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The Second Zagreb Indices and Wiener Polarity Indices of Trees with Given Degree Sequences *

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Abstract. Given a tree $T = (V, E)$, the second Zagreb index of T is denoted by $M_2(T) = \sum_{uv \in E} d(u)d(v)$ and the Wiener polarity index of T is equal to $W_P(T) = \sum_{uv \in E}(d(u)-1)(d(v)-1)$. Let $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d'_1, d'_2, ..., d'_n)$ be two different non-increasing tree degree sequences. We write $\pi \lhd \pi'$, if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, ..., n$. Let $\Gamma(\pi)$ be the class of connected graphs with degree sequence π. In this paper, we characterize one of many trees that achieve the maximum second Zagreb index and maximum Wiener polarity index in the class of trees with given degree sequence, respectively. Moreover, we prove that if $\pi \lhd \pi'$, T^* and T^{**} have the maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively, then $M_2(T^*) < M_2(T^{**})$.

1 Introduction

Throughout the paper, $G = (V, E)$ is a connected undirected simple graph. The symbol $N(v)$ denotes the neighbor set of vertex v, then $d(v) = |N(v)|$ is called the degree of v.

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As usually, let S_n and P_n be the star and path of order n, respectively.

The *distance* $dist(u, v)$ between the vertices u and v of G is equal to the length of (number of edges in) the shortest path that connects u and v. The *Wiener polarity index* of a graph G, denoted by $W_P(G)$, is equal to the number of unordered vertex pairs of distance 3 of G, and the *Wiener index* $W(G)$ is equal to the sum of all pairwise distances of vertices of G. The "Wiener polarity index" and "Wiener index" were introduced by Harold Wiener [1] in 1947. In [1], Wiener used a linear formula of $W(G)$ and $W_P(G)$ to calculate the boiling points t_B of the paraffins, i.e.,

$$t_B = aW(G) + bW_P(G) + c$$

where a, b, and c are constants for a given isomeric group.

This simple numerical representation of a molecule has shown to be a very useful quantity to use in the quantitative structure-property relationships (QSPR) [2, 3]. Thus, the research of Wiener polarity index have drawn much attention recently. For instance, Hosoya [3] found a physico-chemical interpretation of $W_P(G)$, and Lukovits et al. [4] used Wiener polarity index to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. And the extremal Wiener polarity indices of all trees, chemical trees and unicyclic graphs of order n were determined in [5, 6, 7], respectively. Very recently, if $T = (V, E)$ is a tree, Du et al. [8] proposed the following equivalent algorithm for $W_P(T)$:

$$W_P(T) = \sum_{uv \in E} (d(u) - 1)(d(v) - 1). \tag{1}$$

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ are also two famous important topological indices. The *first Zagreb index* and the *second Zagreb index* were defined as [9]:

$$M_1(G) = \sum_{v \in V} d(v)^2 \qquad , \qquad M_2(G) = \sum_{uv \in E} d(u)d(v) \ . \tag{2}$$

Recent research showed that they have been closely correlated with many chemical and mathematical properties [10, 11, 12, 13, 14].

The sequence $\pi = (d_1, d_2, ..., d_n)$ is called the *degree sequence* of G if $d_i = d(v)$ holds for some $v \in V(G)$. Throughout this paper, we enumerate the degrees in non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. A non-increasing sequence $\pi = (d_1, d_2, ..., d_n)$ is call *graphic* if there exists a graph having π as its degree sequence. Specially, if there exists a tree with π as its degree sequence, then π is called a *tree degree sequence*.

Suppose $\pi = (d_1, d_2, ..., d_n)$ and $\pi' = (d'_1, d'_2, ..., d'_n)$ are two different non-increasing graphic degree sequences, we write $\pi \lhd \pi'$ if and only if $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$, and $\sum_{i=1}^{j} d_i \leq \sum_{i=1}^{j} d'_i$ for all $j = 1, 2, ..., n$. Such an ordering is sometimes called *majorization* (see [15]).

We use $\Gamma(\pi)$ to denote the class of connected graphs with degree sequence π. If $G \in \Gamma(\pi)$ and $M_2(G) \geq M_2(G')$ for any other $G' \in \Gamma(\pi)$, then we say that G has *maximum second Zagreb index* in $\Gamma(\pi)$. Similarly, if $G \in \Gamma(\pi)$ and $W_P(G) \geq W_P(G')$ for any other $G' \in \Gamma(\pi)$, then we say that G has *maximum Wiener polarity index* in $\Gamma(\pi)$.

In [16], Wang characterized trees that achieve the maximum and minimum Wiener indices in the class of trees with given degree sequence. Vukičević et al. determined the trees with maximal second Zagreb index and prescribed number of vertices of the given degree in [17], while Deng et al. consider the maximum Wiener polarity index of trees with k pendents in [18]. Motivated by the results of [16, 17, 18], we shall consider the following problem:

Problem 1.1 *Given a tree degree sequence π, which trees have the maximum second Zagreb index and which trees have the maximum Wiener polarity index in $\Gamma(\pi)$.*

To solve Problem 1.1, we need the following definitions, which one can refer to [19] for their detail description.

We use the method of [19] to define a special tree T^* with a given non-increasing tree degree sequence $\pi = (d_0, d_1, ..., d_{n-1})$ as follows: Select a vertex v_0 in layer 0 and create a sorted list of vertices beginning with v_0; choose d_0 new vertices in layer 1, says $v_{11}, v_{12}, ..., v_{1d_0}$, such that $v_{11}, v_{12}, ..., v_{1d_0}$ are adjacent to v_0, then $d(v_0) = d_0$; choose $d_1 + d_2 + \cdots + d_{d_0} - d_0$ new vertices in layer 2 such that $d_1 - 1$ vertices, says $v_{21}, v_{22}, ..., v_{2,d_1-1}$, are adjacent to v_{11}, $d_2 - 1$ vertices are adjacent to v_{12}, ..., $d_{d_0} - 1$ vertices are adjacent to v_{1d_0}, then $d(v_{11}) = d_1$, $d_{v_{12}} = d_2$, ..., $d_{v_{1d_0}} = d_{d_0}$; now choose $d_{d_0+1} - 1$ new vertices in layer 3 such that they are adjacent to v_{21} and hence $d(v_{21}) = d_{d_0+1}$, $\cdots$ continue recursively with v_{22}, v_{23}, $\cdots$ until all vertices of layer 3 are processed. We repeat the above process until all vertices are processed. In this way, a tree T^* of order n and degree sequence π is obtained.

It is easy to see that T^* has layers where each vertex v in layer i has distance i from root v_0, which we call its *height* $h(v) = dist(v, v_0)$. Moreover, v $(v \neq v_0)$ is adjacent to a unique vertex w in layer $i-1$. We call w the *parent* of v, and v a *child* of w. By the definition, if $uv \in E(T^*)$, then either u is the parent or the child of v. For example, v_0 is the unique parent of v_{11}, and v_{21}, ..., v_{2,d_1-1} are all the children of v_{11}.

For example, for a given tree degree sequence $\pi_1 = (4, 4, 3, 3, 3, 3, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)$, T_1^* is the tree of order 19 (see Fig. 1). To construct T_1^*, we first choose v_0 in layer 0; and choose four vertices, says v_{11}, v_{12}, v_{13}, v_{14}, in layer 1 such that they are adjacent to v_0; choose nine new vertices, says v_{21}, v_{22},..., v_{29} in layer 2 such that v_{21}, v_{22}, v_{23} are adjacent to v_{11}, v_{24} and v_{25} are adjacent to v_{12}, v_{26} and v_{27} are adjacent to v_{13}, and v_{28} and v_{29} are adjacent to v_{14}; now choose five new vertices, says v_{31}, v_{32},..., v_{35} in layer 3 such that v_{31} and v_{32} are adjacent to v_{21}, v_{33} is adjacent to v_{22}, v_{34} is adjacent to v_{23}, and v_{35} is adjacent to v_{24}. Then, v_0 is the parent of v_{11}, while v_{21}, v_{22}, v_{23} are all the children of v_{11}. If $\pi_2 = (4, 4, 3, 3, 3, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1)$, with the similar method, we can construct the tree T_2^* with degree sequence π_2, see Fig. 2.

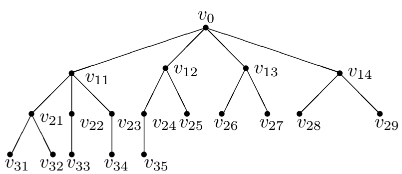

Fig. 1. The BFS-tree with degree sequence π_1.

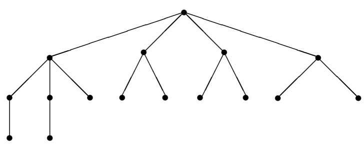

Fig. 2. The BFS-tree with degree sequence π_2.

Definition 1.1 [19] *Let $T = (V, E)$ be a tree with root v_0. A well-ordering $\prec$ of the vertices is called breath-first search ordering with non-increasing degrees (BFS-ordering for short) if the following holds for all vertices $u, v \in V$:*

($B1$) *$u \prec v$ implies $h(u) \leq h(v)$;*

($B2$) *$u \prec v$ implies $d(u) \geq d(v)$;*

(B3) if there are two edges $uu_1 \in E(T)$ and $vv_1 \in E(T)$ such that $u \prec v$, $h(u) = h(u_1) + 1$ and $h(v) = h(v_1) + 1$, then $u_1 \prec v_1$.

We call tree that has a BFS-ordering of its vertices a $BFS-$tree.

For a given tree degree sequence, it is easy to see that

Proposition 1.1 [19] *For a given tree degree sequence π, there exists a unique BFS-tree T^* in $\Gamma(\pi)$, i.e., T^* is uniquely determined up to isomorphism.*

Now we give the main result of this paper, which is the answer to Problem 1.1.

Theorem 1.1 *Given a tree degree sequence π, the $BFS-$tree T^* has the maximum second Zagreb index, and the maximum Wiener polarity index in $\Gamma(\pi)$, respectively.*

For a given tree degree sequence π, by Proposition 1.1 and Theorem 1.1, we can conclude that there is a unique BFS-tree, which has the maximum second Zagreb index, and the maximum Wiener polarity index in $\Gamma(\pi)$, respectively. But it cannot deduce that the BFS-tree is the unique tree with the maximum second Zagreb index or the maximum Wiener polarity index in $\Gamma(\pi)$ because we have the following example.

Example 1.1 Let $\pi = (4, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1)$. Let H_1 and H_2 be two trees as shown in Fig. 3. It is easy to see that H_1 is the unique BFS-tree in $\Gamma(\pi)$, H_2 is not a BFS-tree in $\Gamma(\pi)$, but $M_2(H_1) = M_2(H_2)$ and $W_P(H_1) = W_P(H_2)$.

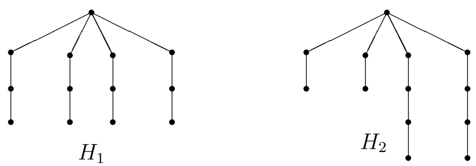

Fig. 3. The trees H_1 and H_2.

Moreover, we shall prove the following interesting result.

Theorem 1.2 *Let π and π' be two different non-increasing tree degree sequences with $\pi \lhd \pi'$. Let T^* and T^{**} be the trees with maximum second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then, $M_2(T^*) < M_2(T^{**})$.*

It is natural to consider the problem: Whether Theorem 1.2 also holds for the maximum Wiener polarity indices between two different non-increasing tree degree sequences? Unfortunately, the answer is negative because we have the following example.

Example 1.2 *Let* $\pi_3 = (3,1,1,1)$ *and* $\pi_4 = (2,2,1,1)$*. Then,* $\pi_4 \lhd \pi_3$*. It is easy to see that* S_4 *and* P_4 *are the unique trees in* $\Gamma(\pi_3)$*, and* $\Gamma(\pi_4)$*, respectively. But we have* $W_P(S_4) = 0 < 1 = W_P(P_4)$ *by Eq.* (1)*.*

Suppose $T \neq S_n$, and T has $\pi = (a_1, a_2, ..., a_n)$ as its degree sequence. Then, $\pi \lhd (n-1, 1, ..., 1)$. By Theorem 1.2, it immediately follows that

Corollary 1.1 [12] *Let* T *be a tree of order* n*, then* $M_2(T) \leq M_2(S_n)$*, where the equality holds if and only if* $T \cong S_n$*.*

Paths P_{l_1}, ..., P_{l_k} are said to *have almost equal lengths* if l_1, ..., l_k satisfy $|l_i - l_j| \leq 1$ for $1 \leq i \leq j \leq k$. By Theorem 1.2, we can also easily deduce the following known result.

Corollary 1.2 *If* T *is a tree of order* n *with* k *pendent vertices, then* $M_2(T) \leq M_2(F_n(k))$*, where* $F_n(k)$ *is the tree on* n *vertices obtained by attaching* k *paths of almost equal lengths to one common vertex.*

2 Proofs of Theorems 1.1 and 1.2

The *girth* $g(G)$ of a connected graph G, is the length of a shortest cycle in G. For the relation between $W_P(G)$, $M_1(G)$ and $M_2(G)$, it has been shown that

Lemma 2.1 [7] *Let* G *be a connected graph with* n *vertices and* m *edges. Then,* $W_P(G) \leq M_2(G) - M_1(G) + m$*, where equality holds if and only if* G *is a tree or* $g(G) \geq 7$*.*

Given a tree degree sequence π, if $T \in \Gamma(\pi)$, then $M_1(T)$ and m are const. By Lemma 2.1, it immediately follows that

Proposition 2.1 *Given a tree degree sequence* π*,* T *has the maximum second Zagreb index in* $\Gamma(\pi)$ *if and only if* T *has the maximum Wiener polarity index in* $\Gamma(\pi)$*.*

Suppose $uv \in E$, the notion $G - uv$ denotes the graph obtained from G by deleting the edge uv. Similarly, if $uv \notin E$, then $G + uv$ denotes the graph obtained from G by adding the edge uv.

Lemma 2.2 *Let $G = (V, E)$ be a connected graph with $v_1u_1 \in E$, $v_2u_2 \in E$, $v_1v_2 \notin E$ and $u_1u_2 \notin E$. Let $G' = G - u_1v_1 - u_2v_2 + v_1v_2 + u_1u_2$. If $d(v_1) \geq d(u_2)$ and $d(v_2) \geq d(u_1)$, then $M_2(G') \geq M_2(G)$, where $M_2(G') > M_2(G)$ if and only if both two inequalities are strict.*

Proof. By Eq. (2), we have

$$M_2(G') - M_2(G) = (d(v_1) - d(u_2))(d(v_2) - d(u_1)) \geq 0.$$

Moreover, $M_2(G') > M_2(G)$ if and only if both two inequalities are strict. ■

Lemma 2.3 *Suppose $G \in \Gamma(\pi)$, and there exist three vertices u, v, w of a connected graph G such that $uv \in E(G)$, $uw \notin E(G)$, $d(v) < d(w) \leq d(u)$, and $d(u) > d(x)$ for all $x \in N(w)$. Then, there exists another connected graph $G' \in \Gamma(\pi)$ such that $M_2(G) < M_2(G')$.*

Proof. We will complete the proof by proving the following two claims.

Claim 1. There exists a vertex $y \in N(w)$ such that $yv \notin E(G)$ and $y \neq v$.

Otherwise, suppose that for each neighbor $x \neq v$ of w, if $xv \in E(G)$, then $N(w)\setminus\{v\} \subseteq N(v) \setminus \{w\}$, which implies that $d(w) \leq d(v)$, a contradiction. So Claim 1 follows.

Claim 2. There exists another connected graph $G' \in \Gamma(\pi)$ such that $M_2(G) < M_2(G')$.

Since G is connected, there exists a path $P_{uw} = (u, ..., s, w)$ from u to w.

Case 1. $uv \notin P_{uw}$ and $vs \notin E(G)$.

Let $G' = G + vs + uw - sw - uv$. Clearly, G' is also connected. Note that $d(u) > d(s)$ and $d(w) > d(v)$. By Lemma 2.2, we have $M_2(G) < M_2(G')$.

We can prove the other cases with a similar method as Case 1. ■

Proof of Theorem 1.1. By Proposition 2.1, we only need to prove that the BFS-tree has the maximum second Zagreb index in $\Gamma(\pi)$.

Assume that T is a tree in $\Gamma(\pi)$ with the maximum second Zagreb index, where $\pi = (d_0, d_1, ..., d_{n-1})$ and $d_0 \geq d_1 \geq \cdots \geq d_{n-1}$. Now we create an ordering $\prec$ by breadth-first search as follows: Choose the vertex of T with maximum degree as root v_0; append all neighbors v_1, ..., v_{d_0} of v_0 to the ordered list; these neighbors are ordered such that $u \prec v$ whenever $d(u) > d(v)$ (in the remaining case the ordering can be arbitrary). Then, with the same method we can append the vertices $N(v_1) \setminus \{v_0\}$ in the ordered list, and then to the vertices $N(v_2) \setminus \{v_0\}$. Continue recursively with all vertices $v_1, v_2, ...$, until all vertices of T are processed. Then, (B1) holds for this ordering. Moreover, if u is the parent of v, then $u \prec v$ by the construction of $\prec$.

Next we shall construct a tree T' from T such that both $(B1)$ and $(B2)$ hold for T', and $M_2(T') \geq M_2(T)$. Assume that $(B2)$ does not hold for T, i.e., there exist two vertices u and v of T with $u \prec v$ but $d(u) < d(v)$. Let v_i be the first vertex in the ordering of $\prec$ with the property $v_i \prec u$ and $d(v_i) < d(u)$ for some u. Clearly, v_i cannot be the root v_0, and if $x \prec v_i$, then $d(x) \geq d(y)$ for each y with $x \prec y$. Suppose v_j is the first vertex in the ordering $\prec$ such that $v_i \prec v_j$ and $d(v_j) = max\{d(v_t) : i+1 \leq t \leq n-1\}$. By the choice of v_i, we can conclude that $v_i \prec v_j$, but $d(v_i) < d(v_j)$.

Let w_i and w_j be the parents of v_i and v_j, respectively. Note that $d(v_i) < d(v_j)$. Then, $w_i \neq w_j$ by the construction of the ordering $\prec$. Moreover, by the construction of the ordering $\prec$ we have $w_i \prec w_j$. Clearly, $w_iv_j \notin E(T)$, otherwise T is not a tree because $w_i \prec w_j \prec v_j$. We consider the following two cases.

Case 1. w_iv_i is in the unique path that connected w_j and v_0.

By the choice of v_i, we can conclude that $w_i \prec v_i \prec w_j \prec v_j$ because w_i is the parent of v_i and $w_i \prec w_j$. By the choice of v_j, we have $d(w_j) < d(v_j)$. Now we shall prove the following Claim.

Claim 1. There exists some $y \in N(v_j)\setminus\{w_j\}$ such that $d(w_i) \leq d(y)$ and $v_iy \notin E(T)$.

Note that T is a tree. Then, $v_iy \notin E(T)$ holds for every $y \in N(v_j)\setminus\{w_j\}$. Now assume that $d(w_i) > d(y)$ holds for every $y \in N(v_j)\setminus\{w_j\}$. Note that $d(w_i) \geq d(v_j) > d(w_j)$ because $w_i \prec v_i \prec v_j$. Then, $d(w_i) > d(y)$ holds for all $y \in N(v_j)$. Recall that $d(w_i) \geq d(v_j) > d(v_i)$ and $w_iv_j \notin E(T)$. By Lemma 2.3, there exists another tree $T' \in \Gamma(\pi)$ such that $M_2(T) < M_2(T')$, a contradiction. Thus, Claim 1 follows.

On the other hand, by $w_i \prec v_i \prec w_j \prec v_j \prec y$ and the choice of v_j, we have $d(w_i) \geq d(v_j) \geq d(y)$, and hence $d(w_i) = d(v_j) = d(y) > d(v_i)$. Let $T_1 = T + w_iv_j + v_iy - w_iv_i - v_jy$. Then, T_1 is also a tree, and $T_1 \in \Gamma(\pi)$. By Lemma 2.2, we can conclude that $M_2(T_1) \geq M_2(T)$.

Case 2. w_iv_i is not in the unique path that connected w_j and v_0.

Then, $v_iw_j \notin E(T)$. Otherwise, T is not a tree. Let $T_1 = T + w_iv_j + w_jv_i - w_iv_i - w_jv_j$. Then, T_1 is also a tree, and $T_1 \in \Gamma(\pi)$. Note that $w_i \prec v_i$ and $w_i \prec w_j$. Then, $d(w_i) \geq$

$d(w_j)$. Moreover, since $d(v_j) > d(v_i)$, we can conclude that $M_2(T_1) \geq M_2(T)$ by Lemma 2.2.

In the above two cases, we can construct a new tree T_1 such that $T_1 \in \Gamma(\pi)$ and $M_2(T_1) \geq M_2(T)$. Now we create a new ordering $\prec'$ to $V(T_1)$ as follows: Let $v_0 \prec' v_1 \prec' \cdots \prec' v_{i-1} \prec' v_j$ be the first i components of $\prec'$. Then, append the vertices $V(T_1) \setminus \{v_0, v_1, ..., v_{i-1}, v_j\}$ by the same method as used in the construction of $\prec$ of $V(T)$. In the new ordering $\prec'$, it is easy to see that if $x \prec' v_j$, then $x \prec v_i$ and hence $d(x) \geq d(y)$ holds for each $x \prec' y$. By the choice of v_j, it follows that $d(v_j) \geq d(y)$ for each $v_j \prec' y$. Moreover, by the construction of $\prec'$, we can conclude that $h(u) \leq h(v)$ if $u \prec' v$.

If $(B2)$ does not hold for T_1, then we can construct a new tree T_2 from T_1 with the same method as used in the construction of T_1 from T such that $M_2(T_2) \geq M_2(T_1)$. Repeat the above process, we can construct the tree T^* from T such that both $(B1)$ and $(B2)$ hold for the ordering $\prec$ of $V(T^*)$ and $M_2(T^*) \geq M_2(T)$.

In T^*, if $h(u) = h(u_1)+1$ and $h(v) = h(v_1)+1$, then u_1 is the parent of u and v_1 is the parent of v. By the ordering $\prec$ of $V(T^*)$, if $u \prec v$, then $u_1 \prec v_1$. Thus, $(B3)$ also holds for T^*. Therefore, the $BFS-$tree T^* has the maximum second Zagreb index in $\Gamma(\pi)$. ■

Our proof of Theorem 1.2 needs more lemmas as follows.

Lemma 2.4 [15, 19] *Let π and π' be two different non-increasing graphic degree sequences. If $\pi \lhd \pi'$, then there exists a series non-increasing graphic degree sequences π_1, ..., π_k such that $(\pi =)\ \pi_0 \lhd \pi_1 \lhd \cdots \lhd \pi_k \lhd \pi_{k+1} (= \pi')$, and π_i and π_{i+1} differ only in two positions, where the differences are* 1 *for $0 \leq i \leq k$.*

Lemma 2.5 *Let u, v be two vertices of a connected graph G, and $w_1, w_2, ..., w_k$ $(1 \leq k \leq d(v))$ be some vertices of $N(v) \setminus \{N(u) \cup u\}$. Let $G' = G + w_1u + w_2u + \cdots + w_ku - w_1v - w_2v - \cdots - w_kv$. If $d(u) \geq d(v)$ and $\sum_{y \in N(u)} d(y) \geq \sum_{x \in N(v)} d(x)$, then $M_2(G') > M_2(G)$.*

Proof. We consider the following two cases.

Case 1. $uv \notin E(G)$.

By Eq. (2), it follows that

$$\begin{aligned}
& M_2(G') - M_2(G) \\
= & (d(v)-k)\left(\sum_{x\in N(v)} d(x) - \sum_{i=1}^{k} d(w_i)\right) + (d(u)+k)\left(\sum_{y\in N(u)} d(y) + \sum_{i=1}^{k} d(w_i)\right) \\
- & \left(d(v)\sum_{x\in N(v)} d(x) + d(u)\sum_{y\in N(u)} d(y)\right) \\
= & k\left(\sum_{y\in N(u)} d(y) - \sum_{x\in N(v)} d(x)\right) + 2k\sum_{i=1}^{k} d(w_i) + (d(u)-d(v))\sum_{i=1}^{k} d(w_i) > 0\ .
\end{aligned}$$

Case 2. $uv \in E(G)$.

By Eq. (2), it can be proved similarly with Case 1.

By Lemma 2.5, it immediately follows that

Corollary 2.1 *Let u, v be two vertices of a connected graph G with $d(u) \geq d(v)$, and $w_1, w_2, ..., w_k$ $(1 \leq k \leq d(v))$ be some vertices of $N(v) \setminus \{N(u) \cup u\}$. Let $G' = G + w_1u + w_2u + \cdots + w_ku - w_1v - w_2v - \cdots - w_kv$. If $uv \notin E(G)$, $d(y) \geq d(x)$ holds for each $y \in N(u)$ and $x \in N(v)$, then $M_2(G') > M_2(G)$.*

Given a graphic degree sequence $\pi = (d_1, d_2, ..., d_n)$, let $d_n(\pi)$ denote the minimum component of π, i.e., $d_n(\pi) = d_n$.

Lemma 2.6 *Let $\pi = (d_1, d_2, ..., d_n)$ be a non-increasing tree degree sequence, and T^* be the BFS-tree in $\Gamma(\pi)$. Suppose $\pi' = (d_1', d_2', ..., d_n')$ $(d_n' = d_n(\pi') \geq 1)$ is a non-increasing graphic degree sequence such that $\pi \lhd \pi'$, and π and π' differ only in two positions, where the differences are 1, then there exists a tree $T' \in \Gamma(\pi')$ such that $M_2(T^*) < M_2(T')$.*

Proof. Recall that π and π' differ only in two positions, where the differences are 1, we may assume that $d_i = d_i'$ for $i \neq p, q$, and $d_p + 1 = d_p'$, $d_q - 1 = d_q'$. Since $\pi \lhd \pi'$, it follows that $1 \leq p < q \leq n$. Note that T^* is a BFS-tree. Then, there exists an ordering $v_1 \prec v_2 \prec \cdots \prec v_n$ of $V(T^*) = \{v_1, v_2, ..., v_n\}$ such that $d(v_i) = d_i$ for $1 \leq i \leq n$, and $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Hence, $v_p \prec v_q$ and $d(v_p) \geq d(v_q)$ because $p < q$.

Suppose $y \in N(v_p)$ and $x \in N(v_q)$. If y is the parent of v_p, and x the parent of v_q, then $y \prec x$ by $(B3)$ and hence $d(y) \geq d(x)$ by $(B2)$. If y is the child of v_p, and x the child of v_q, then $y \prec x$. Otherwise, $v_q \prec v_p$ by $(B3)$, a contradiction. Thus, $d(y) \geq d(x)$ also holds by $(B2)$. Note that $d(v_p) \geq d(v_q)$ and the fact that every neighbor of any vertex $u \in V(T^*)$ is either the parent or a child of u. Then, $\sum_{y \in N(v_p)} d(y) \geq \sum_{x \in N(v_q)} d(x)$.

Let $P_{v_p v_q}$ be the unique path from v_p to v_q in T^*. Note that $d_q = d'_q + 1 \geq d'_n + 1 \geq 2$. Then, there exists some $w \in N(v_q) \backslash N(v_p)$ such that $w \notin P_{v_p v_q}$. Let $T' = T^* - v_q w + v_p w$. Clearly, T' is a tree and $T' \in \Gamma(\pi')$. Moreover, Lemma 2.5 implies that $M_2(T^*) < M_2(T')$.

Combining the above arguments, we then complete the proof. ■

Proof of Theorem 1.2. Since $\pi \lhd \pi'$, by Lemma 2.4 there exists a series non-increasing graphic degree sequences π_2, ..., π_{k-1} such that $(\pi =)\pi_1 \lhd \pi_2 \lhd \cdots \lhd \pi_{k-1} \lhd \pi_k (= \pi')$, and π_i and π_{i+1} differ only in two positions, where the differences are 1 for $1 \leq i \leq k-1$.

By Theorem 1.1, we may suppose that T^* and T^{**} are two BFS-trees. Note that $T^{**} \in \Gamma(\pi')$. Then, $d_n(\pi_i) \geq d_n(\pi') \geq 1$ for $2 \leq i \leq k$ because $(\pi =)\pi_1 \lhd \pi_2 \lhd \cdots \lhd \pi_{k-1} \lhd \pi_k (= \pi')$, and hence there exists at least one tree in $\Gamma(\pi_2)$ by Lemma 2.6. Thus, π_2 is also a tree degree sequence. By Theorem 1.1 and Lemma 2.6, π_i is a tree degree sequence for $1 \leq i \leq k$.

Let T_i be the BFS-tree in $\Gamma(\pi_i)$ for $2 \leq i \leq k-1$. By Lemma 2.6, we can conclude that $M_2(T^*) < M_2(T_2) < \cdots < M_2(T_{k-1}) < M_2(T^{**})$. Thus, Theorem 1.2 follows. ■

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References

[1] H. Wiener, Structrual determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[2] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[3] H. Hosoya, Y. Gao, Mathematical and chemical analysis of Wiener's polarity number, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry-Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 38–57.

[4] I. Lukovits, W. Linert, Polarity-numbers of cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **38** (1998) 715–719.

[5] H. Deng, H. Xiao, F. Tang, On the extremal Wiener polarity index of trees with a given diameter, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 257–264.

[6] H. Deng, On the extremal Wiener polarity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 305–314.

[7] M. H. Liu, B. L. Liu, On the Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 293–304.

[8] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commum. Math. Comput. Chem.* **62** (2009) 235–244.

[9] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi-$electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[10] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals, Part XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[11] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[12] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.

[13] L. Sun, R. S. Chen, The second Zagreb index of acyclic conjuaged molecules, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 57–64.

[14] D. Vukičević, I. Gutman, B. Furtula, V. Andova, D. Dimitrov, Some observations on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 627–645.

[15] A. W. Marshall, I. Olkin, *Inequalities: Theory of Majorization and its Applications*, Academic Press, New York, 1979.

[16] H. Wang, The extremal values of the Wiener index of a tree with given degree sequence, *Discr. Appl. Math.* **156** (2008) 2647–2654.

[17] D. Vukičević, S. M. Rajtmajer, N. Trinajstić, Trees with maximal second Zagreb index and prescribed number of vertices of the given degree, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 65–70.

[18] H. Deng, H. Xiao, The maximum Wiener polarity index of trees with k pendents, *Appl. Math. Lett.* **23** (2010) 710–715.

[19] X. D. Zhang, The Laplacian spectral radii of trees with degree sequences, *Discr. Math.* **308** (2008) 3143–3150.