On the Wiener Index of Trees with Given Number of Branching Vertices[*]

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Abstract

The Wiener index of a connected graph is defined as the sum of distances between all unordered pairs of its vertices. A vertex of a tree T with degree 3 or greater is called a branching vertex of T. In this paper, the lower bound and the upper bound of the Wiener index of an $n-$vertex tree with given number of branching vertices are obtained respectively.

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 $E(G)$. The degree $deg(v)$ of a vertex v in G is the number of edges of G incident with v. A vertex of a tree T with degree 3 or greater is called a *branching vertex* of T. A vertex of degree one is called a *pendent vertex*. Let S_n and P_n denote the star and path with n vertices, respectively. The distance of a vertex v, denoted by $d_G(v)$, is the sum of distances between v and all other vertices of G. 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 [2]. The Wiener index of a connected graph G is defined as

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

The Wiener index belongs among the oldest graph-based structure descriptors (topological indices) which was first introduced by Wiener [23] and has been extensively studied in many literatures. Numerous of its chemical applications and mathematical properties are well studied. For detailed results on this topic, the readers may referred to two surveys by Dobrynin et al. [2] and Gutman et al. [3] and two recent monographs by Gutman and Furtula [11, 12].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. Many researches are devoted to studying the extremal trees that maximize or minimize the Wiener index within certain classes of trees. For instance, see [6] for trees with given matching number, [16, 22] for trees with a given diameter, [13, 24] for trees with a given radius and [7, 8, 9, 14, 15, 18, 19, 20, 21, 25, 26] for trees with some specific degree conditions.

Note that each tree different from the path possesses at least one branching vertices, in this paper, we will investigate how the number of branching vertices influences the Wiener index.

Doyle and Graver [5] discovered a result that is suitable for calculation of the Wiener index of trees with few branching vertices.

Theorem 1 ([5]). Let T be a tree on n vertices. Then

$$W(T) = \binom{n+1}{3} - \sum_{u} \sum_{1 \leq i < j < k \leq deg(u)} n_i(u)n_j(u)n_k(u),$$

where the first summation goes over all branching vertices u of T, and $n_1(u)$, $n_2(u)$, ..., $n_{deg(u)}(u)$ are the number of vertices in each of the components of $T - u$.

Many applications of this formula have been summarized by Dobrynin et al. in Section 5 of [2]. Gutman et al. [10] gave a partial order among the starlike trees, i.e., trees possessing exactly one branching vertex. By this partial order, one can order some starlike trees with respect to their Wiener indices, but not all starlike trees. This implies that the behavior of branching vertices influencing the Wiener index is complicated.

To better understand the relationship between the branching vertices of trees and their Wiener indices, one possible research direction is to determine the upper bound and lower bound of the Wiener index of an $n-$vertex tree T with exactly r branching vertices. For such a tree T, it is easy to find that $r \leq \frac{n}{2}-1$. Otherwise, if $r > \frac{n}{2}-1$, assume that x and y

are the numbers of vertices of degree 1 and 2 of T respectively, recall that $|E(T)| = n-1$, then $\sum\limits_{v \in V(T)} deg(v) \geq x + 2y + 3r = (x + y + r) + 2r + y > n + (n-2) + y = 2|E(T)| + y$, a contradiction.
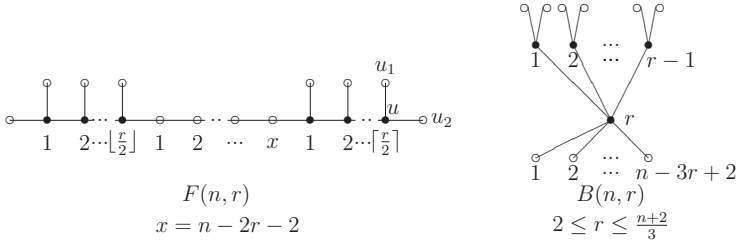

Fig. 1 Two trees $F(n,r)$ and $B(n,r)$

Let $\mathbb{BT}_{n,r}$ be the set of all $n-$vertex trees having exactly r branching vertices. Let $F(n,r)$ and $B(n,r)$ be the trees shown in Figure 1. Clearly, $F(n,r) \in \mathbb{BT}_{n,r}$.

The main work of the present paper is as follows.

Theorem 2. Let $T \in \mathbb{BT}_{n,r}$, where $1 \leq r \leq \frac{n}{2} - 1$, then the following holds.

(a) $W(T) \leq W(F(n,r))$,

with equality if and only if $T = F(n,r)$.

(b) If $r = 1$, then

$$W(T) \geq W(S_n),$$

with equality if and only if $T = S_n$,

if $2 \leq r \leq \frac{n}{2} - 1$, then

$$W(T) \geq (n-r)(n-1) + 3(r-1)(n-3),$$

moreover, if n and r satisfy one of the following conditions:

(b-1) $r = 2$, $n \geq 6$,

(b-2) $r = 3$, $n \geq 8$,

(b-3) $4 \leq r \leq \frac{n+2}{3}$,

then the above bound is sharp and $B(n,r)$ is the unique tree realizing this bound.

The rest of this paper is organized as follows. In Section 2, we introduce some known results on the Wiener index of trees which will help to prove our main result. We close this paper in Section 3 by proving the Theorem 2.

2   Preliminaries

The following theorem is useful for computing the Wiener index of a tree.

Theorem 3 ([23]). Let T be a tree and e its edge. Let $n_1(e)$ and $n_2(e)$ be the numbers of vertices of two components of $T - e$. Then

$$W(T) = \sum_{e \in E(T)} n_1(e)n_2(e).$$

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 $\sum_{i=1}^{n} d_n = 2(n - 1)$. A tree T is called a *caterpillar* if the tree obtained from T by removing all pendent vertices is a path. Shi [18] obtained the following result.

Theorem 4 ([18]). Let $(d_1, d_2, ..., d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_i = 2(n - 1)$, and T_{max} be the tree with maximal Wiener index among all trees with this prescribed degree sequence. Then T_{max} is a caterpillar.

Recently, Sills and Wang [19] characterized the maximal Wiener index of chemical trees with prescribed degree sequence by proving the following result, see also [14].

Theorem 5 ([19]). Let $(d_1, ..., d_k, d_{k+1}, ..., d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_n = 2(n - 1)$ and $4 \geq d_1 \geq ... \geq d_k > d_{k+1} = ... = d_n = 1$. Let T_{max} be the tree with maximal Wiener index among all trees with this prescribed degree sequence. If $(d_1, d_2, ..., d_k) = (\underbrace{a_s, ..., a_s}_{m_s}, \underbrace{a_{s-1}, ..., a_{s-1}}_{m_{s-1}}, ..., \underbrace{a_1, ..., a_1}_{m_1})$ with $a_s > a_{s-1} > ... > a_1 \geq 2$, then T_{max} can be formed by attaching pendent edges to a path $P = v_1 v_2 ... v_k$ such that

$$(deg(v_1), ..., deg(v_k)) = (\underbrace{a_s, ..., a_s}_{l_s}, \underbrace{a_{s-1}, ..., a_{s-1}}_{l_{s-1}}, ..., \underbrace{a_1, ..., a_1}_{m_1}, ..., \underbrace{a_{s-1}, ..., a_{s-1}}_{r_{s-1}}, \underbrace{a_s, ..., a_s}_{r_s}),$$

where $|l_i - r_i| \leq 1$ and $l_i + r_i = m_i$ for $i = 2, ..., s$.

3   Proof of Theorem 2

Proof. First we will determine the upper bound of $W(T)$. Let T^* be a tree with maximal Wiener index in $\mathbb{BT}_{n,r}$. Suppose $(d_1, d_2, ..., d_n)$ is the degree sequence of T^*. Let $\mathcal{T}_d$ be the set of all trees with this prescribed degree sequence. Clearly $\mathcal{T}_d$ is a subclass of $\mathbb{BT}_{n,r}$, so T^* is a tree with maximal Wiener index in $\mathcal{T}_d$. By Theorem 4, T^* is a caterpillar.

We can further claim that T^* possesses only vertices of degree 1, 2 and 3. Otherwise, suppose $P = y_0y_1...y_ly_{l+1}$ is the longest path of T^*, then there exists a vertex y_i $(1 \leq i \leq l)$ such that $deg(y_i) \geq 4$. Assume that $\{y_{i-1}, y_{i+1}, u_1, u_2, ..., u_t\}$ is the set of the neighbors of y_i, where $u_1, u_2, ..., u_t$ $(t = deg(y_i) - 2)$ are pendent vertices. Let T' be the tree obtained from T^* by deleting the edge y_iu_1 and joining u_1 to u_2. See Figure 2 for an example. Clearly, $T' \in \mathbb{BT}_{n,r}$.

$$T^* \qquad\qquad T'$$
Fig. 2   Two trees T^* and T'

But now we can get $W(T') - W(T^*) = d_{T'}(u_1) - d_{T^*}(u_1) > 0$, a contradiction to the maximality of T^*.

Consequently, T^* is a chemical tree with exactly r branching vertices of degree 3. Suppose that t_1 and t_2 are the numbers of the vertices of degree 1 and degree 2 of T^* respectively. Note that T^* is a caterpillar, thus $t_1 = r + 2$. The relation $\sum\limits_{v \in V(T^*)} deg(v) = 2|E(T^*)| = 2n - 2$ gives that $t_1 + 2t_2 + 3r = 2n - 2$, and hence $t_2 = n - 2r - 2$. So the degree sequence of T^* is $(\underbrace{3, ..., 3}_{r}, \underbrace{2, ..., 2}_{n-2r-2}, \underbrace{1, ..., 1}_{r+2})$.

Since T^* is the tree with maximal Wiener index among all trees with this prescribed degree sequence and T^* is a chemical tree, from Theorem 5, we have $T^* = F(n, r)$.

Now we turn to determine the lower bound of $W(T)$.

If $r = 1$, the result clearly holds by the well known fact [2] that if T is any $n-$vertex tree different from S_n and P_n, then $W(S_n) < W(T) < W(P_n)$.

If $r \geq 2$, assume that T has exactly p pendent edges and q non-pendent edges, say $e_1, e_2, ..., e_q$. By Theorem 3,

$$W(T) = \sum_{e \in E(T)} n_1(e)n_2(e) = \sum_{e \text{ is pendent}} n_1(e)n_2(e) + \sum_{i=1}^{q} n_1(e_i)n_2(e_i). \qquad (1)$$

Let n be fixed and define an auxiliary function $f(x) = x(n - x)$, where $1 \leq x \leq n-1$. Then $f'(x) = n - 2x$. So $f(x)$ is increasing strictly in the interval $[1, n/2]$ and decreasing strictly in the interval $[n/2, n - 1]$. Thus

$$(n-1) < 2(n-2) < 3(n-3) < 4(n-4) < ... < \lceil \tfrac{n}{2} \rceil \lfloor \tfrac{n}{2} \rfloor. \tag{2}$$

Call an edge $e_j \in \{e_1, e_2, ..., e_q\}$ is *large* if either $n_1(e_j) \geq 3$ or $n_2(e_j) \geq 3$. Assume that q' is the number of such large edges. Let T'' be the tree obtained from T by deleting vertices of degree 2 in which each is adjacent to a pendent vertex of T and all pendent vertices of T. See Figure 3 for an example.
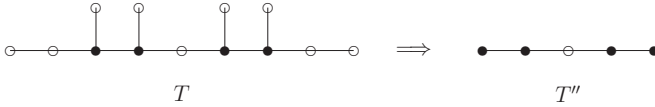

$$T \qquad\qquad\qquad T''$$

Fig. 3   Two trees T and T''

Note that there is a bijection between the set of the large edges of T and the set of the edges of T'' and each branching vertex of T corresponds to a vertex of T'', thus $q \geq q' = |E(T'')| = |V(T'')| - 1 \geq r - 1$.

This fact together with the relation (2) result in

$$\sum_{i=1}^{q} n_1(e_i)n_2(e_i) \geq q'[3(n-3)] \geq 3(r-1)(n-3), \tag{3}$$

with equality if and only if $q = r - 1$ and for each $e_i \in \{e_1, e_2, ..., e_q\}$, either $n_1(e_i) = 3$ or $n_2(e_i) = 3$. It should be noted that if $q = r - 1$, then p (the number of pendent edges of T) has the maximal possible value $(n - 1) - (r - 1) = n - r$. Because the product $n_1(e)n_2(e)$ in (1) has the minimal possible value $n - 1$ if e is a pendent edge, we thus arrive at

$$W(T) \geq (n-r)(n-1) + 3(r-1)(n-3), \tag{4}$$

with equality if and only if T satisfies the following conditions:

(c-1) $p = n - r$, $q = r - 1$,

(c-2) for each non-pendent edge e of T, either $n_1(e) = 3$ or $n_2(e) = 3$.

It is easily checked that if n and r satisfy one of the conditions (b-1), (b-2) and (b-3) stated in Theorem 2, then the graph $B(n, r)$ belongs to $\mathbb{BT}_{n,r}$, satisfies the conditions (c-1), (c-2) and realizes the bound in (4).

To see that $B(n,r)$ is the unique extremal tree, we may assume that $R \in \mathbb{BT}_{n,r}$ is a tree different from $B(n,r)$ which also realizes the bound in (4). Then R satisfies the conditions (c-1) and (c-2). Let R' be the r-vertex tree obtained from R by deleting $n-r$ pendent vertices, then $R' \neq S_r$. Otherwise if $R' = S_r$, by the condition (c-2), one can deduce that $R = B(n,r)$, a contradiction. Now we can choose an non-pendent edge, say e', of the tree R'. Note that each component of $R' - e'$ contains at least two vertices, in which at least one is a branching vertex of R. Therefore, each component of $R - e'$ contains at least four vertices of R, that is $n_1(e') \geq 4$ and $n_2(e') \geq 4$, a contradiction to the condition (c-2).

This completes the proof of this theorem. □

Remark 1. Theorem 2 determines the sharp upper bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$ with all possible values r and the sharp lower bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$ when $r \in [1, \frac{n+2}{3}]$. If $r \in (\frac{n+2}{3}, \frac{n}{2} - 1]$, we can not obtain the sharp lower bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$, since the trees satisfying both conditions (c-1) and (c-2) can not be constructed when r belongs to this interval.

Remark 2. If $r = 1$, the upper bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$ can also be determined by Theorem 8 of [1] or Theorem 1.1 of [17]. In [1] and [17], an ordering of trees with the first up to seventeenth greatest Wiener indices was obtained by Deng and Liu et al. respectively, all these extremal trees possess at most 3 branching vertices. On the other hand, if $r = 2$ or $r = 3$, the lower bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$ can also be determined by Theorem 4.1 of [4]. In [4], an ordering of trees with the first up to fifteenth smallest Wiener indices was given by Dong and Guo, all these extremal trees possess at most 4 branching vertices.

Remark 3. Define two auxiliary functions:

$$f_l(n,r) = \min\{W(T): T \in \mathbb{BT}_{n,r}\},$$

$$f_u(n,r) = \max\{W(T): T \in \mathbb{BT}_{n,r}\}.$$

Thus if $T \in \mathbb{BT}_{n,r}$, then $W(T)$ belongs to the interval $[f_l(n,r), f_u(n,r)]$. By Theorem 2, $f_u(n,r) = W(F(n,r))$. Let u, u_1, u_2 be the vertices of $F(n,r)$ depicted in Figure 1. Let F' be the tree obtained from $F(n,r)$ by deleting the edge uu_1 and joining u_1 to u_2. It is easily checked that $W(F') - W(F(n,r)) = d_{F'}(u_1) - d_{F(n,r)}(u_1) > 0$. Note

that $F' \in \mathbb{BT}_{n,r-1}$, where $r \geq 2$. By theorem 2, we have $W(F(n, r-1)) \geq W(F')$. So $W(F(n,r)) < W(F(n, r-1))$, giving

$$f_u(n,r) < f_u(n, r-1) \quad for \quad 2 \leq r \leq \frac{n}{2} - 1. \tag{5}$$

On the other hand, by Theorem 2, $f_l(n,1) = W(S_n)$ and $f_l(n,r) = W(B(n,r)) = (n-r)(n-1) + 3(r-1)(n-3)$ for $r \in [2, \frac{n+2}{3}]$. Clearly, $f_l(n,2) > f_l(n,1)$. If $r \in [3, \frac{n+2}{3}]$, then $f_l(n,r) - f_l(n, r-1) = [(n-r)(n-1) + 3(r-1)(n-3)] - [(n-r+1)(n-1) + 3(r-2)(n-3)] = 2n - 8 > 0$, so

$$f_l(n,r) > f_l(n, r-1) \quad for \quad 2 \leq r \leq \frac{n+2}{3}. \tag{6}$$

Combining (5) and (6), we can conclude that if $r \in [1, \frac{n+2}{3}]$, then the intervals $[f_l(n, r), f_u(n, r)]$ (r=1, 2, ..., $\lfloor \frac{n+2}{3} \rfloor$) satisfy the following nest relation:

$$[f_l(n,1), f_u(n,1)] \supset [f_l(n,2), f_u(n,2)] \supset ... \supset [f_l(n, \lfloor \frac{n+2}{3} \rfloor), f_u(n, \lfloor \frac{n+2}{3} \rfloor)].$$

In the end of the paper, we leave the following problems which might be worthwhile to study.

Problem A. Determine the sharp lower bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$, where $r \in (\frac{n+2}{3}, \frac{n}{2} - 1]$.

Problem B. Order the trees in $\mathbb{BT}_{n,r}$ by the smallest or greatest Wiener indices.

References

[1] H. Y. Deng, The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 393–402.

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

[3] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

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

[5] J. K. Doyle, J. E. Graver, Mean distance in a graph, *Discr. Math.* **7** (1977) 147–154.

[6] Z. Du, B. Zhou, Minimum Wiener indices of trees and unicyclic graphs of given matching number, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 101–112.

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

[8] 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.

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

[10] I. Gutman, J. Rada, O. Araujo, The Wiener index of starlike trees and a related partial order, *MATCH Commun. Math. Comput. Chem.* **42** (2000) 145–154.

[11] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs - Theory*, Univ. Kragujevac, Kragujevac, 2012.

[12] I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs — Applications*, Univ. Kragujevac, Kragujevac, 2012.

[13] A. Ilić, A. Ilić, D. Stevanović, On the Wiener index and Laplacian coefficients of graphs with given diameter or radius, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 91–100.

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

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

[16] H. Liu, X. F. Pan, On the Wiener index of trees with fixed diameter, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 85–94.

[17] M. Liu, B. Liu, Q. Li, Erratum to 'The trees on $n \geq 9$ vertices with the first to seventeenth greatest Wiener indices are chemical trees', *MATCH Commun. Math. Comput. Chem.* **64** (2010) 743–756.

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

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

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

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

[22] S. Wang, X. Guo, Trees with extremal Wiener indices, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 609–622.

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

[24] Z. You, B. Liu, Note on the minimal Wiener index of connected graphs with n vertices and radius r, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 343–344.

[25] 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.

[26] 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.