

Maximum Wiener Index of Trees with Given Segment Sequence*

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Abstract

A segment of a tree is a path whose ends are branching vertices (vertices of degree greater than 2) or leaves, while all other vertices have degree 2. The lengths of all the segments of a tree form its segment sequence.

In this note we consider the problem of maximizing the Wiener index among trees with given segment sequence or number of segments, answering two questions proposed in a recent paper on the subject. We show that the maximum is always obtained for a so-called quasi-caterpillar, and we also further characterize its structure.

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1 Introduction

The *Wiener index* of a graph G is defined as the sum of all distances between pairs of vertices in G :

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$$

where $d_G(u, v)$ (or simply $d(u, v)$ when there is no ambiguity) is the distance between u and v . Introduced in 1947 [18], the Wiener index has received much attention in the past decades, and several variants and generalizations have been proposed as well. Extremal problems in particular have been studied extensively. Here, the general question is: given a family of graphs, what can be said about the maximum and minimum values of the Wiener index and the graphs for which these are attained? It is very well known that the maximum and minimum are attained by the path and the star respectively (see [2, Equation (3)]) if the family of all trees is considered. Much further work has been done, however, on characterizing the trees that maximize or minimize the Wiener index under various additional conditions: given maximum degree [4, 14, 17], degree sequence [13, 15, 16, 20], diameter [11, 12, 17], independence or matching number [1, 3, 10], and many more [5-8]. Here, we will specifically be interested in the family of trees with a given *segment sequence*, as studied in a recent paper by Lin and Song [9].

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 *branching vertex* (vertex whose degree is at least 3) and that all internal vertices of the path have degree 2. The *segment sequence* of T is the non-increasing sequence of the lengths of all segments of T , in analogy to the degree sequence. There are several formulas that allow for the efficient calculation of the Wiener index based on segment lengths, see [2, Section 5]. To give one example, let us denote the length of a segment S by ℓ_S and the number of vertices in the two components that result when all internal vertices and edges of S are removed by $n_1(S)$ and $n_2(S)$ respectively. Then (see [2, Theorem 10])

$$W(T) = \sum_S \ell_S n_1(S) n_2(S) + \frac{1}{6} \sum_S \ell_S (\ell_S - 1) (3n - 2\ell_S + 1),$$

where both sums are taken over all segments of T . This relation between the Wiener index and segments was also the motivation for considering extremal problems based on

segments. Specifically: given the segment sequence of a tree, what are the maximum and minimum values of the Wiener index, and what are the corresponding extremal trees?

For a given segment sequence (l_1, l_2, \dots, l_m) , the *starlike tree* $S(l_1, l_2, \dots, l_m)$ 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 a recent paper [9] that $S(l_1, l_2, \dots, l_m)$ minimizes the Wiener index among all trees with segment sequence (l_1, l_2, \dots, l_m) .

This leaves the natural question which trees with segment sequence (l_1, l_2, \dots, l_m) maximize the Wiener index. The answer to this question seems to be much more complicated, but the authors of [9] presented a conjecture. Specifically, they asked for the following:

Question 1 Define a *quasi-caterpillar* to be a tree with the property that all its branching vertices (vertices of degree greater than 2) lie on a path (see Figure 1). Does the tree maximizing the Wiener index among all trees with a given segment sequence always have to be a quasi-caterpillar?

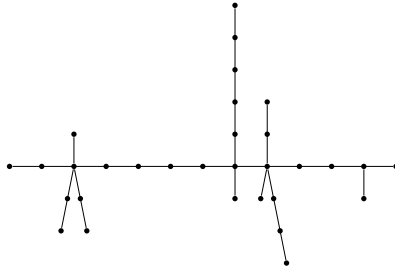


Figure 1: A quasi-caterpillar with segment sequence $(5, 5, 3, 3, 2, 2, 2, 2, 1, 1, 1, 1, 1)$.

Also in [9], the tree with minimal Wiener index among all trees with given number of segments is characterized. Again, we are interested in the analogous question for the maximum, for which a conjecture was presented in [9] as well.

For given n and m , we define trees $O(n, m)$ (for odd m) and $E(n, m)$ (for even m) respectively. The graph $O(n, m)$ is obtained from a path $v_0 v_1 \dots v_\ell$ of length $\ell = n - \frac{m+1}{2}$ by attaching a total of $\frac{m-1}{2}$ leaves to vertices $v_1, v_2, \dots, v_{\lfloor (m-1)/4 \rfloor}$ and $v_{\ell-1}, v_{\ell-2}, \dots, v_{\ell - \lceil (m-1)/4 \rceil}$; see Figure 2 (left) for the case $n = 11, m = 7$. Note that $O(n, m)$ has exactly m segments.

Likewise, $E(n, m)$ is a tree with n vertices and m segments obtained from a path $v_0 v_1 \dots v_\ell$ of length $\ell = n - \frac{m}{2} - 1$ by attaching a total of $\frac{m}{2}$ leaves to vertices $v_1, v_2, \dots, v_{\lfloor (m-2)/4 \rfloor}$ and $v_{\ell-1}, v_{\ell-2}, \dots, v_{\ell - \lfloor (m-2)/4 \rfloor}$, where two leaves are attached to vertex v_1 (so that it becomes the only vertex of degree 4), see Figure 2 (right) for the case $n = 11, m = 8$.



Figure 2: The trees $O(11, 7)$ and $E(11, 8)$.

We remark that $O(n, m)$ and $E(n, m)$ are very similar to the trees that maximize the Wiener index among trees with given number of vertices n and domination number γ (if $\gamma \geq n/3$), see [19, Corollary 3.3].

Question 2 Do $O(n, m)$ (if m is odd) and $E(n, m)$ (if m is even) always maximize the Wiener index among all trees of order n with m segments?

In this note positive answers are provided to both questions. We also present some further characterization of the extremal quasi-caterpillars.

2 Trees with given segment sequence

In this section, we answer Question 1 affirmatively. The main theorem reads as follows:

Theorem 1 *If a tree T maximizes the Wiener index among all trees with the same segment sequence, then it must be a quasi-caterpillar.*

Proof: Before we start with the actual proof, let us fix some terminology and notation. We will call a tree with maximum Wiener index among all trees with the same segment sequence an *optimal tree*. We also write $P(v, w)$ for the unique path between vertices v and w in a tree T (which does not necessarily have to be a segment).

Now let T be an optimal tree, and let P be a path with the greatest possible number of segments on it. Clearly, the two ends of P have to be leaves; we will denote the ends of P by v_0 and v_k and the branching vertices on P by v_1, v_2, \dots, v_{k-1} (in the order of their distances from v_0). For each i ($1 \leq i \leq k - 1$), let the neighbors of v_i that do not lie

on P be v_{i1}, \dots, v_{il_i} , and let T_{ij} ($1 \leq j \leq l_i$) denote the component containing v_{ij} after removing the edge between v_i and v_{ij} .

In each of the subtrees T_{ij} , consider the branching vertex (or leaf if there is no branching vertex) closest to v_i and call it u_{ij} . Finally, we write S_{ij} for the component containing u_{ij} in $T - E(P(v_i, u_{ij}))$ (Figure 3).

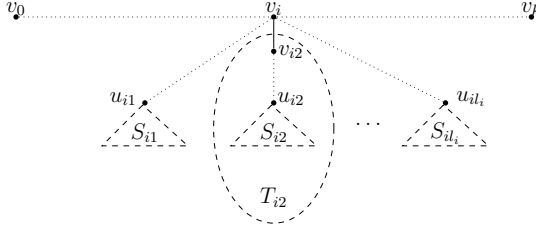


Figure 3: The labeling of T

If S_{ij} is a single vertex for every i and j , then T is a quasi-caterpillar, and we are done.

Otherwise, let $S = S_{i_0 j_0}$ have the greatest number of vertices among all S_{ij} ($1 \leq i \leq k-1, 1 \leq j \leq l_i$). Let $T_{< i_0}$ 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 $T - E(P(v_{i_0}, v_{i_0+1}))$. The subtrees $T_{< i_0}$ and $T_{\geq i_0}$ are defined analogously. Suppose, without loss of generality, that

$$|T_{< i_0}| \geq |T_{> i_0}|, \tag{1}$$

where $|G|$ denotes, here and in the following, the number of vertices of a graph G . Moreover, we can assume that $|S| > |S_{ij}|$ for all $i > i_0$ and all j ; for if not, we could consider a subtree S_{ij} with $|S_{ij}| = |S|$ for which the index i is maximal instead of S itself, and (1) still holds.

By our choice of the path $P = P(v_0, v_k)$ as a path with the greatest number of segments on it, $i_0 \neq k-1$, i.e., v_{i_0} cannot be the last branching vertex (since then there would be a path through $u_{i_0 j_0}$ rather than v_k that contains more segments). Thus v_{i_0+1} is still a branching vertex. 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 4).

Next we distinguish two cases, depending on the lengths of the paths $P(v_{i_0}, u_{i_0 j_0})$ and $P(v_{i_0+1}, u_{i_0+1,1})$, which we denote by p and p' respectively:

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

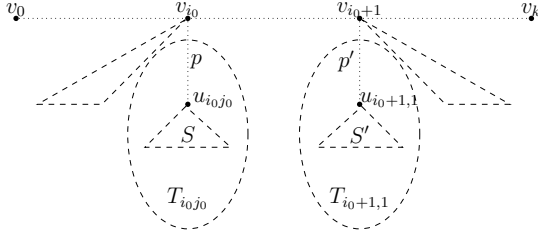


Figure 4: The branches that are switched.

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

It is easy to see that in either case T' has the same segment sequence as T . Let us determine how the Wiener index changes through these operations.

- In the first case, the changes from T to T' are:
 - the distance between any vertex in $T_{i_0 j_0}$ and any vertex in $T_{\leq i_0} - T_{i_0 j_0}$ increases by $d(v_{i_0}, v_{i_0+1})$;
 - the distance between any vertex in $T_{i_0 j_0}$ and any vertex in $T_{> i_0} - T_{i_0+1, 1}$ decreases by $d(v_{i_0}, v_{i_0+1})$;
 - the distance between any vertex in $T_{i_0+1, 1}$ and any vertex in $T_{\leq i_0} - T_{i_0 j_0}$ decreases by $d(v_{i_0}, v_{i_0+1})$;
 - the distance between any vertex in $T_{i_0+1, 1}$ and any vertex in $T_{> i_0} - T_{i_0+1, 1}$ increases by $d(v_{i_0}, v_{i_0+1})$;
 - the distances between vertices of $T_{i_0 j_0}$ and the vertices on the segment between v_{i_0} and v_{i_0+1} change, but the total contribution to the Wiener index remains the same; the same is true for $T_{i_0+1, 1}$.
 - all distances between other pairs of vertices stay the same.

Consequently, the total change is

$$W(T') - W(T) = d(v_{i_0}, v_{i_0+1}) (|T_{i_0 j_0}| - |T_{i_0+1, 1}|) (|T_{\leq i_0} - T_{i_0 j_0}| - |T_{> i_0} - T_{i_0+1, 1}|) .$$

Note that

$$|T_{\leq i_0} - T_{i_0 j_0}| > |T_{< i_0}| \geq |T_{> i_0}| > |T_{> i_0} - T_{i_0+1, 1}| ,$$

and that $|S| > |S'|$ by the assumptions on $S = S_{i_0j_0}$ that we made, so $|T_{i_0j_0}| > |T_{i_0+1,1}|$. Thus $W(T') > W(T)$, a contradiction.

- In the second case, we only need to consider the change of distance between vertices in S and S' and the rest of the tree. In the same way as before, we obtain

$$W(T') - W(T) = (d(v_{i_0}, v_{i_0+1}) + p' - p)(|S| - |S'|)(|T_{\leq i_0} - T_{i_0j_0}| - |T_{> i_0} - T_{i_0+1,1}|),$$

which is again positive, and we reach another contradiction.

In both cases, we see that T cannot be optimal, which completes our proof. ■

3 Further characterization of the extremal trees

Let the longest path of a quasi-caterpillar containing all the branching vertices be called the *backbone*; all segments that do not lie on the backbone (and thus connect a leaf with a branching vertex) are called *pendant segments*. Let a segment sequence (l_1, l_2, \dots, l_m) be given; we know from Theorem 1 that the maximum of the Wiener index can only be attained for a quasi-caterpillar. In this section, we present some further characteristics of extremal quasi-caterpillars. The technical details are somewhat similar to the proof of Theorem 1, and we skip some details.

Theorem 2 *A quasi-caterpillar that maximizes the Wiener index among trees with segment sequence (l_1, l_2, \dots, l_m) must satisfy the following:*

1. *If the number of segments is odd, all branching vertices have degree exactly 3. If the number of segments is even, all but one of the branching vertices have degree 3. The only exception must be a branching vertex of degree 4, which must be the first (or last) branching vertex on the backbone. This also means that the number of segments on the backbone is $k = \lfloor (m+1)/2 \rfloor$, the number of pendant segments is $k' = \lceil (m-1)/2 \rceil$.*
2. *The lengths of the segments on the backbone, listed from one end to the other, form a unimodal sequence r_1, r_2, \dots, r_k , i.e.,*

$$r_1 \leq r_2 \leq \dots \leq r_j \geq \dots \geq r_k$$

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

3. The lengths of the pendant segments, starting from one end of the backbone towards the other, form a sequence of values $s_1, s_2, \dots, s_{k'}$ such that

$$s_1 \geq s_2 \geq \dots \geq s_{j'} \leq \dots \leq s_{k'}$$

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

Proof: We provide justification for each of the above claims as follows:

(1) Let the backbone be the path $P(v_0, v_k)$ between leaves v_0 and v_k with branching vertices v_1, v_2, \dots, v_{k-1} (in the order of their distances from v_0). First we claim that no branching vertex is of degree greater than 4. Otherwise, let v_i be of degree at least 5 with neighbors $v_{i1}, v_{i2}, v_{i3}, \dots$ not on $P(v_0, v_k)$. Let $T_{<i}$ ($T_{>i}$) denote the component containing v_{i-1} (v_{i+1}) in $T - E(P(v_{i-1}, v_{i+1}))$ as before, and let $T_{\leq i} = T_{<i+1}$ and $T_{\geq i} = T_{>i-1}$ be defined as in the proof of Theorem 1 as well. Finally, let T_{i1}, T_{i2}, T_{i3} be the pendant segments at v_i containing v_{i1}, v_{i2}, v_{i3} respectively.

Suppose, without loss of generality, that

$$|T_{<i}| \geq |T_{>i}|,$$

so that

$$|T_{\leq i} - T_{i1} - T_{i2}| > |T_{>i}|.$$

Let T' be obtained from T by detaching T_{i1} and T_{i2} from v_i and reattaching them to v_{i+1} . Note that T' has the same segment sequence as T , even if $i = k - 1$. The same argument as in the proof of Theorem 1 shows that $W(T') - W(T) = d(v_i, v_{i+1}) (|T_{i1}| + |T_{i2}|) \cdot (|T_{\leq i} - T_{i1} - T_{i2}| - |T_{>i}|) > 0$, and we reach a contradiction.

Now we know that all branching vertices are of degree 3 or 4. We can repeat the same argument as before with a vertex v_i of degree 4 (moving only one segment instead of two) to obtain a contradiction, unless $v_i = v_1$ or $v_i = v_{k-1}$ (in which case we would have to move a single segment to the end of the backbone, which changes the segment sequence). Thus the only branching vertices that could possibly have degree 4 are v_1 and v_{k-1} .

Now assume that both v_1 and v_{k-1} are vertices of degree 4. Let $S = T_{11}$ and $S' = T_{k-1,1}$ be two segments attached to v_1 and v_{k-1} respectively, and let R be obtained from T by removing these two segments (Figure 5). Suppose, without loss of generality, that

$$\sum_{v \in V(R)} d(v_k, v) \leq \sum_{v \in V(R)} d(v_0, v).$$

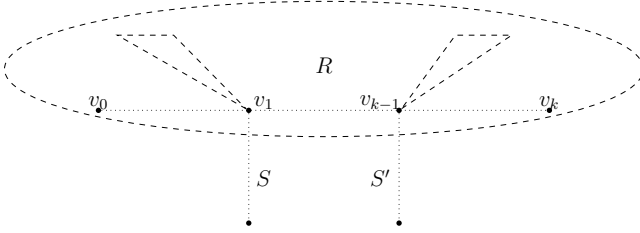


Figure 5: The segments S and S' and the rest of the tree (denoted R).

Let T' be obtained from T by removing both S and S' and attaching them to v_0 . Evidently, T' and T have the same segment sequence. Let us again see how the Wiener index changes:

- the distance between any two vertices in S , any two vertices in S' , or any two vertices in R does not change;
- the total distance between all vertices in S and all vertices in S' decreases by $d(v_1, v_{k-1})|S||S'|$;
- the total distance between vertices in S and $P(v_0, v_1)$ does not change, while the total distance between vertices in S and the rest of R increases by $d(v_0, v_1)(|R| - d(v_0, v_1) - 1)|S|$;
- if S' is moved to v_k , the total distance between vertices in S' and R increases by $d(v_{k-1}, v_k)(|R| - d(v_{k-1}, v_k) - 1)|S'|$ as before;
- moving S' further to v_0 changes the total distance further by

$$|S'| \left(\sum_{v \in V(R)} d(v_0, v) - \sum_{v \in V(R)} d(v_k, v) \right).$$

Since the backbone is the longest path that contains all the branching vertices, we have $|S| \leq d(v_0, v_1)$ and $|S'| \leq d(v_{k-1}, v_k)$. Moreover, we trivially have

$$|R| > d(v_0, v_k) + 1 = d(v_0, v_1) + d(v_1, v_{k-1}) + d(v_{k-1}, v_k) + 1.$$

Thus the total change is

$$\begin{aligned}
 W(T') - W(T) &= |S'| \left(\sum_{v \in V(R)} d(v_0, v) - \sum_{v \in V(R)} d(v_{k+1}, v) \right) \\
 &\quad + d(v_{k-1}, v_k) (|R| - d(v_{k-1}, v_k) - 1) |S'| \\
 &\quad + d(v_0, v_1) (|R| - d(v_0, v_1) - 1) |S| - d(v_1, v_{k-1}) |S| |S'| \\
 &> d(v_{k-1}, v_k) (d(v_0, v_1) + d(v_1, v_{k-1})) |S'| \\
 &\quad + d(v_0, v_1) (d(v_1, v_{k-1}) + d(v_{k-1}, v_k)) |S| - d(v_1, v_{k-1}) |S| |S'| \\
 &> d(v_1, v_{k-1}) (|S'|^2 + |S|^2 - |S| |S'|) > 0 .
 \end{aligned}$$

Consequently $W(T') > W(T)$, a contradiction. Thus there is at most one vertex of degree 4, and it has to be either v_1 or v_{k-1} , if there is such a vertex at all. This happens if and only if the number of segments is even, since the total number of segments is $2k - 1$ if all branching vertices have degree 3, and $2k$ if there is also a single vertex of degree 4.

(2) Consider the segments $P(v_0, v_1), P(v_1, v_2), \dots, P(v_{k-1}, v_k)$ on the backbone, let r_1, r_2, \dots, r_k be the lengths of these segments, and let M be the maximum length of a backbone segment. Let j be the smallest index such that $r_j = d(v_{j-1}, v_j) = M > r_{j+1} = d(v_j, v_{j+1})$. Such an index always exists (if necessary, after reversing the backbone) unless all segments on the backbone have the same length. In this case, however, there is nothing to prove.

Moreover, let $T_{\leq j-1}$, T_j and $T_{\geq j+1}$ denote the components containing v_{j-1} , v_j and v_{j+1} respectively in $T - E(P(v_{j-1}, v_{j+1}))$ (Figure 6). We must have $|T_{\leq j-1}| \geq |T_{\geq j+1}|$, for otherwise interchanging $T_{\leq j-1}$ and $T_{\geq j+1}$ will increase the Wiener index by

$$(|T_j| - 1)(r_j - r_{j+1})(|T_{\geq j+1}| - |T_{\leq j-1}|) > 0 .$$

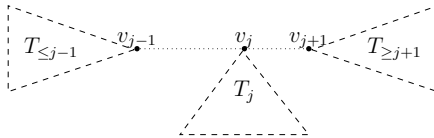


Figure 6: The subtrees $T_{\leq j-1}$, T_j and $T_{\geq j+1}$.

Consequently, we must also have

$$|T_{\leq i-1}| > |T_{\leq j-1}| \geq |T_{\geq j+1}| > |T_{\geq i+1}|$$

for any $i > j$, implying that $r_i \geq r_{i+1}$ by the same argument. It follows that $r_j \geq r_{j+1} \geq \dots \geq r_k$. Similarly, one can show that $r_1 \leq \dots \leq r_j$.

(3) We only consider the case of an odd number of segments in T (the even case can be argued in exactly the same way). Then all branching vertices have degree 3. Let S_i denote the pendant segment at v_i ($1 \leq i \leq k' = k - 1$), let s_i denote the length of S_i , and let μ be the minimum length of all pendant segments.

Let j' be the smallest index such that $s_{j'} = \mu < s_{j'+1}$ (again, such an index exists, if necessary after reversing the backbone, unless all branching segments have the same length), and let $T_{\leq j'}$ and $T_{\geq j'+1}$ denote the components containing $v_{j'}$, and $v_{j'+1}$ respectively in $T - E(P(v_{j'}, v_{j'} + 1))$.

Then we have $|T_{\leq j'} - S_{j'}| \geq |T_{\geq j'+1} - S_{j'+1}|$, or interchanging $S_{j'}$ and $S_{j'+1}$ will increase the Wiener index by

$$d(v_{j'}, v_{j'+1})(s_{j'+1} - s_{j'}) (|T_{\geq j'+1} - S_{j'+1}| - |T_{\leq j'} - S_{j'}|) > 0 .$$

Thus

$$|T_{\leq i} - S_i| \geq |T_{\leq j'}| > |T_{\leq j'} - S_{j'}| \geq |T_{\geq j'+1} - S_{j'+1}| \geq |T_{\geq i+1}| > |T_{\geq i+1} - S_{i+1}|$$

for any $i > j'$, which implies that $s_{i+1} \geq s_i$ by the same argument. It follows that $s_j \leq s_{j'+1} \leq \dots \leq s_{k'}$. Similarly, one can show that $s_1 \geq \dots \geq s_{j'}$. ■

4 Trees with given number of segments

In this section, we answer Question 2 affirmatively by proving the following theorem:

Theorem 3 *Among all trees of order n with m segments, $O(n, m)$ ($E(n, m)$) maximizes the Wiener index if m is odd (even).*

Proof: We only consider the case of odd m , the other case is similar. Let T be an optimal tree, given the number of vertices and segments.

From Theorems 1 and 2, it is clear that T has to be a quasi-caterpillar, and that every branching vertex has degree 3. Let the backbone be the path $P(v_0, v_k)$, and let v_1, v_2, \dots, v_{k-1} be the branching vertices on the backbone. Note that the total number of segments is $m = 2k - 1$. Moreover, let a and b be the lengths of $P(v_0, v_1)$ and the

other pendant segment ending at v_1 , and let T' be the tree that remains when those two segments (including v_1) are removed.

Suppose that $\min\{a, b\} > 1$. If we replace the two segments by segments of lengths 1 and $a + b - 1$, the Wiener index increases by $(a - 1)(b - 1)|T'|$: this transformation amounts to moving $b - 1$ vertices from one segment to the other, so that their distance to the vertices in T' increases by $a - 1$, while the sum of the distances to the other vertices remains the same. This contradicts the choice of T .

Thus the pendant segment at v_1 (and by the same argument, the pendant segment at v_{k-1}) has to have length 1, and by statement (3) of Theorem 2, all pendant segments have length 1. In other words, T is a caterpillar.

From the (partial) characterization of trees with given degree sequence that maximize the Wiener index (see [13, Theorem 3.3]), we also know that the degrees of the internal vertices along the backbone have to be decreasing at first, then increasing, i.e., the sequence of degrees has to be of the form $3, 3, \dots, 3, 2, 2, \dots, 2, 2, 3, 3, \dots, 3$. It only remains to show that the number of vertices of degree 3 on the two sides is as equal as possible (difference at most 1). Let us rename the vertices on the backbone as follows: $u_0 = v_0, u_1, u_2, \dots, u_{n-k} = v_k$; this includes all vertices, not just the branching vertices. Assume that there is a leaf attached to u_1, u_2, \dots, u_x and $u_{n-k-1}, u_{n-k-2}, \dots, u_{n-k-y}$, where $x + y = k - 1$. If $k - 1 = n - k - 1$ (equivalently, $n = 2k = m + 1$), there is nothing to prove, as there is only one possibility left for T : all vertices on the backbone have to have degree 3. Otherwise, assume that $|x - y| > 1$; without loss of generality, $x > y + 1$. If we move the one leaf from u_x to $u_{n-k-y-1}$, the Wiener index increases by $2(x - y - 1)(n - 2k)$, and we reach yet another contradiction. Thus $|x - y| \leq 1$, which means that T is isomorphic to $O(n, m)$. ■

5 Conclusion

We found that a tree maximizing the Wiener index, given the segment sequence, has to be a quasi-caterpillar, and we managed to characterize the structure somewhat further. A complete characterization of the extremal trees seems difficult, as it is for the problem of maximizing the Wiener index of trees given the degree sequence. For the problem of maximizing the Wiener index among trees with a given number of vertices and segments,

however, we did prove such a complete characterization.

It is quite probable that similar results hold for other graph invariants (in particular, distance-based invariants), and we think that it would be worthwhile to further pursue this line of research.

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