MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **74** (2015) 81-96

ISSN 0340 - 6253

On the Maximum and Minimum Zagreb Indices of Trees with a Given Number of Vertices of Maximum Degree

Bojana Borovićanin[1], Tatjana Aleksić Lampert[2]

Department of Mathematics and Informatics, Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
e-mail: [1]bojanab@kg.ac.rs
e-mail: [2]taleksic@kg.ac.rs

(Received January 26, 2015)

Abstract

For a (molecular) graph G the first Zagreb index $M_1(G)$ is defined as the sum of the squares of the vertex degrees, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the pairs of adjacent vertices' vertex degrees. Let $\mathcal{T}_{n,k}$ be the class of trees with n vertices of which k vertices have the maximum degree. In this paper we determine the extremal trees of the class $\mathcal{T}_{n,k}$, i.e., those with minimal (maximal) first Zagreb index or minimal (maximal) second Zagreb index.

1 Introduction

All graphs considered in this paper are simple, connected graphs. Let $G = (V, E)$ be such a graph, where $V = V(G)$ is its vertex set and $E = E(G)$ is its edge set. An edge connecting two vertices u and v in the graph G is denoted by uv. The degree $d_G(v)$ (or $d(v)$ for short) of a vertex $v \in V(G)$ is the number of edges that are incident with v in the graph G. A vertex v for which $d_G(v) = 1$ is called a *pendent* vertex and a vertex of degree three or more is called a *branching* vertex. The *maximum vertex degree* in the graph G is denoted by $\Delta(G)$. A graph T that has n vertices and $n - 1$ edges is called a *tree*. For a vertex $v \in V(T)$, such that $2 \leq d_T(v) \leq \Delta(T)-1$, we say that its *edge rotating capacity* is equal to $d_T(v) - 1$. The *total edge rotating capacity* of a tree T is equal to the sum of the edge rotating capacities of its vertices that satisfy the condition $2 \leq d_T(v) \leq \Delta(T) - 1$.

A sequence of positive integers $\pi = (d_1, d_2, \ldots, d_n)$ is called the *degree sequence* of G if $d_i = d_G(v)$ $(i = 1, \ldots, n)$ holds for some $v \in V(G)$. Throughout this paper, we order the vertex degrees non-increasingly, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. Also, a sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called a *tree degree sequence* if there exists a tree T having π as its degree sequence. Furthermore, it is well know that the sequence $\pi = (d_1, d_2, \ldots, d_n)$ is a degree sequence of an n-vertex tree if and only if

$$\sum_{i=1}^{n} d_i = 2(n-1) \ . \tag{1}$$

If $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ are two different 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 $j = 1, 2, \ldots, n$. Such an ordering is called *majorization* [18, 19]. Also, we use $\Gamma(\pi)$ to denote the class of connected graphs that have the degree sequence π.

Molecular structure descriptors (topological indices) are used in mathematical chemistry to describe the properties of chemical compounds.

Some of the well studied molecular structure descriptors are the *first* and *second Zagreb indices,* $M_1(G)$ and $M_2(G)$, respectively. They were introduced in 1972 by Gutman and Trinajstić [8, 9], as follows

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v) \tag{2}$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v) \ . \tag{3}$$

These indices reflect the extent of branching within the molecular carbon-atom skeleton, which allows them to be viewed as molecular structure descriptors [1, 21]. The main properties of M_1 and M_2 were summarized in [10, 20] and the references therein. There has been great interest in studing extremal graphs that minimize (or maximize) Zagreb indices in different classes of graphs, recently [12, 13, 15]. Goubko and Gutman [4, 7] described the trees with minimal first and second Zagreb indices among the trees with a fixed number of pendent vertices. Lin [17] characterized trees with a fixed number of vertices of degree two that maximize and minimize the first Zagreb index. In 2007, Deng [3] described the graphs that have the largest and smallest Zagreb indices within the classes of trees, unicyclic, and bicyclic graphs, by introducing some new transformations of the graphs in these classes. One of the present authors [2] characterized the trees that maximize and minimize the first and second Zagreb indices among the trees with a given number of segments or given number of branching vertices.

Every tree contains at least two minimum degree vertices (i.e., pendent vertices) and some maximum degree vertices. It is interesting to consider the trees with fixed number of maximum degree vertices. Let $\mathcal{T}_{n,k}$ be the class of trees with n vertices that have exactly k $(\leq n-2)$ vertices having the maximum degree. Recently, Lin [16] determined the trees that maximize the Wiener index in the class $\mathcal{T}_{n,k}$. In this paper we characterize the trees that maximize (minimize) the first Zagreb index in this class, as well as the trees that maximize (minimize) the second Zagreb index in the class $\mathcal{T}_{n,k}$.

It is obvious that the path P_n is the unique element of $\mathcal{T}_{n,n-2}$. So, in the following we consider the class $\mathcal{T}_{n,k}$ where $k \leq n-3$.

Let T be a tree from the class $\mathcal{T}_{n,k}$ with maximum vertex degree Δ. By n_i $(i = 1, 2, \ldots, \Delta)$ we denote the number of vertices of degree i in T. Then,

$$\sum_{i=1}^{\Delta} n_i = n \ . \tag{4}$$

Also, from (1) it is obvious that

$$\sum_{i=1}^{\Delta} i n_i = 2(n-1) \ . \tag{5}$$

By combining (4) and (5) we obtain

$$-n_1 + n_3 + 2n_4 + \cdots + (\Delta - 2)n_\Delta = -2 \ .$$

This leads to the conclusion that

$$n_1 \geq 2 + (\Delta - 2)n_\Delta = 2 + k(\Delta - 2) \tag{6}$$

and

$$n \geq n_1 + n_\Delta \geq 2 + k(\Delta - 1)\,, \tag{7}$$

i.e.,

$$n \geq 2 + k(\Delta - 1) \ . \tag{8}$$

Therefore,

$$k \leq \frac{n-2}{\Delta - 1} \ . \tag{9}$$

Since we assumed that $k \leq n-3$ (i.e., $T \neq P_n$), then $\Delta \geq 3$, which implies that

$$k \leq \frac{n-2}{2} \ . \tag{10}$$

Also, from (8) we see that

$$\Delta \leq \frac{n-2}{k} + 1 \ . \tag{11}$$

Since Δ is a positive integer number we obtain

$$\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1 \ . \tag{12}$$

By the previous considerations the following lemma holds.

Lemma 1.1. *If $T \in \mathcal{T}_{n,k}$ is a tree with the maximum vertex degree Δ then $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$.*

2 The first Zagreb index

In this section, we first characterize the trees with maximal first Zagreb index in the class $\mathcal{T}_{n,k}$.

Lemma 2.1. *If T^1_{max} is a tree with maximal first Zagreb index in $\mathcal{T}_{n,k}$, then its maximum vertex degree is equal to $\lfloor \frac{n-2}{k} \rfloor + 1$.*

Proof. Let Δ be the maximum vertex degree in the tree T^1_{max}. Then, by Lemma 1.1, $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$. Let $\Delta_{max} = \lfloor \frac{n-2}{k} \rfloor + 1$ and $n-2 = k\lfloor \frac{n-2}{k} \rfloor + r$, where $0 \leq r < k$.

Assume that $\Delta < \Delta_{max}$.

Let $\{v_1, \ldots, v_n\}$ be the vertex set of a tree T^1_{max} with the degree sequence $\pi = (d_1, \ldots, d_n)$. Then

$$\Delta = d_1 = \cdots = d_k = \Delta_{max} - t, \qquad t > 0 \ .$$

By (6) we see that

$$n_1 \geq k(\Delta - 2) + 2 \ . \tag{13}$$

Therefore, $n_1 = k(\Delta-2) + 2 + n_1'$, where $n_1' \geq 0$. Using (4) we obtain

$$n = k(\Delta - 2) + 2 + n_1' + \sum_{i=2}^{\Delta-1} n_i + k \, ,$$

which implies

$$\sum_{i=2}^{\Delta-1} n_i + n_1' = r + kt \ . \tag{14}$$

Also, from (5), by direct calculation, we have

$$\sum_{i=2}^{\Delta-1} i n_i + n_1' = 2(r+kt) \ . \tag{15}$$

By subtracting the relation in (14), from the relation in (15), we obtain

$$\sum_{i=2}^{\Delta-1} (i-1) n_i = r + kt \geq kt \geq k \ . \tag{16}$$

Since the sum in (16) is equal to the total edge rotating capacity of T^1_{max}, we conclude that the total edge rotating capacity of this tree is greater than or equal to k.

Let $v_i \in V(T^1_{max})$ $(k < i \leq n)$ be a vertex that has positive edge rotating capacity and let d_i $(2 \leq d_i \leq \Delta - 1)$ be its degree. If we define a tree T_1 with the vertex degree sequence $\pi_1 = (d^1_1, \ldots, d^1_n)$ such that $d^1_1 = \Delta + 1$, $d^1_i = d_i - 1$ and $d^1_j = d_j$ $(j \in \{2, \ldots, n\}$, $j \neq i)$ then

$$M_1(T_1) - M_1(T^1_{max}) = (d_1 + 1)^2 - d_1^2 + (d_i - 1)^2 - d_i^2 = 2(\Delta - d_i + 1) > 0 \ .$$

Therefore, $M_1(T_1) > M_1(T^1_{max})$, but $T_1 \notin \mathfrak{T}_{n,k}$. Since the total edge rotating capacity of T^1_{max} is at least k, then we can conclude the following.

We can repeat the above described transformation of the tree T^1_{max} k times on every vertex of degree Δ. In each step we define a tree T_l with the degree sequence $\pi_l = (d^l_1, \ldots, d^l_n)$ such that $d^l_l = \Delta + 1$, $d^l_i = d^{l-1}_i - 1$ and $d^l_j = d^{l-1}_j$ $(j \in \{1, \ldots, n\}$, $j \neq i, l)$, where $l = 2, \ldots k$ and d^{l-1}_i is a degree of an arbitrary vertex $v_i \in V(T_{l-1})$ $(k < i \leq n)$ that has positive edge rotating capacity (this vertex exists since the total edge rotating capacity of a tree T_{l-1} is at least $k - l + 1$). It is possible that after some of the described transformations we obtain a tree whose degrees $d_{k+1}, \ldots, d_n$ are not in non-increasing order. Besides, each application of this transformation strictly increases the first Zagreb index. Finally, we obtain a tree $T_k \in \mathfrak{T}_{n,k}$ that has the maximum vertex degree equal to $\Delta + 1 = (\Delta_{max} - t) + 1$ and satisfies the condition $M_1(T_k) > M_1(T_{k-1}) > \cdots > M_1(T_1) > M_1(T^1_{max})$. This contradicts the fact that T^1_{max} has the maximum first Zagreb index in the class $\mathfrak{T}_{n,k}$.

This proves that $\Delta = \Delta_{max} = \lfloor \frac{n-2}{k} \rfloor + 1$. ■

Remark 2.1. *The statement of Lemma 2.1 also holds for* $k = n - 2$, *i.e.,* $T = P_n$.

Theorem 2.1. *Let $T \in \mathcal{T}_{n,k}$, where $1 \le k \le \frac{n}{2} - 1$. Then*

$$M_1(T) \le k\Delta^2 + p(\Delta-1)^2 + \mu^2 + n - k - p - 1,$$

and the equality holds if and only if T has the vertex degree sequence $(\underbrace{\Delta,\ldots,\Delta}_{k}, \underbrace{\Delta-1,\ldots,\Delta-1}_{p}, \mu, \underbrace{1,\ldots,1}_{n-k-p-1})$, where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$, $p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and $\mu = n - 1 - k(\Delta-1) - p(\Delta-2)$.

Proof. Let $\pi = (d_1, \ldots, d_n)$ be the vertex degree sequence of a tree T^1_{max} with maximal first Zagreb index in the class $\mathcal{T}_{n,k}$. By Lemma 2.1 we have that $d_1 = d_2 = \cdots = d_k = \Delta = \lfloor \frac{n-2}{k} \rfloor + 1$. As in the previous lemma, let $n-2 = k(\Delta-1)+r$, where $0 \le r < k$. Now, from (6) it follows that $n_1 \ge k(\Delta-2)+2 = n-k-r$. Therefore, $d_n = d_{n-1} = \cdots = d_{k+r+1} = 1$.

Bearing in mind that $n_\Delta = k$ and $n_1 = n'_1 + k(\Delta-2) + 2$, where $n'_1 \ge 0$, after using (4) and (5) in the same manner as in (14) and (16) we obtain

$$\sum_{i=2}^{\Delta-1} n_i + n'_1 = r \tag{17}$$

and

$$\sum_{i=2}^{\Delta-1} (i-1)n_i = r\ . \tag{18}$$

Since $n_i \ge 0$ $(i = 2, \ldots, \Delta-1)$, from (18) it follows that $p = n_{\Delta-1} \le \frac{r}{\Delta-2}$. Since p is a non-negative integer number we obtain $p \le \lfloor \frac{r}{\Delta-2} \rfloor$.

Suppose that $\lfloor \frac{r}{\Delta-2} \rfloor > 0$ and $p < \lfloor \frac{r}{\Delta-2} \rfloor$. Then, by (18), $\sum_{i=2}^{\Delta-2} (i-1)n_i \ge \Delta - 2$ and there exist n_i and n_j $(2 \le i < j \le \Delta-2)$, where $n_i \ne 0$ and $n_j \ne 0$ (or there exists $n_i \ge 2$, where $2 \le i \le \Delta-2$) and the relation (18) is satisfied. Furthermore, since $\pi = (\underbrace{\Delta,\ldots,\Delta}_{k}, d_{k+1}, \ldots, d_{k+r}, 1, \ldots, 1)$, there exist numbers d_{k+j_1} and d_{k+i_1} $(1 \le j_1 < i_1 \le r)$, such that $d_{k+j_1} = j > d_{k+i_1} = i$ (or $d_{k+j_1} = d_{k+i_1} = i$, if $n_i \ge 2$).

Let $\pi' = (d'_1, \ldots, d'_n)$ be a sequence of positive integers such that $d'_x = d_x$ for $x \ne k+j_1$ and $x \ne k+i_1$, $d'_{k+j_1} = d_{k+j_1} + 1 = j+1$ and $d'_{k+i_1} = d_{k+i_1} - 1 = i-1$. Since $\sum_{i=1}^{n} d'_i = 2n-2$, then π' is the vertex degree sequence of a tree T', and

$$M_1(T') - M_1(T^1_{max}) = 2(j-i+1) > 0\ .$$

Since $T' \in \mathcal{T}_{n,k}$ and $M_1(T') > M_1(T^1_{max})$ we obtain a contradiction.

From the previous observation we conclude that $p = n_{\Delta-1} = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and the relation (18) now becomes

$$\sum_{i=2}^{\Delta-2} (i-1)n_i = r - p(\Delta-2) \le \Delta - 3\ .$$

In the same manner as previously, it can easily be proved that it has to be $n_\mu = 1$, where $\mu = r - p(\Delta - 2) + 1$, i.e., $\mu = n - 1 - k(\Delta - 1) - p(\Delta - 2)$, and $n_i = 0$ for $i \neq \mu$, $2 \leq i \leq \Delta - 2$, since in the opposite case we can again construct a tree whose M_1 is greater than $M_1(T^1_{max})$.

Therefore, the tree T^1_{max} with maximal first Zagreb index in the class $\mathcal{T}_{n,k}$ has the vertex degree sequence $\pi = (\underbrace{\Delta, \ldots, \Delta}_{k}, \underbrace{\Delta - 1, \ldots, \Delta - 1}_{p}, \mu, \underbrace{1, \ldots, 1}_{n-k-p-1})$.

The first Zagreb index of the tree T^1_{max} can now be easily calculated. ∎

Remark 2.2. *Theorem 2.1 also holds for $k = n - 2$, i.e., $T = P_n$.*

In the following theorem we will describe the trees that have the minimum first Zagreb index in the class $\mathcal{T}_{n,k}$, using the similar idea as in [2].

Lemma 2.2. *Let T^1_{min} be a tree with minimal first Zagreb index in the class $\mathcal{T}_{n,k}$, where $1 \leq k \leq \frac{n}{2} - 1$. Then, its maximum vertex degree Δ equals 3.*

Proof. Suppose that $\Delta \geq 4$ and u is a vertex of maximum degree Δ in T^1_{min}.

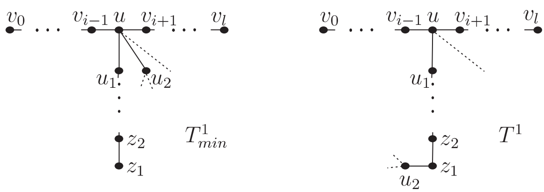

Fig. 1. The graphs T^1_{min} and T^1 in Lemma 2.2

Let $P = v_0 v_1 \ldots v_{i-1} u (= v_i) v_{i+1} \ldots v_l$ be the longest path in T^1_{min} that contains u. Also, let $v_{i-1}, v_{i+1}, u_1, u_2, \ldots, u_{\Delta-2}$ be the vertices adjacent to u in T^1_{min}, and z_1 a pendent vertex connected to u via u_1 (it is possible that $z_1 \equiv u_1$) (Fig. 1). If we define a tree T^1 in the following way

$$T^1 = T^1_{min} - uu_2 + u_2 z_1 \,, \tag{19}$$

then

$$M_1(T^1) - M_1(T^1_{min}) = (\Delta - 1)^2 + 2^2 - \Delta^2 - 1 < 0 \,.$$

Obviously, the tree T^1 has $k - 1$ vertices of degree Δ.

In the same manner, we can apply the transformation described in (19) on every vertex u of degree Δ. In each step from a tree T^i we will obtain a tree T^{i+1} $(1 \leq i \leq k-1)$ that has smaller first Zagreb index than its predecessor. After k repetitions of the transformation we arrive at the tree T^k that has k vertices having the maximum degree $\Delta - 1$. Obviously, $T^k \in \mathcal{T}_{n,k}$ and

$$M_1(T^k) < M_1(T^1_{min}) \ .$$

This contradicts the choice of T^1_{min} as the tree that minimizes M_1 in the class $\mathcal{T}_{n,k}$. ■

Theorem 2.2. *Let $T \in \mathcal{T}_{n,k}$ where $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$M_1(T) \geq 2k + 4n - 6\,,$$

and the equality holds if and only if the tree T has the vertex degree sequence $(\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n-2k-2},\underbrace{1,\ldots,1}_{k+2})$.

Proof. Let T^1_{min} be a tree with minimal M_1 in the class $\mathcal{T}_{n,k}$. According to Lemma 2.2 the vertex degree sequence of this tree is $\pi = (\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n_2},\underbrace{1,\ldots,1}_{n_1})$, when $k \leq \frac{n}{2} - 1$. Hence, using the equality (1) we obtain

$$n_1 + 2n_2 + 3k = 2(n_1 + n_2 + k) - 2\,, \tag{20}$$

which implies that $n_1 = k + 2$ and $n_2 = n - 2k - 2$. Therefore,

$$M_1(T^1_{min}) = k \cdot 3^2 + (n - 2k - 2) \cdot 2^2 + (k + 2) = 2k + 4n - 6 \ .$$ ■

Corollary 2.1. *Let T^k be a tree with minimal first Zagreb index in the class $\mathcal{T}_{n,k}$ and T^p a tree with minimal first Zagreb index in the class $\mathcal{T}_{n,p}$ $(1 \leq k, p \leq \frac{n}{2} - 1)$. If $k > p$ then $M_1(T^k) > M_1(T^p)$.*

Proof. This result is a direct consequence of Theorem 2.2. ■

3 The second Zagreb index

Let π be a degree sequence. If $G \in \Gamma(\pi)$ and $M_2(G) \geq M_2(G')$ holds for any other graph $G' \in \Gamma(\pi)$, then we say that the graph G has the maximumum second Zagreb index in $\Gamma(\pi)$. To prove our main result in this section we will use the following two lemmas.

Lemma 3.1. [18] *Let π and π' be two different non-increasing tree degree sequences such that $\pi \lhd \pi'$. Let T and T' be the trees with maximal second Zagreb indices in $\Gamma(\pi)$ and $\Gamma(\pi')$, respectively. Then, $M_2(T) < M_2(T')$.*

Lemma 3.2. [22] *Let T be a tree with maximal second Zagreb index, with n_i vertices of degree i and maximum vertex degree Δ, and let T_s be a subgraph induced by vertices of degree $\geq s$. Then T_s is connected.*

Theorem 3.1. *Let $T \in \mathfrak{T}_{n,k}$, where $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$M_2(T) \leq (k-1)\Delta^2 + 2p(\Delta-1)^2 + \mu(\Delta+\mu-1) + \Delta(n-k-(\Delta-1)p-\mu),$$

where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$, $p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and $\mu = n-1-k(\Delta-1)-p(\Delta-2)$. The equality holds if and only if the following conditions are satisfied.

(i) The tree T has the vertex degree sequence $(\underbrace{\Delta,\ldots,\Delta}_{k},\underbrace{\Delta-1,\ldots,\Delta-1}_{p},\mu,\underbrace{1,\ldots,1}_{n-k-p-1})$.

(ii) Every vertex of degree $\Delta-1$ is adjacent to a vertex of degree Δ and to $\Delta-2$ pendent vertices.

(iii) The vertex of degree μ (when $\mu > 1$) is adjacent to a vertex of the degree Δ and to $\mu-1$ pendent vertices.

(iv) The remaining pendent vertices are attached to the vertices of degree Δ.

Proof. Let Δ be the maximum vertex degree in a tree T^2_{max} with maximal second Zagreb index in the class $\mathfrak{T}_{n,k}$. By Lemma 1.1 we know that $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$.

Let $\Delta_{max} = \lfloor \frac{n-2}{k} \rfloor + 1$, and $n-2 = k\lfloor \frac{n-2}{k} \rfloor + r$ $(0 \leq r < k)$. With $\pi = (d_1,\ldots,d_n)$ we will denote a tree degree sequence such that

$$\pi = (\underbrace{\Delta_{max},\ldots,\Delta_{max}}_{k},\underbrace{\Delta_{max}-1,\ldots,\Delta_{max}-1}_{p},\mu,\underbrace{1,\ldots,1}_{n-k-p-1})$$

where $p = \lfloor \frac{r}{\Delta_{max}-2} \rfloor$ and $\mu = r+1-p(\Delta_{max}-2)$.

Assume that $\Delta < \Delta_{max}$. Therefore, T^2_{max} has a degree sequence $\pi' = (d'_1,\ldots,d'_n) \neq \pi$. Then $d'_1 = d'_2 = \cdots = d'_k = \Delta = \Delta_{max} - t$, $t > 0$ and

$$\sum_{i=1}^{k} d'_i = k\Delta = k\Delta_{max} - kt < \sum_{i=1}^{k} d_i \ .$$

Also, by (14), it holds that $\pi' = (\underbrace{\Delta, \dots, \Delta}_{k}, d'_{k+1}, \dots, d'_{k+(r+kt)}, 1, \dots, 1)$ and

$$\sum_{i=1}^{k+p} d'_i \leq (k+p)\Delta_{max} - p - (k+p)t < \sum_{i=1}^{k+p} d_i = (k+p)\Delta_{max} - p \ . \tag{21}$$

Having in mind that

$$\sum_{i=k+1}^{k+(r+kt)} d_i = \sum_{i=k+1}^{k+(p+1)} d_i \ + \ (r+kt-p-1)\cdot 1 = p(\Delta_{max}-1) + \mu + r + kt - p - 1 = 2r + kt$$

and

$$\sum_{i=1}^{k+(r+kt)} d'_i = 2(n-1) - (n-k-r-kt)\cdot 1 = r + k(\Delta_{max}-1) + k + r + kt = 2r + k\Delta_{max} + kt$$

we obtain

$$\sum_{i=1}^{k+(r+kt)} d'_i = k\Delta_{max} + 2r + kt = \sum_{i=1}^{k+(r+kt)} d_i \ . \tag{22}$$

Now, from relations (21) and (22) we conclude that there exists j $(p \leq j < r+kt)$, such that $\sum_{i=1}^{s} d'_i < \sum_{i=1}^{s} d_i$ for $s = 1, \dots, j$ and $\sum_{i=1}^{l} d'_i = \sum_{i=1}^{l} d_i$ for $l = j+1, \dots, n$, which implies

$$\pi' \lhd \pi \ . \tag{23}$$

Let T be a tree with maximal second Zagreb index among the trees with the degree sequence π. Then $T \in \mathfrak{T}_{n,k}$ and by Lemma 3.1 and (23), we have that $M_2(T) > M_2(T^2_{max})$. This contradicts the choice of T^2_{max}. Therefore, $\Delta = \Delta_{max} = \lfloor \frac{n-2}{k} \rfloor + 1$.

Next, we notice that for two different vertex degree sequences

$$\pi = (\underbrace{\Delta, \dots, \Delta}_{k}, \underbrace{\Delta-1, \dots, \Delta-1}_{p}, \mu, \underbrace{1, \dots, 1}_{n-k-p-1}) \ (p = \lfloor \frac{r}{\Delta-2} \rfloor \text{ and } \mu = r + 1 - p(\Delta-2))$$

and

$$\pi' = (\underbrace{\Delta, \dots, \Delta}_{k}, d'_{k+1}, \dots, d'_{k+r}, 1, \dots, 1), \ \text{where} \ \sum_{i=1}^{r} d'_{k+i} = 2r \, ,$$

it holds

$$\pi' \lhd \pi \ . \tag{24}$$

In order to prove this, notice that the sum $\sum_{i=1}^{r} d'_{k+i} = 2r$ can be reduced to the sum $\sum_{i=2}^{\Delta-1}(i-1)n_i = r$ (n_i is the number of vertices of degree i) in the same way as was done in (18). Next, we conclude that $n_{\Delta-1} \leq p = \lfloor \frac{r}{\Delta-2} \rfloor$. Also, for $n_{\Delta-1} = p$, let $\mu - 1 = \sum_{i=2}^{\Delta-2}(i-1)n_i = r - p(\Delta-2) \leq \Delta - 3$. If $\mu > 1$, then, by setting $n_\mu = 1$, and the remaining n_i's ($2 \leq i \leq \Delta-2$) equal zero, we will get the degree sequence $(\underbrace{\Delta-1, \ldots, \Delta-1}_{p}, \mu, \underbrace{1, \ldots, 1}_{r-p-1})$ such that $(d'_{k+1}, \ldots, d'_{k+r}) \lhd (\underbrace{\Delta-1, \ldots, \Delta-1}_{p}, \mu, \underbrace{1, \ldots, 1}_{r-p-1})$, for any degree sequence $(d'_{k+1}, \ldots, d'_{k+r})$, satisfying $\sum_{i=1}^{r} d'_{k+i} = 2r$, different from it.

The previous consideration leads us to the conclusion that a tree T^2_{max} with maximal second Zagreb index in the class $\mathcal{T}_{n,k}$ must belong to $\Gamma(\pi)$, i.e., it has to be $(d'_{k+1}, \ldots, d'_{k+r}) = (\underbrace{\Delta-1, \ldots, \Delta-1}_{p}, \mu, \underbrace{1, \ldots, 1}_{r-p-1})$. In the opposite case, if T is a tree with maximal second Zagreb index among the trees with the degree sequence π, then $T \in \mathcal{T}_{n,k}$ and by Lemma 3.1 and (24), we have that $M_2(T) > M_2(T^2_{max})$. This contradicts the choice of T^2_{max}.

Furthermore, using Lemma 3.2 we can conclude that the vertices in T^2_{max} of degree Δ induce a connected subgraph T_k of T^2_{max}. The tree T_k contains $k-1$ edges that connect vertices of degree Δ in T^2_{max}. As there are $k\Delta$ edges with at least one end vertex in $V(T_k)$, we conclude that there exist exactly $R = k\Delta - (k-1) = k(\Delta-2) + 2$ edges with one end vertex in $V(T_k)$. Since $\Delta \geq 3$, it holds $R \geq k+2$. Also, as $p = \lfloor \frac{r}{\Delta-2} \rfloor$, and $r < k$, it is obvious that $p < k < R$, i.e., the number of vertices of degree $\Delta - 1$ is smaller than the number of vertices of degree Δ in T^2_{max} and for an arbitrary vertex of degree $\Delta - 1$ there exists a corresponding vertex of degree Δ that can be adjacent to it.

In the following, we prove that vertices in T^2_{max} have to be connected in a certain way. Namely, we prove that each vertex of degree $\Delta - 1$ has exactly one neighbor of degree Δ and $\Delta - 2$ pendent neighbors. In the opposite case, since vertices of degree $\geq \Delta - 1$ are connected in T^2_{max} (by Lemma 3.2), there exists a vertex (say u) of degree $\Delta - 1$ connected to a vertex v of degree $\Delta - 1$. Besides, let $vw_1 \in E(T^2_{max})$, where w_1 is a vertex of degree Δ. Since $R > k > p$, then there exists a vertex w_2 of degree Δ (it may be $w_1 \equiv w_2$), with a neighbor x ($d(x) = 1$ or $d(x) = \mu$) (Fig. 2).

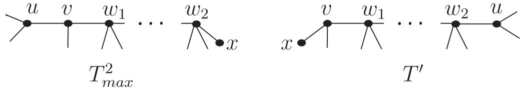

Fig. 2. The graphs T^2_{max} and T' in Theorem 3.1

Suppose that $w_1 \not\equiv w_2$ and let $T' = T^2_{max} - uv - w_2x + vx + w_2u$. Then

$$M_2(T') - M_2(T^2_{max}) = \Delta - 1 - d(x)\ .$$

Since $d(x) = 1$ or $d(x) = \mu \leq \Delta - 2$, in both cases it holds $M_2(T') - M_2(T^2_{max}) > 0$, and therefore, $M_2(T') > M_2(T^2_{max})$. This contradicts the choice of T^2_{max}.

The proof is analogous if $w_1 \equiv w_2$.

Also, it is obvious that a vertex u of degree μ (when $\mu > 1$) is adjacent to a vertex of degree Δ and to $\mu - 1$ pendent vertices. Namely, having in mind Lemma 3.2, we conclude that a vertex u has a neighbor of degree Δ or $\Delta - 1$, and its remaining neighbors are pendent vertices. If u has a neighbor v of degree $\Delta - 1$, and w is a vertex of degree Δ with a pendent neighbor x, then for a tree T', obtained from T^2_{max} by deleting the edges uv and wx, and adding the edges ux and wu, it is satisfied

$$M_2(T') - M_2(T^2_{max}) = \mu - 1 > 0\,,$$

and therefore $M_2(T') > M_2(T^2_{max})$. This contradicts the choice of T^2_{max}.

By the previous considerations we can calculate $M_2(T^2_{max})$ as follows.

$$\begin{aligned} M_2(T^2_{max}) &= (k-1)\Delta^2 + p\Delta(\Delta-1) + \Delta\mu + p(\Delta-1)(\Delta-2) + \mu(\mu-1) \\ &\quad + \Delta(n-k-p(\Delta-1)-\mu) \\ &= (k-1)\Delta^2 + 2p(\Delta-1)^2 + \mu(\Delta+\mu-1) + \Delta(n-k-(\Delta-1)p-\mu)\ . \end{aligned}$$

This proves the theorem. ■

Remark 3.1. *Theorem 3.1 also holds for $k = n-2$, i.e. $T = P_n$.*

In the following we will characterize the trees with minimal second Zagreb index in the class $\mathcal{T}_{n,k}$, using the similar idea as in [2].

Lemma 3.3. *Let T^2_{min} be a tree with minimal second Zagreb index in the class $\mathcal{T}_{n,k}$, where $1 \leq k \leq \frac{n}{2} - 1$. Then, its maximum vertex degree Δ equals 3.*

Proof. Suppose that $\Delta \geq 4$ and u is a vertex of maximum degree Δ in T^2_{min}.

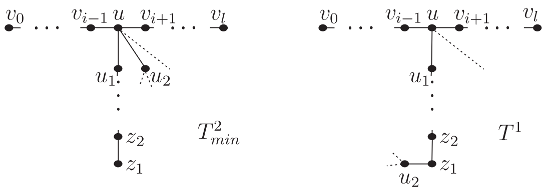

Fig. 3. The graphs T^2_{min} and T^1 in Lemma 3.3

Let $P = v_0 v_1 \dots v_{i-1} u (= v_i) v_{i+1} \dots v_l$ be the longest path in T^2_{min} that contains u. Also, let $v_{i-1}, v_{i+1}, u_1, u_2, \dots, u_{\Delta-2}$ be the vertices adjacent to u in T^2_{min}, and z_1 a pendent vertex connected to u via u_1 (it is possible that $z_1 \equiv u_1$) (Fig. 3). We define a tree T^1 as

$$T^1 = T^2_{min} - uu_2 + u_2 z_1. \tag{25}$$

If $z_1 \equiv u_1$ then

$$M_2(T^1) - M_2(T^2_{min}) = -\left(d(v_{i-1}) + d(v_{i+1}) + \sum_{j=3}^{\Delta-2} d(u_j) \right) - (\Delta - 2)(d(u_2) - 1) < 0 \ .$$

Otherwise, let z_2 be the vertex that is adjacent to z_1. Then

$$\begin{aligned} & M_2(T^1) - M_2(T^2_{min}) \\ & = -\left(d(v_{i-1}) + d(v_{i+1}) + d(u_1) + \sum_{j=3}^{\Delta-2} d(u_j) + (\Delta-2) d(u_2) \right) + d(z_2) \\ & < d(z_2) - \Delta - d(u_2) < 0 \ . \end{aligned}$$

In both cases we obtained the tree T^1 that has $k-1$ vertices of degree Δ.

After applying the transformation described in (25) k times, on every vertex u of degree Δ (as described in the proof of Lemma 2.2), we will obtain a tree T^k that has k vertices having the maximum degree $\Delta - 1$ and $M_2(T^k) < M_2(T^2_{min})$. Obviously, $T^k \in \mathcal{T}_{n,k}$ and this contradicts the choice of T^2_{min}. ∎

The following lemma proves that the vertices in the tree that minimizes M_2 in the class $\mathcal{T}_{n,k}$ have to be connected in a certain way.

Lemma 3.4. *Let T be a tree from the class $\mathcal{T}_{n,k}$.*

(i) Let $u, z, v, w \in V(T)$ be the vertices such that $uz, zv, vw \in E(T)$ and $d_T(u) = 1$, $d_T(z) = 2$, $d_T(v) = 3$, $d_T(w) = 2$ or $d_T(w) = 3$. If $T' \in \mathcal{T}_{n,k}$ is a

tree defined as

$$T' = T - uz - vw + zw + uv\,,$$

then $M_2(T') < M_2(T)$.

(ii) *Let* $u, y, z, v, w, t \in V(T)$ *be the vertices such that* $uy, yz, zv, wt \in E(T)$ *and* $d_T(u) = d_T(v) = d_T(w) = d_T(t) = 3$ *and* $d_T(y) = d_T(z) = 2$. *Let* $T' \in \mathcal{T}_{n,k}$ *be a tree defined as*

$$T' = T - yz - zv - wt + zw + zt + yv\ .$$

Then $M_2(T') < M_2(T)$.

Proof. (i) It is easy to see that

$$M_2(T) - M_2(T') = (d_T(v) - 2)(d_T(w) - 1) > 0\ .$$

Therefore, $M_2(T') < M_2(T)$.

(ii) It holds that $M_2(T) - M_2(T') = 1$, which implies $M_2(T') < M_2(T)$. ■

Lemma 3.4 implies that in the tree that minimizes M_2 in the class $\mathcal{T}_{n,k}$ $(1 \leq k \leq \frac{n}{2} - 1)$ between any two vertices of degree 3 there has to be at least one vertex of degree 2 (if possible). The remaining vertices of degree 2 (if they exist) can be placed arbitrarily between two vertices of degree 2, or between a vertex of degree 2 and a vertex of degree 3.

Theorem 3.2. *Let* $T \in \mathcal{T}_{n,k}$, *where* $1 \leq k \leq \frac{n}{2} - 1$. *Then*

$$M_2(T) \geq \begin{cases} 3k + 4n - 10, & \text{if } n \geq 3k + 1 \\ 6k + 3n - 9, & \text{if } n < 3k + 1\ . \end{cases} \tag{26}$$

The equality holds if and only if the following three conditions are satisfied.

(i) *The tree* T *has the vertex degree sequence* $(\underbrace{3, \ldots, 3}_{k}, \underbrace{2, \ldots, 2}_{n-2k-2}, \underbrace{1, \ldots, 1}_{k+2})$.

(ii) *Between any two vertices of degree* 3 *in* T *there should be at least one vertex of degree* 2, *if possible.*

(iii) *The remaining vertices of degree* 2 *(if they exist) in* T *are placed between two vertices of degree* 2, *or between a vertex of degree* 2 *and a vertex of degree* 3.

Proof. Let T^2_{min} be a tree that minimizes M_2 in the class $\mathcal{T}_{n,k}$. According to Lemma 3.3 this tree has the vertex degree sequence $\pi = (\underbrace{3,\dots,3}_{k}, \underbrace{2,\dots,2}_{n_2}, \underbrace{1,\dots,1}_{n_1})$, when $k \leq \frac{n}{2} - 1$. Also, by the equality in (1) we obtain

$$n_1 + 2n_2 + 3k = 2(n_1 + n_2 + k) - 2, \tag{27}$$

which implies that $n_1 = k+2$ and $n_2 = n-2k-2$. By the considerations discussed above, between two vertices of degree 3 in T^2_{min} there should be at least one vertex of degree 2. If this is possible for every two vertices of degree 3, then we obtain $n-2k-2 \geq k-1$, i.e. $n \geq 3k+1$. Also, the condition in (iii) follows from the previous discussion. The second Zagreb index of T^2_{min} can now be easily calculated. This completes the proof. ■

Acknowledgement. The research of the authors is supported by the Serbian Ministry of Education, Science and Technological Development (Grant No. 174033).

References

[1] A. T. Balaban, I. Motoc, D. Bonchev, O. Makanyan, Topological indices for structure–activity corrections, *Topics Curr. Chem.* **114** (1983) 21–55.

[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) 000–000 .

[3] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs an bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[4] M. Goubko, Minimizing degree–based topological indices for trees with given number of pendant vertices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 33–46.

[5] I. Gutman, B. Furtula, *Distance in Molecular Graphs – Applications*, Univ. Kragujevac, Kragujevac, 2012.

[6] I. Gutman, B. Furtula, *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012.

[7] I. Gutman, M. Goubko, Trees with fixed number of pendent vertices with minimal first Zagreb index, *Bull. Int. Math. Virt. Inst.* **3** (2013) 161–164.

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

[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, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[11] S. Li, H. Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most k, *Appl. Math. Lett.* **23** (2010) 128–132.

[12] S. C. Li, M. J. Zhang, Sharp bounds for the Zagreb indices of bipartite graphs with a given diameter, *Appl. Math. Lett.* **24** (2011) 131–137.

[13] S. Li, H. Yang, Q. Zhao, Sharp bounds on Zagreb indices of cacti with k pendent vertices, *Filomat* **26** (2012) 1189–1200.

[14] Q. Zhao, S. Li, On the maximum Zagreb indices of graphs with k cut vertices, *Acta Appl. Math.* **111** (2010) 93–106.

[15] S. C. Li, Q. Zhao, Sharp upper bounds on zagreb indices of bicyclic graphs with a given matching number, *Math. Comput. Model.* **54** (2011) 2869–2879.

[16] 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.

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

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

[19] A. W. Marshall, I. Olkin, *Inequalities: Theory of Majorization and Its Applications*, Acad. Press, New York, 1979.

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

[21] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[22] 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.