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A Note on the Maximal Wiener Index of Trees with Given Number of Vertices of Maximum Degree*

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Abstract

The Wiener index of a connected graph is defined as the sum of the distances between all unordered pairs of its vertices. Let $\mathbb{MT}_{n,k}$ be the set of trees of order n with exactly k vertices of maximum degree. In this note, we characterize the trees with the maximal Wiener index in $\mathbb{MT}_{n,k}$.

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 $deg_G(v)$ of a vertex v in G is the number of edges of G incident with v. A vertex of degree one is called a *pendent vertex*. A vertex of a tree T with degree 3 or greater is called a *branching vertex* of T. Let P_n denote the path with n vertices. 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 $d_G(u, v)$. The diameter of G, denoted by $diam(G)$, is the maximum distance between two vertices of G. 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 is the oldest and very important topological index in chemical graph theory which was first introduced by Wiener [18] and has been extensively studied by many chemical and mathematical researchers. For its details, the readers may see two surveys by Dobrynin et al. [2] and Gutman et al. [3] and two recent monographs by Gutman and Furtula [8, 9].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. Since every atom has a certain valency, chemists are also in particular interested in trees with some degree restrictions and having maximal or minimal Wiener index. Many researches are devoted to this topics, see [5, 16] for trees with fixed maximum degree, [6, 7, 11] for trees with all degrees odd, [12] for trees with given number of branching vertices, [13] for trees with given number of vertices of even degree and [10, 14, 15, 17, 19, 20] for trees with given degree sequence. As for trees with given number of pendent vertices, Burns and Entringer [1] determined the lower bound of the Wiener index of an $n-$vertex tree with exactly k pendent vertices, and the upper bound was obtained by Shi [14] and Entringer [4] independently. The tree $S(n,m)$ is 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 end–vertex of each path to a new vertex. The *dumbbell* $D(n,a,b)$ consists of the path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P and b independent vertices adjacent to the other pendent vertex. Then the main results of [1, 4, 14] (see also Section 12 of [2]) can be stated as:

Theorem 1 ([1, 4, 14]). If T is a tree on n vertices with k pendent vertices, $2 \leq k \leq n-1$, then

$$W(S(n,k)) \leq W(T) \leq W\left(D\left(n, \left\lfloor \frac{k}{2} \right\rfloor, \left\lceil \frac{k}{2} \right\rceil\right)\right) ,$$

the lower bound is attained if and only if $T = S(n,k)$, and the upper bound is attained if and only if $T = D(n, \lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil)$.

Observe that any tree contains at least two minimum degree vertices (i.e., two pendent vertices) and some maximum degree vertices. It is interesting to obtain results analogous to Theorem 1 in the opposite direction by considering the maximum degree vertices.

Let $\mathbb{MT}_{n,k}$ be the set of trees of order n with exactly $k(\leq n-2)$ vertices of maximum degree. Note that the path P_n is the unique element in $\mathbb{MT}_{n,n-2}$. So in the following we only consider the class $\mathbb{MT}_{n,k}$ with $k \leq n-3$. Let $M(n,k)$ be the tree shown in Figure 1.

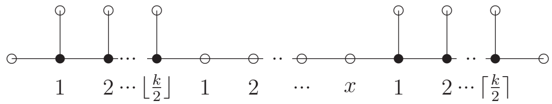

Fig. 1 The tree $M(n,k)$

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

Theorem 2. Let $T \in \mathbb{MT}_{n,k}$, where $1 \leq k \leq n-3$. Then

$$W(T) \leq W(M(n,k)),$$

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

Let $\mathbb{BT}_{n,r}$ (resp. $\mathbb{ET}_{n,r}$) be the set of trees of order n with exactly r branching vertices (resp. r even-degree vertices). In [12] and [13], the present author determined the upper bound and lower bound of the Wiener index of trees in $\mathbb{BT}_{n,r}$ and $\mathbb{ET}_{n,r}$, respectively. Using a argument similar to that of [12] and [13], we give a proof of Theorem 2 in Section 2, while in the following we provide a sequence of results to make the proof more compact.

If a graph G has vertices v_1, v_2, ...,v_n, then $(deg_G(v_1), deg_G(v_2), ..., deg_G(v_n))$ is called a *degree sequence* of G. A tree T is called a *caterpillar* if the tree obtained from T by removing all pendent vertices is a path. The following is a long known result due to Shi [14].

Theorem 3 ([14]). 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.

Very recently, Sills and Wang [15] characterized the maximal Wiener index of chemical trees (trees with maximum degrees at most 4) with prescribed degree sequence by proving the following result, see also [10].

Theorem 4 ([15]). Let $(d_1, ..., d_k, d_{k+1}, ..., d_n)$ be a degree sequence with $\sum_{i=1}^{n} d_i = 2(n-1)$ 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

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

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

Lemma 5. Let T be a caterpillar with the longest path $P = y_0 y_1 ... y_l y_{l+1}$. Assume that there exists a vertex y_i $(1 \leq i \leq l)$ such that $deg_T(y_i) \geq 3$, suppose u is a pendent vertex $(u \neq y_0$ and $u \neq y_{l+1})$ adjacent to y_i and T' is the tree obtained from T by deleting the edges $y_i u$ and joining u to y_0, then $W(T') > W(T)$.

Proof. Let T_u be the tree obtained from T by deleting the vertices u and let T'_u be the tree obtained from T' by deleting the vertices u. Note that $W(T') = W(T'_u) + d_{T'}(u)$, $W(T) = W(T_u) + d_T(u)$ and $T_u = T'_u$.

It is easily verified that $W(T') - W(T) = d_{T'}(u) - d_T(u) > 0$. $\square$

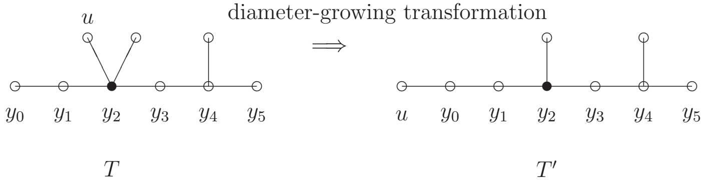

Fig. 2 The diameter-growing transformation of a caterpillar T relative to the vertex y_2.

It is easy to see that if a caterpillar T contains a vertex y_i of degree greater than 2, then by the operation stated in Lemma 5, one can get another caterpillar T' with $W(T') > W(T)$ and $diam(T') = diam(T) + 1$, see Figure 2 for an example. For the convenience of the subsequent discussion, such a transfer operation will be called a *diameter-growing transformation of* T *relative to the vertex* y_i.

2 Proof of Theorem 2

Proof. Let T^* be a tree with the maximal Wiener index in $\mathbb{MT}_{n,k}$. Suppose $(d_1, d_2, ..., d_n)$ is the degree sequence of T^*. Let $\mathbb{T}_d$ be the set of trees of order n with this degree sequence. Clearly $\mathbb{T}_d \subseteq \mathbb{MT}_{n,k}$, so T^* also is a tree with the maximal Wiener index in $\mathbb{T}_d$. By Theorem 3, T^* is a caterpillar. Let $P = y_0y_1...y_ly_{l+1}$ be the longest path of T^* and let $\triangle$ be the maximum degree of vertices of T^*. The condition $k \leq n-3$ implying that $\triangle \geq 3$.

We can further claim that $\triangle = 3$.

Suppose, to the contrary, $\triangle \geq 4$. Since T^* is a caterpillar, any vertex of degree greater than 2 belongs to $\{y_1, y_2, ..., y_l\}$. Then for each $y_i \in \{y_1, y_2, ..., y_l\}$ such that $deg_{T^*}(y_i) \geq 3$, we carry out diameter-growing transformation relative to y_i, repeatedly r_i times, where

$$r_i = deg_{T^*}(y_i) - 2 \quad \text{if } 3 \leq deg_{T^*}(y_i) \leq \triangle - 1\,,$$

and

$$r_i = deg_{T^*}(y_i) - 3 \quad \text{if } deg_{T^*}(y_i) = \triangle\ .$$

Finally, we will get another caterpillar T' possessing only k vertices of degree 3 and $n-k$ vertices of degree 1 and 2. Thus $T' \in \mathbb{MT}_{n,k}$. According to Lemma 5, $W(T') > W(T^*)$, but this contradicts the choice of T^*.

Consequently, T^* is a chemical tree with exactly k 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 $t_1 = k+2$. The relation $\sum\limits_{v \in V(T^*)} deg_{T^*}(v) = 2|E(T^*)| = 2n-2$ gives that $t_1 + 2t_2 + 3k = 2n-2$, and hence $t_2 = n-2k-2$. So the degree sequence of T^* is $(\underbrace{3, ..., 3}_{k}, \underbrace{2, ..., 2}_{n-2k-2}, \underbrace{1, ..., 1}_{k+2})$.

Since T^* is the tree with the maximal Wiener index among all trees with this prescribed degree sequence and T^* is a chemical tree, from Theorem 4, we arrive at

$$T^* = M(n,k)\,,$$

by which the proof of Theorem 2 is completed. □

Theorem 2 only determines the trees with the maximal Wiener index in $\mathbb{MT}_{n,k}$. To better understand the behavior of the maximum degree vertices influencing the Wiener index, it might be worthwhile to consider the following problem.

Problem. Characterize the tree(s) with the minimal Wiener index in $\mathbb{MT}_{n,k}$.

Dendrimers are highly regular trees that model various chemical molecules (see Section 2 of [2] for its details). The regular dendrimer tree $T_{k,d}$ is defined as follows. For any $d \geq 3$, $T_{0,d}$ is the one-vertex graph and $T_{1,d}$ is the star with $d+1$ vertices. Then for $k = 2, 3, ...,$ and $d \geq 3$, the tree $T_{k,d}$ is obtained by attaching $d-1$ new vertices of degree one to each vertex of degree one of $T_{k-1,d}$. The tree $T_{k,d}$ has order (see Section 2 of [2])

$$n(T_{k,d}) = 1 + \frac{d}{d-2}[(d-1)^k - 1] \ .$$

In view of the construction of $T_{k,d}$, the tree $T_{k,d}$ has exactly $n(T_{k-1,d})$ vertices of maximum degree d, hence $T_{k,d} \in \mathbb{MT}_{n(T_{k,d}),n(T_{k-1,d})}$.

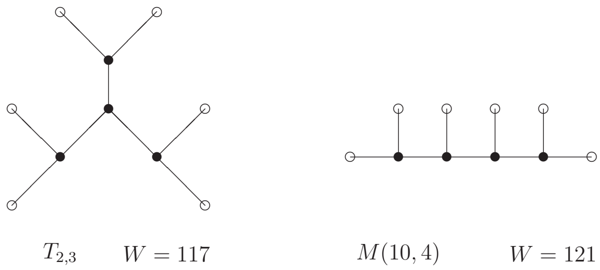

Fig. 3 All trees in $\mathbb{MT}_{10,4}$ and their Wiener indices.

In Figure 3, we list all trees in the class $\mathbb{MT}_{10,4}$ together with their Wiener indices, the regular dendrimer $T_{2,3}$ is tree with the minimal Wiener index in $\mathbb{MT}_{10,4}$. So, it is also interesting to consider the above problem for the special class $\mathbb{MT}_{n(T_{k,d}),n(T_{k-1,d})}$ for every k and $d \geq 3$.

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