MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **75** (2016) 81-89

ISSN 0340 - 6253

On Segment Sequences and the Wiener Index of Trees*

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(Received December 23, 2014)

Abstract

The Wiener index of a connected graph is defined as the sum of distances between all unordered pairs of its vertices. A segment of a tree is a path-subtree whose terminal vertices are branching or pendent vertices. The length of a segment S is equal to the number of edges in S and it is denoted by l_S. If a tree T has segments S_1, S_2, ...,S_m, then the sequence $(l_{S_1}, l_{S_2}, ..., l_{S_m})$ is called the segment sequence of T. In this paper, we characterize the trees which minimize the Wiener index among all trees of given order with prescribed segment sequence.

1 Introduction

All graphs considered in this paper are simple, connected graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A vertex of degree one of a tree is called a *pendent vertex*. A vertex of a tree T with degree 3 or greater is called a *branching vertex* of T. As usual, S_n and P_n denote, respectively, the star and path on n vertices. The distance between vertices u and v of G is denoted by $d_G(u,v)$. For other terminologies and notations not defined here we refer the readers to [4]. The Wiener index of a connected graph G is defined as

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

*This project is supported by the Li Shangda Natural Science Foundation of Jimei University

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The Wiener index belongs to the oldest graph-based structure descriptors (topological indices). It was first introduced by Wiener [22] and has been extensively studied in many articles. Chemists are often interested in the Wiener index of trees which represent acyclic molecular structures. Since every atom has a certain valency, researchers are also interested in trees with degree restrictions and having maximal or minimal Wiener index [6–8, 10–13, 19].

The degree $deg(v)$ of a vertex v in G is the number of edges of G incident with v. If a graph G has vertices v_1, v_2, ...,v_n, then the sequence $(deg(v_1), deg(v_2), ..., deg(v_n))$ is called a degree sequence of G. It is well known that a sequence $(d_1, d_2, ..., d_n)$ of positive integers is a degree sequence of an $n-$vertex tree if and only if

$$d_1 + d_2 + ... + d_n = 2(n-1) \ .$$

The extremal questions of maximizing or minimizing various topological indices among trees with a given degree sequence have been widely studied, see [1] for the spectral radius, [9, 16–18, 20, 21, 23, 24] for the Wiener index, [16] for the terminal Wiener index and [15] for the second Zagreb index and Wiener polarity index.

The aim of this paper is to introduce a new graphical sequence which encodes the structure of trees and investigate how this sequence influences the Wiener index of trees.

Recall that a *segment* of a tree T [4, p. 219] is a path-subtree S whose terminal vertices are branching or pendent vertices of T (i.e., every internal vertex v of S has $d_T(v) = 2$). The length of a segment S is equal to the number of edges in S and it is denoted by l_S. Dobrynin, Entringer and Gutman (see Section 5 of [4]) summarized many applications of this concept to the calculation of the Wiener index of trees. If a tree T has segments S_1, S_2, ...,S_m, then the sequence $(l_{S_1}, l_{S_2}, ..., l_{S_m})$ is called the *segment sequence* of T. It is known that [4, p. 229] a sequence $(t_1, t_2, ..., t_m)$ $(m \geq 3)$ of positive integers is a segment sequence of an $n-$vertex tree if and only if

$$t_1 + t_2 + ... + t_m + 1 = n \ . \qquad (1)$$

Given a sequence $(l_1, l_2, ..., l_m)$ of positive integers, denote by $\mathbb{S}_{l_1,l_2,...,l_m}$ the set of all trees with the segment sequence $(l_1, l_2, ..., l_m)$, and by $S(l_1, l_2, ..., l_m)$ the tree obtained from m disjoint paths P_{l_1}, P_{l_2}, ..., P_{l_m} by adding a new vertex u and joining u to each of the vertices w_1, w_2, ..., w_m, where w_i is a terminal vertex of the path P_{l_i} for $i = 1, 2, ..., m$. Clearly, $S(l_1, l_2, ..., l_m) \in \mathbb{S}_{l_1,l_2,...,l_m}$. Note that the path P_{l_1} is the unique element in $\mathbb{S}_{l_1}$

and the set $\mathbb{S}_{l_1,l_2}$ is empty. So in the following we only consider the class $\mathbb{S}_{l_1,l_2,\ldots,l_m}$ with $m \geq 3$. In Figure 1, all trees in $\mathbb{S}_{2,1,1,1,1}$ are depicted.

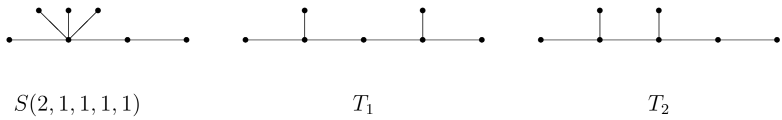

Fig. 1 The trees in $\mathbb{S}_{2,1,1,1,1}$

As mentioned above, the problem of maximizing and minimizing the Wiener index of trees with prescribed degree sequence were studied a lot. The segment sequence is a natural characteristic of the structure of a tree. Given a tree T, one can easily get its segment sequence. So it is natural to consider the analogous problem for the trees with prescribed segment sequence.

Problem A. Characterize the trees which maximize and minimize the Wiener index among all trees with prescribed segment sequence.

In this paper, we give a partial solution of the above problem by proving the following theorem.

Theorem 1. For any tree $T \in \mathbb{S}_{l_1,l_2,\ldots,l_m}$, $m \geq 3$, it holds that

$$W(T) \geq W(S(l_1, l_2, ..., l_m)\,,$$

with equality if and only if $T = S(l_1, l_2, ..., l_m)$.

2 Proof of the main result and discussion

If all internal vertices and all edges of a segment S are deleted from a tree T, we have two nontrivial connected components. Denote by $n_1(S)$ and $n_2(S)$ the number of vertices of these components.

Lemma 2 ([4, p.220]). Let T be a tree on n vertices. Then

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

where the summations go over all segments S of T.

With the aid of the lemma above, we shall prove a simple lemma which will help to prove our main result.

For a segment S of a tree T, if one terminal vertex of S is a pendent vertex, then S is called a *pendent segment* of T. Otherwise, it is called a *nonpendent segment* of T.

Given a tree $T \in \mathbb{S}_{l_1,l_2,\ldots,l_m}$, $m \geq 3$, if T contains a nonpendent segment S_0, then T must comprise the structure as shown in Figure 2, where u and v are two terminal vertices of S_0, T_1 and T_2 are two subtrees of T linked by the segment S_0. Let T' be the tree obtained from T by contracting the segment S_0 and adding a pendent segment S_0' to the vertex $u(=v)$ with $l_{S_0'} = l_{S_0}$ (see Figure 2). Clearly, $T' \in \mathbb{S}_{l_1,l_2,\ldots,l_m}$. Such a transformation will be called a *starlike-operation* of T.

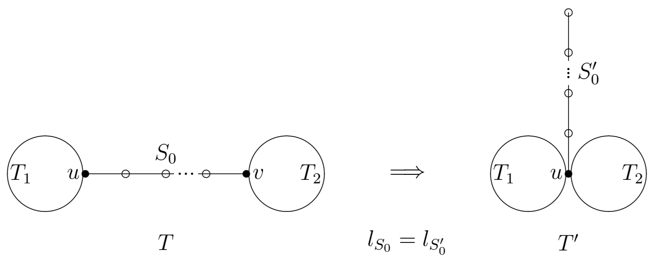

Fig. 2 Two trees T and T' in $\mathbb{S}_{l_1,l_2,\ldots,l_m}$.

Lemma 3. Let T and T' be two trees whose structures are specified above. Then

$$W(T) - W(T') = (n_1 - 1)(n_2 - 1)l_{S_0} > 0\,,$$

where $n_1 = |V(T_1)|$ and $n_2 = |V(T_2)|$.

Proof. Set $n = l_1 + l_2 + \ldots + l_m + 1$, according to (1), $|V(T)| = |V(T')| = n$. Let $A = \{S_0, S_1, \ldots, S_{m-1}\}$ be the set of segments of T, where S_0 is the nonpendent segment depicted in Figure 2. We may assume that the segment S_i in T becomes the corresponding segment S_i' in T' under the starlike-operation, $i = 0, 1, \ldots, m-1$. Then $B = \{S_0', S_1', \ldots, S_{m-1}'\}$ is the set of segments of T', and

$$l_{S_i} = l_{S_i'} \; \textit{for each}\; i \in \{0, 1, \ldots, m-1\}. \tag{2}$$

By Lemma 2,

$$W(T) = \sum_{S\in A} n_1(S)n_2(S)l_S + \frac{1}{6}\sum_{S\in A} l_S(l_S - 1)(3n - 2l_S + 1)\,, \tag{3}$$

and,

$$W(T') = \sum_{S' \in B} n_1(S')n_2(S')l_{S'} + \frac{1}{6}\sum_{S' \in B} l_{S'}(l_{S'}-1)(3n-2l_{S'}+1)\ . \tag{4}$$

It is easily checked that $n_1(S_i)n_2(S_i) = n_1(S_i')n_2(S_i')$ for each $i \in \{1, 2, ..., m-1\}$,

$$n_1(S_0)n_2(S_0)l_{S_0} = n_1 n_2 l_{S_0}\ ,$$

and

$$n_1(S_0')n_2(S_0')l_{S_0'} = (n_1+n_2-1)l_{S_0}\ .$$

Thus, by (2)

$$\begin{aligned}\sum_{S \in A} n_1(S)n_2(S)l_S - \sum_{S' \in B} n_1(S')n_2(S')l_{S'} &= n_1 n_2 l_{S_0} - (n_1+n_2-1)l_{S_0}\\ &= (n_1-1)(n_2-1)l_{S_0}, \end{aligned} \tag{5}$$

and further,

$$\frac{1}{6}\sum_{S \in A} l_S(l_S-1)(3n-2l_S+1) = \frac{1}{6}\sum_{S' \in B} l_{S'}(l_{S'}-1)(3n-2l_{S'}+1)\ . \tag{6}$$

Combining (3), (4), (5) and (6), we arrive at

$$W(T) - W(T') = (n_1-1)(n_2-1)l_{S_0} > 0 \quad (\text{since } n_1 \geq 3,\ n_2 \geq 3)\,,$$

as required. ■

Remark. A special case for $l_{S_0} = 1$ of Lemma 3 was found by Dong and Guo (see Theorem 2.5 of [5]).

Proof of Theorem 1. For a $T \in \mathbb{S}_{l_1,l_2,\ldots,l_m}$, if $T \neq S(l_1, l_2, ..., l_m)$, then T must have some nonpendent segments, thus T can be transformed into the tree $S(l_1, l_2, ..., l_m)$ by carrying out the starlike-operarton repeatedly. By Lemma 3, we have

$$W(T) > W(S(l_1, l_2, ..., l_m))\ .$$

This completes the proof of Theorem 1. ■

In regard to maximizing and minimizing the Wiener index of trees with prescribed degree sequence, it has been proved that the minimum is attained by the greedy trees [20, 23]. The maximization problem can be reduced to the study of caterpillars [17], but a complete solution is still open [9, 16, 24]. Theorem 1 gives a complete solution to the minimization problem in Problem A, but the solution to the maximization problem seems to be difficult.

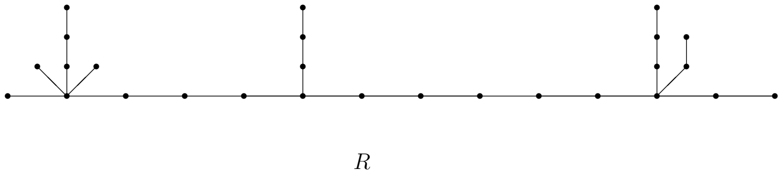

Fig. 3 A quasi caterpillar R

Recall a tree is called a *caterpillar* if the removal of all pendent vertices results in a path. We further define that a tree is a *quasi caterpillar* if the removal of all pendent vertices and all vertices of degree two that lie in the pendent segments of the tree results in a path, see Figure 3 for an example. Numerical testing of trees with a small number of segments revealed that the trees with the maximum Wiener index among all trees with prescribed segment sequence are quasi caterpillars. So, it might be worthwhile to consider the following problem, which might provide a clue to the solution of the maximization problem in Problem A.

Problem B. Let T_{max} be the tree with the maximum Wiener index among all trees with prescribed segment sequence, does T_{max} have to be a quasi caterpillar?

Recently, the first author of the present paper [14] characterized the trees which minimize and maximize the first Zagreb index among all trees with fixed number of segments, respectively. Borovićanin [2] characterized the trees which minimize and maximize the second Zagreb index among all trees with fixed number of segments, respectively. So it is natural to consider the analogous extremal problem for the Wiener index. In the following, we shall give a partial solution of this problem.

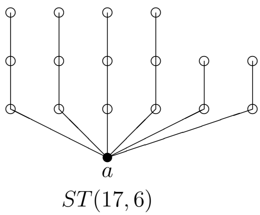

Fig. 4 The tree $ST(17,6)$

Let $ST(n,m)$ be an $n-$vertex tree obtained from m disjoint paths (each has $\lceil \frac{n-1}{m} \rceil$ or $\lfloor \frac{n-1}{m} \rfloor$ vertices) by attaching one endvertex of each path to a new vertex a. The vertex a is called the *center* of $ST(n,m)$, see Figure 4 for an example. Note that $ST(n,2) = P_n$ and $ST(n,n-1) = S_n$. Burns and Entringer [3] obtained the following result (see also Theorem 31 of [4]).

Theorem 4 ([3]). Let T be a tree on n vertices with k pendent vertices, then

$$W(T) \geq W(ST(n,k)) ,$$

with equality if and only if $T = ST(n,k)$.

Denote by $\mathbb{ST}_{n,k}$ the set of all $n-$vertex trees with exactly k segments. Note that the path P_n is the unique element in $\mathbb{ST}_{n,1}$, the star S_n is the unique element in $\mathbb{ST}_{n,n-1}$ and the set $\mathbb{ST}_{n,2}$ is empty. So in the following we only consider the class $\mathbb{ST}_{n,k}$ with $3 \leq k \leq n-2$.

Now we can state the following.

Theorem 5. For any tree $T \in \mathbb{ST}_{n,k}$, where $3 \leq k \leq n-2$, it holds that

$$W(T) \geq W(ST(n,k)) ,$$

with equality if and only if $T = ST(n,k)$.

Proof. In view of Theorem 1, a tree that minimizes the Wiener index in $\mathbb{ST}_{n,k}$ has to be the form $S(l_1, l_2, ..., l_k)$, where $l_1, l_2, ..., l_k$ are positive integers with $l_1 + l_2 + ... + l_k + 1 = n$. But this means that it has k pendent vertices, so the statement of Theorem 5 follows directly from Theorem 4. $\square$

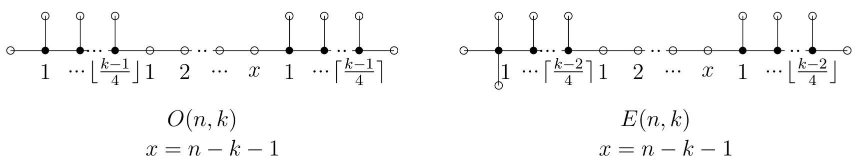

Fig. 5 Two trees $O(n,k)$ and $E(n,k)$

Let $O(n,k)$ and $E(n,k)$ be the trees depicted in Figure 5. Clearly, $O(n,k) \in \mathbb{ST}_{n,k}$, $E(n,k) \in \mathbb{ST}_{n,k}$, $O(n,k)$ and $E(n,k)$ are chemical trees (trees with maximum degrees at most 4). Numerical testing of trees in $\mathbb{ST}_{n,k}$ with small values of n and k revealed that

$O(n,k)$ uniquely attains the maximum value of the Wiener index for odd k and $E(n,k)$ uniquely attains the maximum value of the Wiener index for even k. So it might be worthwhile to consider the following problem.

Problem C. Among all trees in $\mathbb{ST}_{n,k}$, does $O(n,k)$ (resp. $E(n,k)$) attain the maximum value of the Wiener index for odd (resp. even) k?

It should be mentioned that in [14], it is proved that among all trees in $\mathbb{ST}_{n,k}$, the trees with the same degree sequence as $O(n,k)$ (resp. $E(n,k)$) attain the minimum value of the first Zagreb index for odd (resp. even) k.

Acknowledgment: The author would like to thank an anonymous referee whose suggestions helped to improve this paper.

References

[1] T. Biyikoğlu, J. Leydold, Graphs with given degree sequence and maximal spectral radius, *El. J. Combin.* **15** (2008) # R119 (pp. 1–9).

[2] B. Borovićanin, On the extremal Zagreb indices of trees with given number of segments or given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 57–79.

[3] K. Burns, R. C. Entringer, A graph–theoretic view of the United States postal service, in: Y. Alavi, A. J. Schwenk (eds), *Graph Theory, Combinatorics, and Algorithms*, Wiley, New York, 1995, pp. 323–334.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[5] H. W. Dong, X. F. Guo, Ordering trees by their Wiener indices, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 527–540.

[6] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Discr. Appl. Math.* **122** (2002) 127–137.

[7] B. Furtula, I. Gutman, H. Lin, More trees with all degrees odd having extremal Wiener index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 293–296.

[8] B. Furtula, Odd–vertex–degree trees maximizing Wiener index, *Kragujevac J. Math.* **37** (2013) 129–134.

[9] Y. L. Jin, X. D. Zhang, On the two conjectures of the Wiener index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 583–589.

[10] H. Lin, Extremal Wiener index of trees with all degrees odd, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 287–292.

[11] H. Lin, On the Wiener index of trees with given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 301–310.

[12] H. Lin, Extremal Wiener index of trees with given number of vertices of even degree, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 311–320.

[13] H. Lin, A note on the maximal Wiener index of trees with given number of vertices of maximum degree, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 783–790.

[14] H. Lin, On segments, vertices of degree two and the first Zagreb index of trees, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 825–834.

[15] M. Liu, B. Liu, The second Zagreb indices and Wiener polarity indices of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 439–450.

[16] N. S. Schmuck, S. G. Wagner, H. Wang, Greedy trees, caterpillars, and Wiener–type graph invariants, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 273–292.

[17] R. Shi, The average distance of trees, *Sys. Sci. Math. Sci.* **6** (1993), 18–24.

[18] A. V. Sills, H. Wang, On the maximal Wiener index and related questions, *Discr. Appl. Math.* **160** (2012) 1615–1623.

[19] D. Stevanović, Maximizing Wiener index of graphs with fixed maximum degree, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 71–83.

[20] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **156** (2009) 2647–2654.

[21] H. Wang, Corrigendum: the extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **157** (2009) 3754–3754.

[22] H. Wiener, Structual determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[23] X. D. Zhang, Q. Y. Xing, L. Q. Xu, R. Y. Pang, The Wiener index of trees with given degree sequences, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 623–644.

[24] X. D. Zhang, Y. Liu, M.X. Han, Maximum Wiener index of trees with given degree sequence, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 661–682.