MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **81** (2019) 105-118

ISSN 0340 - 6253

The Wiener Index of Trees with Given Degree Sequence and Segment Sequence*

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(Received March 28, 2018)

Abstract

The Wiener index of a graph is defined as the sum of distances between all pairs of vertices. As one of the most well known chemical indices, the extremal structures that maximize or minimize the Wiener index have been extensively studied for many different classes of graphs, among which trees with a given degree sequence or segment sequence. In this note we consider trees in which both the degree sequence and segment sequence are predetermined, and examine the extremal problems. Characteristics of the extremal structures are presented, some directly from previously established methods. We also pose some questions from our study.

*This work is supported by the National Natural Science Foundation of China (Nos.11701372; 11526140; 11531001); the Joint NSFC-ISF Research Program (jointly funded by the National Natural Science Foundation of China and the Israel Science Foundation (No.11561141001)); Shanghai Natural Science Foundation (No.16ZR1422400); Shanghai YangFan Program (No.16YF1415900).

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1 Introduction

The study of chemical indices has been an important part of chemical graph theory. One of the most well known such indices is called the Wiener index, defined as the sum of distances between all pairs of vertices:

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

where $d(u,v)$ is the distance between vertices u and v in G [27, 28].

Many studies related to the Wiener index have been published over the years [2, 3, 6, 7, 10, 11, 13, 14, 20, 22, 25]. Among these studies we are particularly interested in the extremal problems. That is, among a given class of graphs, find the ones that maximize or minimize the Wiener index. Because of the important role that acyclic structures play in many chemists' and mathematicians' research interests, the examination of extremal trees has attracted much attention. For recent results in this direction one may see [4, 9, 12, 15, 17–19, 21].

Of various different constraints one may put on trees, the *degree sequence* (the non-increasing sequence of vertex degrees) is a natural condition corresponding to the valences of atoms in a molecular graph. The extremal tree with a given degree sequence, that minimizes the Wiener index, was identified in [26] and [30]. The trees that maximize the Wiener index, although they cannot be characterized completely, were shown to be caterpillars (trees that turn into paths when all leaves are removed) [24]. Such caterpillars must satisfy the so called $\vee$-property, that the vertex degrees on the backbone of the caterpillar must decrease from the two ends towards the middle [29].

A *segment* of a tree T is a path in T with the property that each of the ends is either a leaf or a branch vertex (of degree at least 3) and that all internal vertices of the path have degree 2. Similar to the degree sequence, the *segment sequence* of T is the non-increasing sequence of the lengths of all segments of T. For a given segment sequence $(l_1, l_2, \ldots, l_m)$, the *starlike tree* $S(l_1, l_2, \ldots, l_m)$ is the tree with exactly one vertex of degree ≥ 3 formed by identifying one end of each of the m segments. It was shown in [16] that $S(l_1, l_2, \ldots, l_m)$ minimizes the Wiener index among all trees with segment sequence $(l_1, l_2, \ldots, l_m)$. The extremal tree with a given segment sequence, that maximizes the Wiener index, was conjectured to be the *quasi-caterpillar* (a tree in which all branch vertices lie on a path, see Figure 1) in [16] and proved in [1].

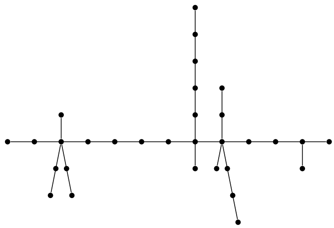

Figure 1: A quasi-caterpillar with segment sequence (5,5,3,3,2,2,2,2,1,1,1,1,1).

In this note we will consider the extremal problems, with respect to the Wiener index, among trees with both of degree sequence and segment sequence predetermined. First, in Section 2, we introduce an operation that increases or decreases the Wiener index under certain conditions. This operation, used in some so-called "sliding lemma", leads to basic properties related to the degrees and segments along a path in an extremal tree. Such properties are analogous to the aforementioned $\vee$-property. We then show in Section 3 that the tree with maximum Wiener index among trees with both given degree and segment sequences must be a quasi-caterpillar. This proof, although technical, is very similar to that in [1]. Through further analysis we present the characteristics of this maximizing quasi-caterpillar in Section 4. Lastly we summarize our findings in Section 5, where we also briefly discuss the difficulty in completely characterizing the extremal trees that minimize the Wiener index.

2 The "sliding lemma" and properties of extremal trees

First let us introduce the following observation on the change of the value of the Wiener index when we "slide" a part of a tree along a path. For this purpose let v be on a path $P(u,w)$ from u to w in T, such that v is the only branch vertex on $P(u,w)$ and $d(u,v) < d(v,w)$. Furthermore, let T_u, T_v, T_w denote the components in $T - E(P(u,w))$ that contain u, v, w, respectively.

Lemma 2.1 *Following the above notations, suppose v' is on $P(u,w)$ such that $d(u,v') = d(v,w)$ and $d(v',w) = d(u,v)$. Let T' be obtained from T by detaching T_v from v and reattaching it to v' (Figure 2).*

- *If $|T_u| \geq |T_w|$, then $W(T') \geq W(T)$ with equality if and only if $|T_u| = |T_w|$.*

- *If $|T_u| \leq |T_w|$, then $W(T') \leq W(T)$ with equality if and only if $|T_u| = |T_w|$.*

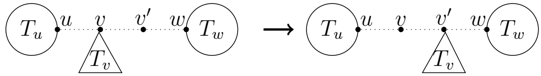

Figure 2: "Sliding" T_v from v to v'.

Proof. We will only prove the first case, the second one is similar.

Note that from T to T', only the distances between vertices in $T_v - \{v\}$ and vertices not in $T_v - \{v\}$ changed. Among such pairs of vertices, the sum of all distances from a vertex x in $T_v - \{v\}$ to all vertices on the path $P(u,w)$ remains the same. Consequently we only need to consider the distances between a vertex in $T_u - \{u\}$ or $T_w - \{w\}$ and a vertex in $T_v - \{v\}$.

- If $x \in V(T_v) - \{v\}$ and $y \in V(T_u) - \{u\}$, then $d(x,y)$ increased by $d(v,v')$ from T to T';

- Similarly, if $x \in V(T_v) - \{v\}$ and $y \in V(T_w) - \{w\}$, then $d(x,y)$ decreased by $d(v,v')$ from T to T'.

Thus

$$W(T') - W(T) = (|T_v| - 1)(|T_u| - |T_w|)d(v,v') \geq 0$$

with equality if and only if $|T_u| = |T_w|$. ■

It is easy to see that the above "sliding" operation does not change the degree sequence or the segment sequence of the tree. Applying Lemma 2.1 to the extremal trees with given degree and segment sequences yields some interesting partial characteristics of the extremal trees.

First we will consider trees, with given degree and segment sequences, that minimize the Wiener index. For such a tree T, let P be a path with the greatest number of segments in T and denote the shortest segment on P by $P(u_1,v_1)$ with $d(u_1,v_1) = c$. We now label the branch vertices on P by $v_1, v_2, \cdots$ on the same side of $P(u_1,v_1)$ as v_1, and $u_1, u_2, \cdots$ on the same side of $P(u_1,v_1)$ as u_1. Let X_i (Y_j) denote the component containing u_i (v_j) in $T - E(P)$, we will consider the relations between $|X_i|$'s, $|Y_j|$'s, as well as $a_i = d(u_i,u_{i+1})$ and $b_j = d(v_j,v_{j+1})$ as illustrated in Figure 3. Here we use $X_{\geq t}$ to denote the graph induced by $X_t, X_{t+1}, \ldots$. Similarly for $Y_{\geq t}$.

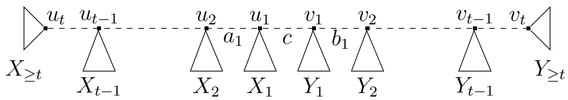

Figure 3: Path P with the greatest number of segments.

Proposition 2.1 *If T minimizes the Wiener index, among all trees with given degree and segment sequences, then for P described as above we may assume*

- $c \leq a_1 \leq b_1$*;*
- $|X_1| \geq |X_2| \geq \ldots$*;*
- $|Y_1| \geq |Y_2| \geq \ldots$*;*
- $c \leq a_1 \leq a_2 \leq \ldots$*;*
- $c \leq b_1 \leq b_2 \leq \cdots$*.*

Proof. First, since $P(u_1, v_1)$ is the shortest segment on P, we may assume, without loss of generality, that $c \leq a_1 \leq b_1$. We now claim that

$$|Y_{\geq 1}| \geq |X_{\geq 2}|. \tag{1}$$

If $c = a_1$, then it is easy to see that (1) can be achieved by relabeling the graph if necessary. Otherwise, let $c < a_1$, if (1) is not true, then $|Y_{\geq 1}| < |X_{\geq 2}|$. Lemma 2.1 implies that sliding X_1 from u_1 towards u_2 would decrease the Wiener index, a contradiction to the extremality of T.

With (1), suppose now, for contradiction, that $|X_1| < |X_2|$. Let T' be obtained from T by "switching" the components X_1 and X_2. From T to T', we have:

- the distance between any vertex in X_2 and any vertex in $Y_{\geq 1} \cup P(u_1, v_1)$ decreases by a_1;
- the distance between any vertex in X_1 and any vertex in $Y_{\geq 1} \cup P(u_1, v_1)$ increases by a_1;
- the distance between any vertex in X_2 and any vertex in $X_{\geq 2} - X_2$ increases by a_1;
- the distance between any vertex in X_1 and any vertex in $X_{\geq 2} - X_2$ decreases by a_1;

- the distances between vertices of X_1 and the vertices on the segment between u_1 and u_2 change, but the total contribution to the Wiener index remains the same; the same is true for X_2.
- all distances between other pairs of vertices stay the same.

Hence

$$W(T') - W(T) = a_1\big(|X_1| - |X_2|\big) \cdot \big(|Y_{\geq 1} \cup P(u_1, v_1)| - |X_{\geq 2} - X_2|\big) < 0,$$

a contradiction.

Note that by $|Y_{\geq 1} \cup X_1 \cup P(u_1, v_1)| > |Y_{\geq 1}| \geq |X_{\geq 2}| > |X_{\geq 3}|$, we can show $|X_2| \geq |X_3|$ through exactly the same argument. And more generally, $|X_1| \geq |X_2| \geq |X_3| \geq \ldots$.

Similarly, we also conclude $|Y_1| \geq |Y_2| \geq \ldots$.

Next we show that $c \leq a_1 \leq a_2$. Otherwise, suppose $a_1 > a_2$. Note that from (1) we must have $|X_{\geq 3}| \geq |X_1 \cup P(u_1, v_1) \cup Y_{\geq 1}|$, a contradiction. Thus $c \leq a_1 \leq a_2$. More generally we have $c \leq a_1 \leq a_2 \leq \ldots$ and similarly $c \leq b_1 \leq b_2 \leq \cdots$. ■

Similar conclusions can be drawn for trees that maximize the Wiener index, we skip the proofs.

Proposition 2.2 *If T maximizes the Wiener index, among all trees with given degree and segment sequences, then for P described as above but with $P(u_1, v_1)$ being the longest segment on P, we may assume*

- $c \geq a_1 \geq b_1$;
- $|X_1| \leq |X_2| \leq \ldots$;
- $|Y_1| \leq |Y_2| \leq \ldots$;
- $c \geq a_1 \geq a_2 \geq \ldots$;
- $c \geq b_1 \geq b_2 \geq \cdots$.

3 Maximum Wiener index in trees with given degree and segment sequences

In this section we show that the tree maximizing the Wiener index, given degree and segment sequences, must be a quasi-caterpillar. The proof is very similar to that of [1] and we skip some details.

Theorem 3.1 *Among trees with given degree sequence and segment sequence, the Wiener index is maximized only by quasi-caterpillars.*

Proof. For convenience we will call an extremal tree T with the maximum Wiener index an *optimal tree*. Let $P = P(v_0, v_k)$ be a path of T with the greatest number of segments, and label the branch vertices on P by $v_1, v_2, \ldots, v_{k-1}$ (from v_0, towards v_k). For each i between 1 and $k-1$, let the neighbors of v_i that do not lie on P be $v_{i,1}, \ldots, v_{i,l_i}$, and let $T_{i,j}$ $(1 \leq j \leq l_i)$ denote the component containing $v_{i,j}$ after removing the edge $v_i v_{i,j}$.

In each of the subtrees $T_{i,j}$, consider the branch vertex (or leaf if there is no branch vertex) closest to v_i and call it $u_{i,j}$. We then use $S_{i,j}$ for the component containing $u_{i,j}$ in $T - E(P(v_i, u_{i,j}))$ (Figure 4).

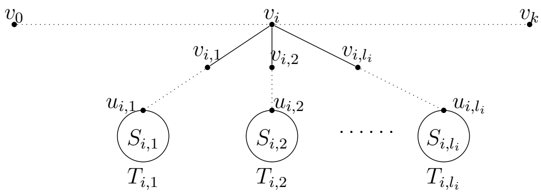

Figure 4: The labeling of T

Supposing, for contradiction, that T is not a quasi-caterpillar, then let $S = S_{i_0,j_0}$ be of the largest order among $S_{i,j}$ $(1 \leq i \leq k,\ 1 \leq j \leq l_i)$. Let $T_{\leq i_0}$ denote the component containing v_{i_0} in $T - E(P(v_{i_0}, v_{i_0+1}))$ and $T_{>i_0}$ the component containing v_{i_0+1} in $T - E(P(v_{i_0}, v_{i_0+1}))$. Similarly for $T_{<i_0}$ and $T_{\geq i_0}$. As in [1], we may assume, without loss of generality, that

$$|T_{<i_0}| \geq |T_{>i_0}| \text{ and } |S| > |S_{i,j}| \text{ for all } i > i_0 \text{ and all } j.$$

By our choice of P as a path with the greatest number of segments, v_{i_0} cannot be the last branch vertex and hence v_{i_0+1} is still a branch vertex. We now consider the subtree $T_{i_0+1,1}$ consisting of the path from v_{i_0+1} to $u_{i_0+1,1}$ and the subtree $S' = S_{i_0+1,1}$ (Figure 5). Denote p (p', respectively) be the length of the path $P(v_{i_0}, u_{i_0,j_0})$ ($P(v_{i_0+1}, u_{i_0+1,1})$, respectively).

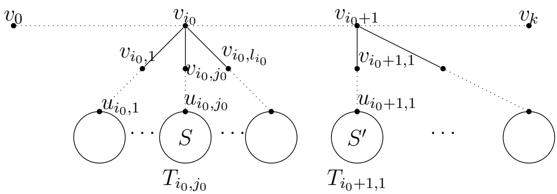

Figure 5: The branches that are switched.

We can now construct a new tree T':

1. If $p \geq p'$, let T' be obtained from T by switching T_{i_0,j_0} and $T_{i_0+1,1}$.

2. If $p < p'$, let T' be obtained from T by switching S and S'.

It has been shown in [1], that we have

$$W(T') - W(T) > 0$$

in either case. We also note that from T to T' both the degree sequence and the segment sequence stay the same, hence yielding a contradiction to the optimality of T. ■

4 Further characterization of the extremal quasi-caterpillar

In a quasi-caterpillar, let the path containing all the branch vertices be called the *backbone*. We call all the segments that do not lie on the backbone (and thus connect a leaf with a branch vertex) *pendant segments*. For a tree with given degree and segment sequences that maximize the Wiener index, knowing that it has to be a quasi-caterpillar from Theorem 3.1, we now show some further properties of such an optimal quasi-caterpillar in terms of the ordering of vertex degrees and segment lengths.

Theorem 4.1 *For a quasi-caterpillar that maximizes the Wiener index among trees with given degree and segment sequences, let the backbone contain k segments which are of lengths $r_1, r_2, \ldots, r_k$ from one end to another. Then there must exist a*

$$j_0 \in \{1, 2, \ldots, k\}$$

such that the following are satisfied:

1. *The sequence* $r_1, r_2, \ldots, r_k$ *is unimodal, i.e.,*

$$r_1 \le r_2 \le \cdots \le r_{j_0} \ge \cdots \ge r_k;$$

2. *Let the branch vertices be* v_i *for* $1 \le i \le k-1$ *such that* $P(v_i, v_{i+1})$ *is the segment with length* r_{i+1}*. Denote the lengths of the pendent segments attached at* v_i *by* $s_{i,t}$*,* $1 \le t \le \ell_i$ *where* $\deg(v_i) = \ell_i + 2$ *for* $1 \le i \le k-1$*. Then*

$$\max_{1\le t\le \ell_{i+1}} s_{i+1,t} \le \min_{1\le t\le \ell_i} s_{i,t} \text{ for } i \le j_0 - 2 \tag{2}$$

and

$$\max_{1\le t\le \ell_{i-1}} s_{i-1,t} \le \min_{1\le t\le \ell_i} s_{i,t} \text{ for } i \ge j_0 \tag{3}$$

3. *Recall that* $\deg(v_i) = \ell_i + 2$ *for* $1 \le i \le k-1$*, we have*

$$\ell_1 \ge \ell_2 \ge \cdots \ge \ell_{j_0-1}, \text{ and } \ell_{j_0} \le \ell_{j_0+1} \le \cdots \le \ell_{k-1},$$

or equivalently,

$$\deg(v_1) \ge \deg(v_2) \ge \cdots \ge \deg(v_{j_0-1}), \text{ and } \deg(v_{j_0}) \le \deg(v_{j_0+1}) \le \cdots \le \deg(v_{k-1}).$$

Proof. Part (1) follows from essentially the same proof as that in [1] through repeated application of Lemma 2.1. We skip the proof here.

(2) Following the notations in Theorem 3.1, note that each $T_{i,j}$ is simply a pendant segment with a common end vertex. Let $i_0 \le j_0 - 2$ be the largest index where (2) failed and

$$s_{i_0,t_0} < s_{i_0+1,t_0'}$$

for some t_0 and t_0'.

Consider, now, the tree T' obtained from T by switching T_{i_0,t_0} and $T_{i_0+1,t_0'}$ (Figure 6).

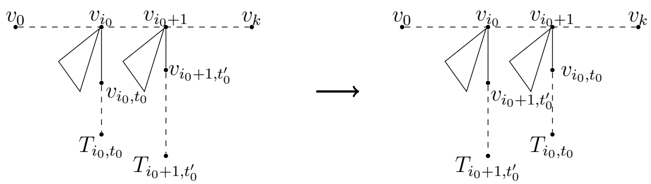

Figure 6: The trees T and T' in case (2)

It is easy to see that T' has the same degree and segment sequences as T. From T' to T, we have the following changes in the distances between vertices:

- the distance between any vertex in $T_{\leq i_0} - T_{i_0,t_0}$ and any vertex in T_{i_0+1,t'_0} decreases by $d(v_{i_0}, v_{i_0+1}) = r_{i_0+1}$;
- the distance between any vertex in $T_{\geq i_0+1} - T_{i_0+1,t'_0}$ and any vertex in T_{i_0+1,t'_0} increases by $d(v_{i_0}, v_{i_0+1}) = r_{i_0+1}$;
- the distance between any vertex in $T_{\leq i_0} - T_{i_0,t_0}$ and any vertex in T_{i_0,t_0} increases by $d(v_{i_0}, v_{i_0+1}) = r_{i_0+1}$;
- the distance between any vertex in $T_{\geq i_0+1} - T_{i_0+1,t'_0}$ and any vertex in T_{i_0,t_0} decreases by $d(v_{i_0}, v_{i_0+1}) = r_{i_0+1}$;
- the distances between vertices of T_{i_0,t_0} and the vertices in $P(v_{i_0}, v_{i_0+1})$ change, but the total contribution to the Wiener index remains the same; the same is true for T_{i_0+1,t'_0}.

Consequently,

$$W(T') - W(T) = r_{i_0+1}\big(s_{i_0+1,t'_0} - s_{i_0,t_0}\big) \cdot \big(|T_{\geq i_0+1} - T_{i_0+1,t'_0}| - |T_{\leq i_0} - T_{i_0,t_0}|\big).$$

Since $r_{i_0+1} \leq r_{i_0+2}$, by Lemma 2.1, $|T_{\geq i_0+2}| \geq |T_{\leq i_0}|$. Then

$$|T_{\leq i_0} - T_{i_0,t_0}| < |T_{\leq i_0}| \leq |T_{\geq i_0+2}| < |T_{\geq i_0+1} - T_{i_0+1,t'_0}|.$$

Thus $W(T') > W(T)$, a contradiction.

(3) can be shown in exactly the same way.

(3) First we show that $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_{j_0-1}$, otherwise, let i_0 $(< j_0)$ be the largest index such that $\ell_{i_0-1} < \ell_{i_0}$.

Let $\ell_{i_0} - \ell_{i_0-1} = x$ and define

$$T_{i_0,\leq x} = T_{i_0,1} \cup T_{i_0,2} \cup \cdots \cup T_{i_0,x}.$$

Consider the tree

$$T' = T - \{v_{i_0}v_{i_0,1}, v_{i_0}v_{i_0,2}, \cdots, v_{i_0}v_{i_0,x}\} + \{v_{i_0-1}v_{i_0,1}, v_{i_0-1}v_{i_0,2}, \cdots, v_{i_0-1}v_{i_0,x}\}.$$

Again it is easy to see that the degree sequence and segment sequence stay the same from T to T' (Figure 7):

- the distance between any vertex in $T_{\leq i_0-1}$ and any vertex in $T_{i_0,\leq x}$ decreases by $d(v_{i_0-1}, v_{i_0}) = r_{i_0}$;
- the distance between any vertex in $T_{\geq i_0} - T_{i_0,\leq x}$ and any vertex in $T_{i_0,\leq x}$ increases by $d(v_{i_0-1}, v_{i_0}) = r_{i_0}$;
- the distances between vertices of $T_{i_0,\leq x}$ and the vertices on $P(v_{i_0-1}, v_{i_0})$ change, but the total contribution to the Wiener index remains the same.

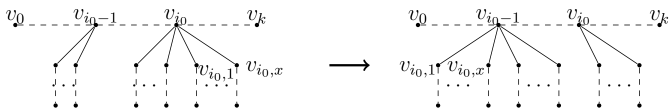

Figure 7: Transformation in case (3)

Hence

$$W(T') - W(T) = r_{i_0} \cdot |T_{i_0,\leq x}| \cdot \big(|T_{\geq i_0} - T_{i_0,\leq x}| - |T_{\leq i_0-1}|\big).$$

Again by Lemma 2.1 and the fact that $r_{i_0} \leq r_{i_0+1}$, we have $|T_{\geq i_0+1}| \geq |T_{\leq i_0-1}|$ and

$$|T_{\leq i_0-1}| \leq |T_{\geq i_0+1}| < |T_{\geq i_0} - T_{i_0,\leq x}|.$$

Thus $W(T') > W(T)$, a contradiction.

Similarly, one can show that $\ell_{j_0} \leq \ell_{j_0+1} \leq \cdots \leq \ell_{k-1}$. ■

5 Concluding remarks

In this note we considered extremal problems, with respect to the Wiener index, among trees with given degree and segment sequences. We first presented a "sliding lemma" that is very similar to other versions of lemmas under the same name, while maintaining both degree and segment sequences. This lemma is then used to find partial characteristics of the extremal trees that minimize or maximize the Wiener index, with given degree and segment sequences. Through more detailed analysis, we show that the tree with the maximum Wiener index must be a quasi-caterpillar, and provide further characterizations of this extremal quasi-caterpillar. Some of the proofs are direct applications of previously established techniques.

On the other hand, the analogue of Proposition 2.1 for trees with only predetermined degree sequence (but not segment sequence), first established in [26], was an important part of a proof that established the extremality of the greedy tree among trees with a given degree sequence. The other part of the proof in [26] requires the comparison between the components X_i and Y_i in Proposition 2.1 for any i. The following examples show that we do not have an easy way to do this even in the $i = 1$ case, where we have $|X_1| < |Y_1|$ in Figure 8 and $|X_1| > |Y_1|$ in Figure 9. But "switching" X_1 and Y_1 in either case would result in an increase in the Wiener index. This presents the main difficulty in identifying the extremal tree that minimizes the Wiener index with given degree and segment sequences, which we leave as an open problem.

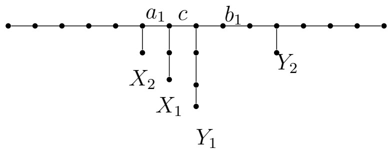

Figure 8: A tree with $|X_1| < |Y_1|$.

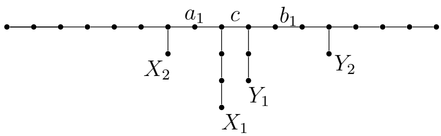

Figure 9: A tree with $|X_1| > |Y_1|$.

Acknowledgments: The authors would like to thank the anonymous referees for many helpful comments.

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