREES

With respect to the number of subtrees, again the path is extremal with minimum value among general trees.

**Theorem 2.5.** [15] *Amongst all trees with a given order  $n$ , the path minimizes the number of subtrees.*

Similarly for binary trees.

**Theorem 2.6.** [15] *Amongst binary trees with  $n$  leaves, the number of subtrees is minimized by some binary caterpillar.*

For trees with a given maximum degree or a given diameter, the following state that the same trees that maximize the Wiener index indeed also minimize the number of subtrees.

**Theorem 2.7.** [23] *Let  $\Delta$  be a positive integer more than two, and let  $T$  be a tree with  $n$  vertices, which has the maximum degree at least  $\Delta$ . Then the number of subtrees is minimized by  $T_{n,\Delta}$ , with equality if and only if  $T = T_{n,\Delta}$ .*

**Theorem 2.8.** [25] *Let  $T$  be a tree on  $n$  vertices with  $k$  pendent vertices,  $D(n, \lfloor \frac{k+1}{2} \rfloor, \lfloor \frac{k}{2} \rfloor)$  maximizes the number of subtrees.*

### 2.3 TREES WITH GIVEN DEGREE SEQUENCE

Next we consider a more general case, when the trees with a given degree sequence are considered. Similar to the binary tree case the sparse trees are caterpillars. Identifying these sparse caterpillars is, however, very difficult. Letting the backbone of the caterpillar be  $P$ , we can then be more specific about these sparse caterpillars.

We say that a tree satisfies  $V$ -properties, if the degrees of vertices on the path  $P$ , listed from one end to the other end, form a sequence  $deg(v_1), deg(v_2), \dots, deg(v_k)$ , and satisfy

$$deg(v_1) \geq deg(v_2) \geq \dots \geq deg(v_j) \leq \dots \leq deg(v_k),$$

for some  $j \in \{1, 2, \dots, k\}$ .

**Theorem 2.9.** [26] *Amongst all trees with given degree sequence, there exists caterpillars satisfying the  $V$ -property which maximize the Wiener index.*

**Theorem 2.10.** [27] *Amongst all trees with degree sequence, there exist caterpillars which minimize the number of subtrees.*

## CHAPTER 3

## STEINER WIENER INDEX AND SPARSE TREES

Based on the Steiner distance, the concept of Steiner Wiener index was introduced recently. We now examine sparse trees with respect to the Steiner Wiener index in different classes of trees. Our brief survey and study here include both the sparse and dense tree cases, as well as other related work.

## 3.1 STEINER WIENER INDEX: SURVEY

**Theorem 3.1.** [9] *Amongst all trees of order  $n$ , the star minimizes the Steiner Wiener index, and the path maximizes the Steiner Wiener index.*

**Theorem 3.2.** [9] *For all trees  $T$ , we have*

$$SW_2(T) = W(T),$$

$$SW_3(T) = \frac{n-2}{2}W(T),$$

$$SW_{n-1}(T) = n(n-1) - p, \text{ where } p \text{ is the number of leaves of } T$$

**Theorem 3.3.** [9] *If  $T$  is a tree, then the Steiner  $k$ -Wiener index*

$$SW_k(T) = \sum_{e=xy \in E(T)} \sum_{i=1}^{k-1} \binom{n_1(e)}{i} \binom{n_2(e)}{k-i},$$

where  $n_1(e)(n_2(e),$  respectively) is the number of vertices in  $T$  closer to  $x(y,$  respectively).

## 3.2 STEINER WIENER INDEX WITH A GIVEN DEGREE SEQUENCE

For trees with a given degree sequence we can once again show that the sparse tree needs to be a caterpillar satisfying the  $V$ -property.

**Theorem 3.4.** [24] *Amongst all trees with given degree sequence, the caterpillar satisfying the  $V$ -property maximizes the Steiner Wiener index.*

### 3.3 COMPUTATIONAL RESULTS OF STEINER WIENER INDEX

As an effort to further examine the structure of the sparse caterpillar, we first provide some computational work.

Let  $a, b, c, x,$  and  $y,$  describe a chemical caterpillar whose backbone has the following properties:

- $a, b, c,$  are the number of vertices with degree 4, 3, 2 respectively;
- $x, y,$  are the number of vertices with degree 4, 3 in the left side of the tree respectively;
- $v_0$  is a pendant leaf of the backbone;
- $v_1, v_2, \dots, v_x$  all have degree 4;
- $v_{x+1}, v_{x+2}, \dots, v_{x+y}$  all have degree 3;
- $v_{x+y+1}, v_{x+y+2}, \dots, v_{x+y+c}$  all have degree 2;
- $v_{x+y+c+1}, v_{x+y+c+2}, \dots, v_{x+b+c}$  all have degree 3;
- $v_{x+b+c+1}, v_{x+b+c+2}, \dots, v_{a+b+c}$  all have degree 4;
- $v_{a+b+c+1}$  is a pendant leaf of the backbone.

Let  $k = 4, 5, 6, 7,$  we compute the values of  $\max SW_i(T), i = 4, 5, 6, 7,$  in the case when  $T$  be a chemical caterpillar, the label of  $T$  is as follows:

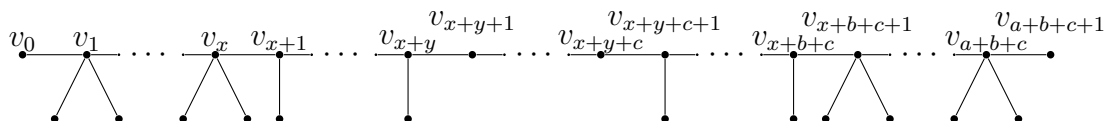


Figure 3.1: A caterpillar with maximum degree 4

It is natural to conjecture that the extremal chemical trees that maximize the Steiner  $k$ -Wiener index is “symmetric”, this is indeed what we observed from the tables and formally stated below.

Here we will give three examples to explain the tables below, which include the different value of  $a$ ,  $b$ ,  $c$ ,  $x$ , and  $y$ . As shown in second line of the left side in Table 3.1,  $a = 11$ ,  $b = 8$ ,  $c = 2$ . Since  $a$  is odd and  $b$  is even, hence  $x = (11 - 1)/2 = 5$ ,  $y = 8/2 + 1 = 5$ , then we obtain the result of maximum values of  $SW_4 = 12552746$ . Last line of right side in Table 3.2,  $a = 19$ ,  $b = 11$ ,  $c = 2$ . Both  $a$  and  $b$  are odd, so  $x = (19 - 1)/2 = 9$ ,  $y = (11 + 1)/2 = 6$ , then obtain the result of maximum values of  $SW_5 = 2040002356$ . The ninth line of left side in Table 3.3,  $a = 12$ ,  $b = 12$ ,  $c = 2$ . Both  $a$  and  $b$  are even, so  $x = 12/2 = 6$ ,  $y = 12/2 = 6$ , then we obtain the result of maximum values of  $SW_6 = 4050773941$ .

To conclude this thesis, we give a conjecture about the structure of the extremal chemical trees that maximize the Steiner  $k$ -Wiener index: For a chemical tree with given degree sequence  $d_1, d_2, \dots, d_n$ , the Steiner  $k$ -Wiener index, for  $k \geq 4$ , is maximized when the chemical tree is of the structure in Figure 3.1 with:

- $x = a/2, y = \lfloor b/2 \rfloor$  if  $a$  is even;
- $x = (a - 1)/2, y = (b + 1)/2$  if both  $a$  and  $b$  are odd;
- $x = (a - 1)/2, y = b/2 + 1$  if  $a$  is odd and  $b$  is even.



Table 3.1: Maximum values of  $SW_4$  with given degree sequence and the extremal trees.

$SW_4$	a	b	c	x	y	$SW_4$	a	b	c	x	y
12552746	11	8	2	5	5	16699509	12	8	2	6	4
18262227	11	10	2	5	6	20005336	12	9	2	6	4
25874586	11	12	2	5	7	23814099	12	10	2	6	5
35827839	11	14	2	5	8	28179089	12	11	2	6	5
48622178	11	16	2	5	9	33160679	12	12	2	6	6
21869883	13	8	2	6	5	38819716	12	13	2	6	6
30631706	13	10	2	6	6	45224857	12	14	2	6	7
41989999	13	12	2	6	7	69888155	14	14	2	7	7
56480362	13	14	2	6	8	80070401	14	15	2	7	7
74706971	13	16	2	6	9	103980784	14	17	2	7	8
85709642	15	14	2	7	8	70074808	16	11	2	8	5
110935973	15	16	2	7	9	80294671	16	12	2	8	6
141761110	15	18	2	7	10	91668195	16	13	2	8	6
179065245	15	20	2	7	11	104292897	16	14	2	8	7
56768510	17	8	2	8	5	65434039	17	9	2	8	5
75123399	17	10	2	8	6	85924267	17	11	2	8	6
97929150	17	12	2	8	7	111235513	17	13	2	8	7
125945907	17	14	2	8	8	179605763	17	17	2	8	9
201063991	17	18	2	8	10	224519775	17	19	2	8	10
250108870	17	20	2	8	11	70215621	18	8	2	9	4
86087796	19	8	2	9	5	80463451	18	9	2	9	4
111468329	19	10	2	9	6	104533448	18	11	2	9	5
142490188	19	12	2	9	7	190352497	18	16	2	9	8
180040477	19	14	2	9	8	212829627	18	17	2	9	8
225094076	19	16	2	9	9	264130592	18	19	2	9	9
278717737	19	18	2	9	10	293238635	18	20	2	9	10

Table 3.2: Maximum values of  $SW_5$  with given degree sequence and the extremal trees.

$SW_5$	a	b	c	x	y	$SW_5$	a	b	c	x	y
125476340	11	8	2	5	5	272517819	12	10	2	6	5
648225526	11	16	2	5	9	334217003	12	11	2	6	5
918311726	11	18	2	5	10	592958183	12	14	2	6	7
1276107057	11	20	2	5	11	709497719	12	15	2	6	7
245482195	13	8	2	6	5	1179116947	12	18	2	6	9
369359507	13	10	2	6	6	1383858171	12	19	2	6	9
775223742	13	14	2	6	8	1617369687	12	20	2	6	10
1087698601	13	16	2	6	9	302176017	13	9	2	6	5
1498520445	13	18	2	6	10	649560770	13	13	2	6	7
650323169	15	10	2	7	6	1279447903	13	17	2	6	9
921848852	15	12	2	7	7	1747938392	13	19	2	6	10
1281696158	15	14	2	7	8	846890675	16	10	2	8	5
1751421719	15	16	2	7	9	1003332080	16	11	2	8	5
2356293127	15	18	2	7	10	1623642767	16	14	2	8	7
1090509138	17	10	2	8	6	1890468368	16	15	2	8	7
1503151177	17	12	2	8	7	2919018587	16	18	2	8	9
2038146645	17	14	2	8	8	3351046296	16	19	2	8	9
2722856302	17	16	2	8	9	3835022321	16	20	2	8	10
3588975644	17	18	2	8	10	922603736	17	9	2	8	5
4672967991	17	20	2	8	11	1753741345	17	13	2	8	7
1283830534	19	8	2	9	5	3131077766	17	17	2	8	9
2362299333	19	12	2	9	7	4101260229	17	19	2	8	10
3134830449	19	14	2	9	8	1621101744	14	17	2	7	8
4106868832	19	16	2	9	9	776258692	15	11	2	7	6
5317544106	19	18	2	9	10	3840995850	18	17	2	9	8
6811457623	19	20	2	9	11	2040002356	19	11	2	9	6

Table 3.3: Maximum values of  $SW_6$  with given degree sequence and the extremal trees.

$SW_6$	a	b	c	x	y	$SW_6$	a	b	c	x	y
1012780165	11	8	2	5	5	1012780165	11	8	2	5	5
1331264987	11	9	2	5	5	1731853951	11	10	2	5	6
3608813138	11	13	2	5	7	10560454511	11	18	2	5	10
4534950599	11	14	2	5	8	15550588149	11	20	2	5	11
5657460420	11	15	2	5	8	1520069287	12	8	2	6	4
7009819461	11	16	2	5	9	2524690253	12	10	2	6	5
8629912837	11	17	2	5	9	4050773941	12	12	2	6	6
4050773941	12	12	2	6	6	8638448434	13	14	2	6	8
5072056334	12	13	2	6	6	12866164659	13	16	2	6	9
6306285405	12	14	2	6	7	18753342267	13	18	2	6	10
7788997943	12	15	2	6	7	26809726522	13	20	2	6	11
9560684147	12	16	2	6	8	3209798013	14	8	2	7	4
11666519353	12	17	2	6	8	5072598241	14	10	2	7	5
14157618741	12	18	2	6	9	7792737757	14	12	2	7	6
17090630090	12	19	2	6	9	11675925315	14	14	2	7	7
20529253585	12	20	2	6	10	17109278133	14	16	2	7	8
2230809113	13	8	2	6	5	24576550725	14	18	2	7	9
2849499660	13	9	2	6	5	34675147413	14	20	2	7	10
3609554789	13	10	2	6	6	4535536561	15	8	2	7	5
4536872092	13	11	2	6	6	7016085327	15	10	2	7	6
5661003560	13	12	2	6	7	10576941961	15	12	2	7	7
11675925315	14	14	2	7	7	26852307547	17	14	2	8	8
14170985717	14	15	2	7	7	37738910924	17	16	2	8	9
12873364697	15	13	2	7	7	22504194271	19	10	2	9	6
15583925551	15	14	2	7	8	31906141453	19	12	2	9	7
18768967316	15	15	2	7	8	44486984775	19	14	2	9	8
26838534790	15	17	2	7	9	82748051279	19	18	2	9	10

Table 3.4: Maximum values of  $SW_7$  with given degree sequence and the extremal trees.

$SW_7$	a	b	c	x	y	$SW_7$	a	b	c	x	y
1418556619	2	8	20	1	4	36550875	3	4	10	1	1
311943405	2	10	9	1	5	250749064	3	4	17	1	1
9480478	4	1	9	2	0	6815667522	5	17	2	2	2
1410192140	4	9	12	2	4	2733232	5	1	3	2	2
1725148897	6	4	17	3	2	81418949602	7	14	20	3	3
12762797695	6	14	9	3	7	56604679058	7	15	15	3	3
2060679963	6	8	10	3	4	17107655060	7	13	10	3	3
2465287834	6	10	7	3	5	145118866	7	4	3	3	3
80771821986	8	20	5	4	10	11046686401	9	7	13	4	4
90975587497	8	19	8	4	9	269950250613	9	19	15	4	4
19802685951	8	10	14	4	5	81507618756	9	12	18	4	4
22525721449	8	16	3	4	8	4958945486	9	7	8	4	4
17171414855	10	7	13	5	3	299171553379	11	16	16	5	5
533280126619	10	20	17	5	10	298912671768	11	17	14	5	5
298312777485	10	20	11	5	10	747441139	11	1	4	5	5
10984094929	10	8	8	5	4	22636924848	11	9	8	5	5
26005196806	12	7	10	6	3	3494203506	13	1	6	6	6
127990789661	12	16	5	6	8	534919367157	13	14	20	6	6
220140245657	14	12	12	7	6	365324821137	15	10	18	7	7
271271782123	14	9	20	7	4	56191006016	15	9	3	7	7
770114429581	16	12	19	8	6	71824937336	17	5	7	8	8
7950884958	16	1	2	8	0	38406698567	17	4	4	8	8
102326615747	18	3	11	9	1	299353872718	19	4	16	9	9
1187801963929	18	11	20	9	5	90868252330	19	3	7	9	9
441278902696	20	8	9	10	4	1400733246698	19	14	13	9	9
485826390403	20	7	12	10	3	2448113446450	19	17	14	9	9

## REFERENCES

- [1] E. Andriantiana, S. Wagner, H. Wang, *Greedy trees, subtrees and antichains*, Electron. J. Combin., 20 (2013), P28.
- [2] J. A. Bondy and U. S. R. Murty, *Graph Theory with Applications*, Macmillan (London) (1976).
- [3] P. Dankelmann, O. R. Oellermann, H. C. Swart, *The average Steiner distance of a Graph*, Journal of Graph Theory, 22 (1) (1996), 15–22.
- [4] P. Dankelmann, H. C. Swart, O. R. Oellermann, *On the average Steiner distance of graphs with prescribed properties*, Discrete Appl. Math., 79 (1997), 91–103.
- [5] A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: Theory and applications*, Acta Appl. Math., 66 (2001), 211–249.
- [6] R. C. Entringer, *Bounds for the average distance-inverse degree product in trees*, in: Y. Alavi, D. R. Lick, A. J. Schwenk (Eds.), *Combinatorics, Graph Theory, and Algorithms*, New Issues Press, Kalamazoo, 1999, 335–352.
- [7] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, *Wiener index versus maximum degree in trees*, Discrete Appl. Math., 122 (2002), 127–137.
- [8] I. Peterin, P. Z. Pleteršek, *Wiener index of strong product of graphs*, Opuscula Math., 38 (1) (2018), 81–94.
- [9] X. Li, Y. Mao, I. Gutman, *The Steiner Wiener index of a graph*, Discuss. Math. Graph Theory, 36 (2016), 455–465.
- [10] X. Li, Y. Mao, I. Gutman, *Inverse problem on the Steiner Wiener index*, Discuss. Math. Graph Theory, 38 (2018), 83–95.
- [11] L. Lu, Q. Huang, J. Hou, X. Chen, *A sharp lower bound on Steiner Wiener index for trees with given diameter*, Discrete Mathematics, 341 (2018), 723–731.
- [12] N. Schmuck, S. Wagner, H. Wang, *Greedy trees, caterpillars, and Wiener-type graph invariants*, MATCH Commun. Math. Comput. Chem., 68 (2012), 273–292.

- [13] R. Shi, *The average distance of trees*, Systems Sci. Math. Sci., 6 (1) (1993), 18–24.
- [14] L. A. Székely, H. Wang, *Binary trees with the largest number of subtrees*, Discrete Appl. Math., 155 (2007), 374–385.
- [15] L. A. Székely, H. Wang, *On subtrees of trees*, Adv. in Appl. Math., 34 (2005), 138–155.
- [16] L. A. Székely, H. Wang, *Extremal values of ratios: distance problems vs. subtree problems in trees*, The Electronic Journal of Combinatorics, 20(1) (2013), P67.
- [17] L. A. Székely, H. Wang, *Extremal values of ratios: distance problems vs. subtree problems in trees II*, Discrete Math., 322 (2014), 36–47.
- [18] S. Wagner, *On the Wiener index of random trees*, Discrete Math., 312 (9) (2012), 1502–1511.
- [19] H. Wang, *The extremal values of the Wiener index of a tree with given degree sequence*, Discrete Appl. Math., 156 (2008), 2647–2654.
- [20] S. Wang, X. Guo, *Trees with extremal Wiener indices*, MATCH Commun. Math. Comput. Chem., 60 (2008), 609–622.
- [21] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc., 69 (1947), 17–20.
- [22] H. Wiener, *Correlation of heats of isomerization, and differences in heats of vaporization of isomers, among the paraffin hydrocarbons*, J. Am. Chem. Soc., 69 (1947), 2636–2638.
- [23] W. Yan, Y-N. Yeh, *Enumeration of subtrees of trees*, Theoretical Computer Science, 369 (2006), 256–268.
- [24] J. Zhang, H. Wang, X.-D. Zhang, *Trees, degree sequences, and the Steiner Wiener index*, Preprint.
- [25] J. Zhang, H. Wang, X.-D. Zhang, *Revisiting the Wiener index and the number of subtrees*, Preprint.

- [26] X.-D. Zhang, Q.-Y. Xiang, L.-Q. Xu, R.-Y. Pan, *The Wiener index of trees with given degree sequences*, MATCH Commun. Math. Comput. Chem., 60 (2008), 623–644.
- [27] X.-M. Zhang, X.-D. Zhang, *The minimal number of subtrees with a given degree sequence*, Graphs and Combinatorics, 31 (2015), 309–318.
- [28] X.-M. Zhang, X.-D. Zhang, D. Gray, H. Wang, *The number of subtrees of trees with given degree sequence*, J. Graph Theory, 73 (2013), 280–295.