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On the Extremal Zagreb Indices of Trees with Given Number of Segments or Given Number of Branching Vertices

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Abstract

The first Zagreb index M_1 of a graph is equal to the sum of squares of its vertex degrees, and the second Zagreb index M_2 is equal to the sum of products of degrees of pairs of adjacent vertices. A vertex of a tree with degree at least three is called a branching vertex and a segment of a tree is a path-subtree whose terminal vertices are branching or pendent vertices. Sharp lower and upper bounds on the second Zagreb index of trees with fixed number of segments are determined and the corresponding extremal trees are characterized. As the number of segments in a tree is determined by the number of vertices of degree two (and vice versa) in this way the extremal trees with prescribed number of vertices of degree two whose second Zagreb index is minimum (or maximum) are determined, too. Also, sharp lower and upper bounds on Zagreb indices M_1 and M_2 of n-vertex trees with given number of branching vertices are determined, and corresponding extremal trees are characterized

1 Introduction

In this paper only simple and finite graphs are considered. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. An edge of G, connecting the vertices u and v is denoted by uv. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices in G adjacent to v. Let $N_G(v)$ be the neighbor set of the vertex $v \in V(G)$. A vertex of degree one in a graph is said to be *pendent* and a vertex of degree three or more is called a *branching vertex*. The maximum vertex degree of G is denoted by $\Delta(G)$.

If G is a graph with $V(G) = \{v_1, v_2, \ldots, v_n\}$ then the sequence $(d_G(v_1), \ldots, d_G(v_n))$ is called a degree sequence of G. It is well known that a sequence $(d_1, d_2, \ldots, d_n)$ of positive integers is a degree sequence of an n-vertex tree if and only if

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

Molecular structure descriptors (topological indices) are widely used in mathematical chemistry to predict properties of chemical compounds. They have been studied intensively in recent years and among the oldest and the most studied being the *first* and *second Zagreb indices*, $M_1(G)$ and $M_2(G)$, respectively. They were first introduced in 1972 by Gutman and Trinajstić in [9] and defined as [9, 10]

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v) \ .$$

For more details on these indices see the recent papers [1–3, 5, 6, 11–15, 18–22] and the references therein. The extremal trees that maximize or minimize Zagreb indices within certain classes of trees have been studied intensively in recent years (see [6, 12–15, 18, 21, 22]).

Recently, Goubko and Gutman [7, 8] characterized the trees with the minimum first and second Zagreb indices among the trees with fixed number of pendent vertices. After that, Lin [16] characterized the trees with fixed number of vertices of degree two that maximize and minimize the first Zagreb index.

In this paper, the trees which maximize and minimize the second Zagreb index among all trees with fixed number of vertices of degree two are characterized. For this purpose, an idea exposed in [16] will be used.

Besides, we investigate the relationship between the number of branching vertices of trees and their Zagreb indices by determining upper an lower bounds on the first and second Zagreb indices of trees with prescribed number of branching vertices. A similar problem for Wiener index of such trees has been solved in [17].

A *segment* of a tree T (see [4]) is a path-subtree S whose terminal vertices are pendent or branching vertices of T, i.e., an internal vertex of a segment S has degree two. We use the notation s_T for the number of segments of a tree T, as in [16].

We need some further notations. Denote by $V_1(T)$, $V_2(T)$ and $V_{\geq 3}(T)$ the set of pendent vertices, vertices of degree two and branching vertices of a tree T, respectively. By $S(T)$ we denote a tree obtained from T by replacing each segment of T by an edge and, as in [16], we call it the squeeze of T. Namely, for a vertex u of degree two with

$N_T(u) = \{v, w\}$ we delete the edges uv and uw and add a new edge vw. Repeating this procedure as long as there are vertices of degree two in T we finally arrive at $S(T)$. Then we have

$$s_T = |E(S(T))| = |V(S(T))| - 1 = |V(T)| - |V_2(T)| - 1 \ . \tag{2}$$

Thus, in a tree T, s_T is determined by the number of vertices of degree two, and vice versa.

As usual, by P_n and S_n we denote the path and the star of order n, respectively. A tree is said to be *starlike of degree* k if it contains exactly one vertex of degree greater than two (the central vertex), and the central vertex has degree k ($k \geq 3$).

Denote by $\mathcal{ST}_{n,k}$ the set of all n-vertex trees with exactly k segments. Then, as noted in [16], the path P_n is the unique element of $\mathcal{ST}_{n,1}$, the star S_n is the unique element of $\mathcal{ST}_{n,n-1}$ and the set $\mathcal{ST}_{n,2}$ is empty. Thus, we need to consider the set $\mathcal{ST}_{n,k}$ for $3 \leq k \leq n-2$.

Besides, denote by $\mathcal{BT}_{n,b}$ the set of all n-vertex trees with exactly b branching vertices. Note that each tree different from the path contains at least one branching vertex, implying $b \geq 1$. Also, for an arbitrary tree $T \in \mathcal{BT}_{n,b}$ it can easily be proved (see [17]) that $b \leq \frac{n}{2} - 1$. Thus, we assume $1 \leq b \leq \frac{n}{2} - 1$.

The paper is organized as follows. In Sections 2 and 3 we determine lower and upper bounds on M_2 of trees from $\mathcal{ST}_{n,k}$ and characterize the extremal trees. In Section 4, lower bounds on first and second Zagreb indices of trees from $\mathcal{BT}_{n,b}$ are determined and the extremal trees are characterized. Finally, in Section 5, we obtain upper bounds on M_1 and M_2 of trees from $\mathcal{BT}_{n,b}$ and characterize the trees that achieve these bounds.

2 On the minimum second Zagreb index of trees with given number of segments

We first consider the structure of a tree that minimizes the second Zagreb index of trees from $\mathcal{ST}_{n,k}$ for given k. Let $ST_{min} \in \mathcal{ST}_{n,k}$ be the tree with minimal second Zagreb index. Then, the following observations hold.

Lemma 2.1. *The tree $ST_{min} \in \mathcal{ST}_{n,k}$ with minimal second Zagreb index does not contain a vertex of degree greater than 4.*

Proof. Assume, on the contrary, there exists a vertex v of degree greater than 4. Let $P : v_0 \cdots v_{i-1}v(= v_i)v_{i+1} \cdots v_{l+1}$ be a longest path in ST_{min} containing $v = v_i$. Since $d_{ST_{min}}(v) \geq 5$, there exist vertices u and w adjacent to v, that are not included in the path P (Fig. 1). We shall distinguish the following two cases.

Fig. 1

Case 1. $i = l$ or $i = 1$

Then, all neighbors of the vertex v, except v_{l-1} (or v_2, for $i = 1$), are pendent. Let T' be the tree obtained from ST_{min} by deleting the edges uv and wv and adding the new edges uv_{l+1} and wv_{l+1} (or edges uv_0 and wv_0 if $i = 1$). It is obvious that $s_{T'} = k$, implying $T' \in \mathcal{ST}_{n,k}$.

We shall consider only the case $i = l$, since for $i = 1$, the proof is analogous.

Note that v and v_{l+1} are the only vertices whose degrees are different in T' and ST_{min}, $d_{T'}(v) = d_{ST_{min}}(v) - 2$ and $d_{T'}(v_{l+1}) = 3$. For the sake of brevity, for an arbitrary vertex $z \in ST_{min}$, let $d(z) = d_{ST_{min}}(z)$. Therefore,

$$\begin{aligned} & M_2(ST_{min}) - M_2(T') \\ & = (d(v) - 1)d(v) + d(v)d(v_{l-1}) \\ & -(d(v) - 2)(d(v) - 4) - 3(d(v) - 2) - (d(v) - 2)d(v_{l-1}) - 3 \cdot 1 \cdot 2 \\ & = 2(d(v) + d(v_{l-1})) - 8 > 0 \, (\text{since } d(v) \geq 5) \,, \end{aligned}$$

a contradiction, since ST_{min} is the tree with minimal M_2 in $\mathcal{ST}_{n,k}$.

Case 2. $2 \leq i \leq l - 1$

By previous case it holds $d(v_l) \leq 4$. Let T' be the tree obtained from ST_{min} as in previous case, so it holds $s_{T'} = k$. Then,

$$\begin{aligned} & M_2(ST_{min}) - M_2(T') \\ & = d(v)(d(u) + d(w) + \sum_{\substack{zv \in E(ST_{min}) \\ z \neq u,w}} d(z)) + 1 \cdot d(v_l) \\ & -((d(v) - 2) \sum_{\substack{zv \in E(ST_{min}) \\ z \neq u,w}} d(z) \, + \, 3(d(u) + d(w) + d(v_l))) \\ & = (d(v) - 3)(d(u) + d(w)) + 2(\sum_{\substack{zv \in E(ST_{min}) \\ z \neq u,w}} d(z) \, - \, d(v_l)) > 0 \\ & (\text{since } d(v) \geq 5, \quad \sum_{\substack{zv \in E(ST_{min}) \\ z \neq u,w}} d(z) \, \geq 5, \; d(v_l) \leq 4) \; . \end{aligned}$$

Thus, again we get a contradiction. ∎

Lemma 2.2. *The tree $ST_{min} \in \mathcal{ST}_{n,k}$ with minimal second Zagreb index contains at most one vertex of degree 4.*

Proof. Suppose, on the contrary, that v_i and v_j $(i \neq j)$ are vertices of degree 4 in ST_{min} and let $P : v_0 \cdots v_i \cdots v_j \cdots v_{l+1}$ be a longest path in ST_{min} containing v_i and v_j. Then there exist vertices u and w, that are not included in the path P, such that $uv_i,\ wv_j \in E(ST_{min})$. Let T' be the tree obtained from ST_{min} by deleting the edges uv_i and wv_j and adding the new edges uv_{l+1} and wv_{l+1} (Fig. 2). Then $s_{T'} = k$, implying $T' \in \mathcal{T}_{n,k}$.

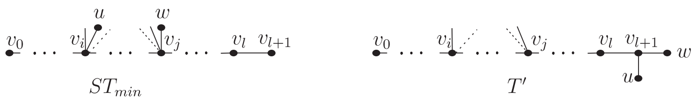


Fig. 2

As before, for an arbitrary vertex $z \in ST_{min}$, let $d(z) = d_{ST_{min}}(z)$. We shall consider the following four cases.

Case 1. $j = l$ and $j \neq i+1$

It holds

$$\begin{aligned}
&M_2(ST_{min}) - M_2(T') \\
&= 4\,(d(u) + \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z)\,) \;+\; 4\,(d(w) + 1 + \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w, v_{l+1}}} d(z)\,) \\
&-3(\sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;+ \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w, v_{l+1}}} d(z) \;+\; d(u) + d(w)) - 3\cdot 3 \\
&= \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;+ \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w, v_{l+1}}} d(z) \;+\; d(u) + d(w) - 5 > 0 \\
&(\text{since } d(u) \geq 1,\ d(w) \geq 1, \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;\geq 4, \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w, v_{l+1}}} d(z) \geq 3\,),
\end{aligned}$$

a contradiction.

Case 2. $j \neq l$ and $j \neq i+1$

We have

$$\begin{aligned}
&M_2(ST_{min}) - M_2(T') \\
&= 4\,(d(u) + \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z)\,) \;+\; 4\,(d(w) + \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w}} d(z)\,) + 1\cdot d(v_l) \\
&-3(\sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;+ \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w}} d(z) \;+\; d(u) + d(w) + d(v_l)\,) \\
&= \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;+ \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w}} d(z) \;+\; d(u) + d(w) - 2d(v_l) > 0 \\
&(\text{since } d(u) \geq 1,\ d(w) \geq 1, \sum_{\substack{zv_i \in E(ST_{min})\\ z\neq u}} d(z) \;\geq 4, \sum_{\substack{zv_j \in E(ST_{min})\\ z\neq w}} d(z) \geq 5,\ d(v_l) \leq 4),
\end{aligned}$$

a contradiction.

Case 3.$j = i+1$ and $j \neq l$

It follows that

$$M_2(ST_{min}) - M_2(T')$$
$$= 4\,(d(u) + \sum_{\substack{zv_i \in E(ST_{min}) \\ z \neq u, v_j}} d(z)\,) \, + \, 4\,(d(w) + \sum_{\substack{zv_j \in E(ST_{min}) \\ z \neq w, v_i}} d(z)\,) + 4 \cdot 4 + 1 \cdot d(v_l)$$
$$-3(\sum_{\substack{zv_i \in E(ST_{min}) \\ z \neq u, v_j}} d(z) \, + \sum_{\substack{zv_j \in E(ST_{min}) \\ z \neq w, v_i}} d(z) \, + \, d(u) + d(w) + d(v_l)\,) - 3 \cdot 3$$
$$= \sum_{\substack{zv_i \in E(ST_{min}) \\ z \neq u, v_j}} d(z) \, + \sum_{\substack{zv_j \in E(ST_{min}) \\ z \neq w, v_i}} d(z) \, + \, d(u) + d(w) - 2d(v_l) + 7 > 0$$
$$\text{(since } d(u) \geq 1,\ d(w) \geq 1, \sum_{\substack{zv_i \in E(ST_{min}) \\ z \neq u, v_j}} d(z) \ \geq 2, \sum_{\substack{zv_j \in E(ST_{min}) \\ z \neq w, v_i}} d(z) \geq 3,\ d(v_l) \leq 4),$$

a contradiction.

Case 4. $j = l = i + 1$

Let $N_{ST_{min}}(v_i) = \{u, v_j, v_{i-1}, x\}$. Note that the vertex $v_j = v_l$ now has three pendent neighbors. Thus, it holds

$$M_2(ST_{min}) - M_2(T')$$
$$= 4(d(u) + d(x) + d(v_{i-1})) + 4 \cdot 4 + 4 \cdot 3 - 3(d(x) + d(v_{i-1}) + d(u)) - 24$$
$$= d(u) + d(x) + d(v_{i-1}) + 4 > 0$$

a contradiction.

Thus, in each case we get a contradiction to the choice of ST_{min} as the tree with minimal M_2 among the trees from $\mathcal{ST}_{n,k}$. Accordingly, the tree with minimal M_2 contains at most one vertex of degree 4. ∎

Denote by n_i $(i \geq 1)$ the number of vertices of degree i in ST_{min}. By Lemmas 2.1 and 2.2, we conclude that $n_4 \leq 1$ and $n_i = 0$ for $i \geq 5$.

Lemma 2.3. *Let ST_{min} be the tree with minimal second Zagreb index among the trees from $\mathcal{ST}_{n,k}$. If $n_4 = 0$ then $n_1 = n_3 + 2$ and $s_{ST_{min}}$ is odd. If $n_4 = 1$, then $n_1 = n_3 + 4$ and $s_{ST_{min}}$ is even.*

Proof. We first consider the case $n_4 = 0$.

The relation (1) now becomes

$$n_1 + 2n_2 + 3n_3 = 2(n-1), \tag{3}$$

i.e.,

$$n_1 + 2n_2 + 3n_3 = 2(n_1 + n_2 + n_3) - 2\,,$$

which yields $n_1 = n_3 + 2$. Next, we prove that in this case $s_{ST_{min}}$ is odd.

$$s_{ST_{min}} = |E(S(ST_{min}))| = |V(S(ST_{min}))| - 1 = n_1 + n_3 - 1 = 2n_3 + 1\,,$$

which is odd. Besides, the relation (3) and $n_2 = n - k - 1$ implies that $n_1 = \frac{k+3}{2}$ and $n_3 = \frac{k-1}{2}$.

Next, we consider the case $n_4 = 1$.

The relation (1) now becomes

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \tag{4}$$

i.e.,

$$n_1 + 2n_2 + 3n_3 + 4 \cdot 1 = 2(n_1 + n_2 + n_3 + 1) - 2\,,$$

which yields $n_1 = n_3 + 4$. Next, we prove that in this case $s_{ST_{min}}$ is even.

$$s_{ST_{min}} = |E(S(ST_{min}))| = |V(S(ST_{min}))| - 1 = n_1 + n_3 + n_4 - 1 = 2n_3 + 4\,,$$

which is even. Besides, the relation (4) and $n_2 = n - k - 1$ implies that $n_1 = \frac{k+4}{2}$ and $n_3 = \frac{k-4}{2}$. ■

In addition, vertices of degree 2 should be placed on the edges of the tree $S(ST_{min})$ such that $M_2(ST_{min})$ is minimal.

Lemma 2.4. *a) Let u, z, v, w be the vertices of a tree $T \in \mathcal{ST}_{n,k}$ such that $uz, zv, vw \in E(T)$ and $d_T(u) = 1$, $d_T(z) = 2$, $d_T(w) = 2$ or $d_T(w) = 3$ and $d_T(v) = 3$ or $d_T(v) = 4$. Let T' be the tree obtained from T as follows*

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

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

b) Let u, y, z, v, w, t be the vertices of a tree $T \in \mathcal{ST}_{n,k}$ such that $uy, yz, zv, wt \in E(T)$ and $d_T(v) = d_T(w) = d_T(t) = 3$, $d_T(y) = d_T(z) = 2$ and $d_T(u) = 3$ or $d_T(u) = 4$ (v may coincide with w). Let T' be the tree obtained from T as follows

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

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

c) Let u, y, z, v, w *be the vertices of a tree* $T \in \mathcal{ST}_{n,k}$ *such that* $uy, zv, vw \in E(T)$ *and* $d_T(u) = 4$, $d_T(y) = d_T(z) = 3$, $d_T(w) = 3$ *or* $d_T(w) = 2$ *and* $d_T(v) = 2$ *(y may coincide with z). Let* T' *be the tree obtained from* T *as follows*

$$T' = T - uy - zv - vw + uv + vy + zw\,.$$

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

Proof. a) It holds

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

since $d_T(v) \geq 3$ and $d_T(w) \geq 2$, which implies $M_2(T') < M_2(T)$;

b) Now, we have

$$M_2(T) - M_2(T') = 1\,,$$

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

c) It holds

$$M_2(T) - M_2(T') = 1\,,\ \text{for}\ d_T(w) = 3\ \text{or}\ \ M_2(T) - M_2(T') = 2\,,\ \text{for}\ d_T(w) = 2\,,$$

which implies $M_2(T') < M_2(T)$.

In addition, in each case it holds $s_{T'} = s_T$. ■

Thus, for $n_4 = 0$, by Lemma 2.4, in order to minimize M_2 we need to place the vertices of degree 2 between the vertices of degree 3 so that there is at least one vertex of degree 2 between any two vertices of degree 3, and then the remaining vertices of degree 2 can be placed arbitrarily between two vertices of degree 2 or one vertex of degree 2 and one vertex of degree 3.

Denote by $\mathcal{ST}_O(n,k)$, for odd k, the set of all n-vertex trees with the degree sequence $(\underbrace{3,\ldots,3}_{\frac{k-1}{2}}, \underbrace{2,\ldots,2}_{n-k-1}, \underbrace{1,\ldots,1}_{\frac{k+3}{2}})$, whose vertices of degree 2 are placed as described above.

Note also that if $n - k - 1 < \frac{k-1}{2} - 1$, i.e., $n < \frac{3k-1}{2}$, there are not enough vertices of degree 2 to be placed between any two vertices of degree 3. This fact will be useful for calculating the index M_2 of such trees from $\mathcal{ST}_O(n,k)$.

If $n_4 = 1$, by Lemma 2.4, the unique vertex of degree 4 in ST_{min} has three pendent neighbors. Also, in order to minimize M_2, we first place a vertex of degree 2 between the vertex of degree 4 and its unique neighbor of degree 3 and then the vertices of degree 2 between any two vertices of degree 3 (at least one vertex of degree 2 between any two vertices of degree 3, if it is possible) and the remaining vertices of degree 2 are placed arbitrarily between two vertices of degree 2 or between the vertex of degree 4 and a vertex of degree 2, or between a vertex of degree 3 and a vertex of degree 2.

Denote by $\mathcal{ST}_E(n,k)$, for even k, the set of all n-vertex trees with the degree sequence $(4, \underbrace{3,\dots,3}_{\frac{k-4}{2}}, \underbrace{2,\dots,2}_{n-k-1}, \underbrace{1,\dots,1}_{\frac{k+4}{2}})$, whose vertices of degree 2 are placed as described above.

Also, we note that if $n < \frac{3k-2}{2}$ there are not enough vertices of degree 2 to be placed between any two vertices of degree 3, what is important for calculating the second Zagreb index M_2 of such trees from $\mathcal{ST}_E(n,k)$,

By previous considerations, the structure of a tree that minimizing M_2 is completely determined, which enables us to state the following result.

Theorem 2.1. *Let $T \in \mathcal{ST}_{n,k}$, where $3 \le k \le n-2$, then*

$$M_2(T) \ge \begin{cases} \dfrac{8n+3k-23}{2}, & n \ge \frac{3k-1}{2} \text{ and } k \text{ odd} \\ 3n+3k-12, & n < \frac{3k-1}{2} \text{ and } k \text{ odd} \\ \dfrac{8n+3k-18}{2}, & n \ge \frac{3k-2}{2} \text{ and } k \text{ even} \\ 3n+3k-10, & n < \frac{3k-2}{2} \text{ and } k \text{ even}. \end{cases}$$

The equality holds if and only if $T \in \mathcal{ST}_O(n,k)$, for odd k, or $T \in \mathcal{ST}_E(n,k)$, for even k.

Proof. Having in mind Lemmas 2.1–2.4 and previous considerations, we conclude that the tree which minimizes M_2 belongs to $\mathcal{ST}_O(n,k)$, for odd k, or to $\mathcal{ST}_E(n,k)$, for even k. By simple calculations, one can easily obtain the second Zagreb indices of trees belonging to these sets, by which the proof is completed. ■

3 On the maximum second Zagreb index of trees with given number of segments

First, we determine the structure of a tree from $\mathcal{ST}_{n,k}$ which maximizes M_2. Denote this tree by ST_{max}.

Lemma 3.1. *If there exists a pendent vertex adjacent to a branching vertex in the tree ST_{max}, than the tree ST_{max} does not contain a vertex of degree 2 with both non-pendent neighbors.*

Proof. Suppose, on the contrary, that a pendent vertex u is adjacent to a vertex v of degree greater than 2, and there exists a vertex w of degree 2, such that $N_{ST_{max}}(w) = \{w_1, w_2\}$ and both w_1 and w_2 are non -pendent vertices (Fig. 3).

Fig. 3

We use the notation $d(x) = d_{ST_{max}}(x)$ for the degree of a vertex x in ST_{max}. Let

$$T' = ST_{max} - ww_1 - ww_2 + uw + w_1w_2 \ .$$

Then, $T' \in \mathcal{ST}_{n,k}$ and

$$\begin{aligned}
&M_2(ST_{max}) - M_2(T') \\
&= 1 \cdot d(v) + 2(d(w_1) + d(w_2)) - (2 \cdot 1 + 2d(v) + d(w_1)d(w_2)) \\
&= -d(v) - 2 + 2(d(w_1) + d(w_2)) - d(w_1)d(w_2) \\
&\leq -5 + 2(d(w_1) + d(w_2)) - d(w_1)d(w_2)
\end{aligned}$$

Note that $I = 2(d(w_1)+d(w_2))-d(w_1)d(w_2) = 2d(w_1)d(w_2)(\frac{1}{d(w_1)}+\frac{1}{d(w_2)}-\frac{1}{2})$, implying that:

i) $I \leq 0$, for $4 \leq d(w_1) \leq d(w_2)$,

ii) $I = 4$, for $2 = d(w_1) \leq d(w_2)$,

iii) $I \leq 3$, for $3 = d(w_1) \leq d(w_2)$.

Thus, in each possible case, we obtain $M_2(ST_{max})-M_2(T') < 0$, implying $M_2(ST_{max}) < M_2(T')$, a contradiction to the choice of ST_{max} as the tree with maximal M_2 among the trees from $\mathcal{ST}_{n,k}$. ■

Lemma 3.2. *Let w be the vertex from $V(ST_{max})$, such that $d_{ST_{max}}(w) = \Delta(ST_{max})$. Then w is the only branching vertex in ST_{max} , i.e. ST_{max} is a starlike tree.*

Proof. We notice first that maximal degree of a vertex in ST_{max} must be greater than 2, since $k \geq 3$ which implies $ST_{max} \neq P_n$.

Suppose there exists a vertex $u \in V(ST_{max})$, such that $u \neq w$ and $3 \leq d_{ST_{max}}(u) \leq d_{ST_{max}}(w)$, and let $P = wv_1 \cdots v_s u$ be a path in ST_{max} connecting w and u. Let $N_{ST_{max}}(u) = \{u_1, \ldots, u_{d(u)-1}, v_s\}$ and $T' = ST_{max} - \{uu_i | 1 \leq i \leq d(u)-1\} + \{wu_i | 1 \leq i \leq d(u)-1\}$ (Fig. 4).

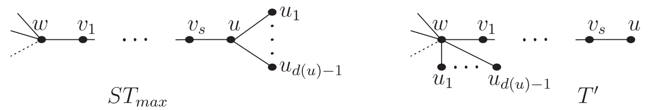


Fig. 4

First, we note that $s_{T'} = s_{ST_{max}}$. We shall consider the difference $M_2(T') - M_2(ST_{max})$, by examine only the contributions coming from edges whose degrees differ in T' and ST_{max}. As before, by $d(x)$ we denote the degree of a vertex $x \in V(ST_{max})$.

Case 1. $uw \notin E(ST_{max})$

$$M_2(T') - M_2(ST_{max})$$
$$= (d(w) + d(u) - 1)\Big(\sum_{ww_i \in E(ST_{max})} d(w_i) + \sum_{i=1}^{d(u)-1} d(u_i)\Big) + 1 \cdot d(v_s)$$
$$-\Big(\, d(w) \sum_{ww_i \in E(ST_{max})} d(w_i) + d(u)\Big(\sum_{i=1}^{d(u)-1} d(u_i) + d(v_s)\Big)\,\Big)$$
$$= (d(u) - 1)\Big(\sum_{ww_i \in E(ST_{max})} d(w_i) - d(v_s)\Big) + (d(w) - 1) \sum_{i=1}^{d(u)-1} d(u_i) > 0$$
$$\Big(\text{ since } d(u) - 1 \geq 2, \sum_{ww_i \in E(ST_{max})} d(w_i) - d(v_s) \geq (d(w) - 1) \cdot 1 + 2 - d(v_s)$$
$$\geq d(w) + 1 - d(v_s) > 0, \sum_{i=1}^{d(u)-1} d(u_i) \geq d(u) - 1 \geq 2\Big).$$

This implies $M_2(T') > M_2(ST_{max})$, a contradiction.

Case 2. $uw \in E(ST_{max})$

$$M_2(T') - M_2(ST_{max})$$
$$= (d(w) + d(u) - 1)\Big(\sum_{\substack{ww_i \in E(ST_{max}) \\ w_i \neq u}} d(w_i) + \sum_{i=1}^{d(u)-1} d(u_i) + 1\Big)$$
$$-\Big(\, d(w) \sum_{\substack{ww_i \in E(ST_{max}) \\ w_i \neq u}} d(w_i) + d(u) \sum_{i=1}^{d(u)-1} d(u_i) + d(w) \cdot d(u)\,\Big)$$
$$= (d(u) - 1) \sum_{\substack{ww_i \in E(ST_{max}) \\ w_i \neq u}} d(w_i) + (d(w) - 1) \cdot \Big(\sum_{i=1}^{d(u)-1} d(u_i) - (d(u) - 1)\Big) > 0$$
$$\Big(\text{ since } d(u) - 1 \geq 2, \sum_{\substack{ww_i \in E(ST_{max}) \\ w_i \neq u}} d(w_i) \geq d(w) - 1 > 0,$$
$$\sum_{i=1}^{d(u)-1} d(u_i) - (d(u) - 1) \geq (d(u) - 1) - (d(u) - 1) \geq 0\Big).$$

Consequently, $M_2(T') > M_2(ST_{max})$, a contradiction.

Thus, the extremal tree ST_{max} contains exactly one branching vertex. As $s_{ST_{max}} = k$, we conclude that ST_{max} is in fact a starlike tree of degree k. ■

Having in mind Lemmas 3.1 and 3.2, denote by $\mathcal{S}(n,k)$ the set of all starlike trees of degree k on n vertices, such that an arbitrary pendent vertex is adjacent to a vertex of degree 2, for $2k+1 \le n$, or the central vertex of degree k has exactly $2k+1-n$ pendent neighbors, for $n < 2k+1$.

Then, the following result can be stated.

Theorem 3.1. *Let $T \in \mathcal{ST}_{n,k}$, where $3 \le k \le n-2$, then*

$$M_2(T) \le \begin{cases} 2k^2 - 6k + 4n - 4\,, & n \ge 2k+1 \\ k(n-3) + 2n - 2\,, & n < 2k+1. \end{cases}$$

The upper bound is attained if and only if $T \in \mathcal{S}(n,k)$.

Proof. By Lemmas 3.1 and 3.2 it follows that a tree $ST_{max} \in \mathcal{ST}_{n,k}$ which maximizes M_2 is a starlike tree of degree k, such that an arbitrary pendent vertex in ST_{max} is adjacent to a vertex of degree 2 (for $n \ge 2k+1$) or there are exactly $n-k-1$ pendent vertices with neighbors of degree 2 (for $n < 2k+1$). Hence, $ST_{max} \in \mathcal{S}(n,k)$ and $M_2(ST_{max}) = 2k^2 - 6k + 4n - 4$ for $n \ge 2k+1$ and $M_2(ST_{max}) = k(n-3) + 2n - 2$ for $n < 2k+1$. ■

Remark 3.1. *According to (2) , Theorems 2.1 and 3.1 also characterize the trees which minimize and maximize the second Zagreb index of n-vertex trees with prescribed number of vertices of degree two.*

4 On the minimum Zagreb indices of trees with fixed number of branching vertices

In this section we examine the influence of the number of branching vertices in a tree on Zagreb indices M_1 and M_2, and find sharp lower bounds on M_1 and M_2 for n-vertex trees from $\mathcal{BT}_{n,b}$ having b branching vertices. We use a similar approach as before. Namely, we first determine the structure of trees that minimizing M_1 and M_2. Let BT^1_{min} (respectively BT^2_{min}) be the tree with minimal first Zagreb index (respectively second Zagreb index) among the n-vertex trees from $\mathcal{BT}_{n,b}$ with exactly b branching vertices. Then the following observations hold.

Lemma 4.1. *The tree $BT^1_{min} \in \mathcal{BT}_{n,b}$ (respectively $BT^2_{min} \in \mathcal{BT}_{n,b}$) that minimizes the first Zagreb index (respectively the second Zagreb index) does not contain a branching vertex of degree greater than 3.*

Proof. Suppose, on the contrary, that the tree BT^1_{min} (respectively BT^2_{min}) contains a branching vertex of degree greater than 3, and let u be such a vertex whose degree is maximum. Let $P = v_0v_1 \dots v_{i-1}u(= v_i)v_{i+1} \dots v_{l+1}$ be a longest path in BT^1_{min} (respectively in BT^2_{min}) containing u. Assume that $N(u) = \{v_{i-1}, v_{i+1}, u_1, u_2, \dots u_{d(u)-2}\}$ is the neighbor set of u in BT^1_{min} (respectively in BT^2_{min}). Denote by z_1 a pendent vertex connected to u via u_1 (z_1 may coincide with u_1 if $d(u_1) = 1$).

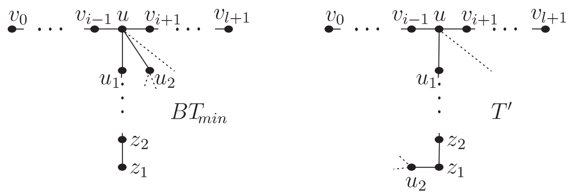


Fig. 5

Let T' be the tree obtained from BT^1_{min} (respectively BT^2_{min}) by deleting the edge uu_2 and adding the new edge z_1u_2 (Fig. 5). Then $T' \in \mathcal{BT}_{n,b}$ and the only vertices whose degrees differ in BT^1_{min} (respectively in BT^2_{min}) and T' are u and z_1. If we denote by $d(x)$ the degree of a vertex x in BT^1_{min} (respectively in BT^2_{min}), then it holds

$$\begin{aligned}
&M_1(T') - M_1(BT^1_{min}) \\
&= (d(u) - 1)^2 + 2^2 - (d^2(u) + 1^2) \\
&= -2(d(u) - 2) < 0 \\
&(\text{ since } \ d(u) \geq 4).
\end{aligned}$$

Thus, $M_1(T') < M_1(BT^1_{min})$, a contradiction to the choice of BT^1_{min} as the tree from $\mathcal{BT}_{n,b}$ with minimal M_1.

Assume that $N_{BT^2_{min}}(z_1) = \{z_2\}$. Then, for the second Zagreb index we obtain

$$\begin{aligned}
&M_2(T') - M_2(BT^2_{min}) \\
&= (d(u)-1)(d(v_{i-1}) + d(v_{i+1}) + \sum_{\substack{j=1\\ j\neq 2}}^{d(u)-2} d(u_j)) + 2\cdot d(z_2) + 2d(u_2) \\
&-(d(u)(d(v_{i-1}) + d(v_{i+1}) + \sum_{j=1}^{d(u)-2} d(u_j)) + 1\cdot d(z_2)) \\
&= -(d(v_{i-1}) + d(v_{i+1}) + \sum_{\substack{j=1\\ j\neq 2}}^{d(u)-2} d(u_j) + (d(u)-2)d(u_2)) + d(z_2) \\
&< d(z_2) - d(u) - d(u_2) < 0 \\
&(\text{ since } d(u) \text{ is maximum}).
\end{aligned}$$

Also, in a special case when $u_1 = z_1$(i.e., $z_2 = u$), it holds

$$\begin{aligned}
&M_2(T') - M_2(BT^2_{min}) \\
&= (d(u)-1)(d(v_{i-1}) + d(v_{i+1}) + \sum_{j\geq 3} d(u_j) + 2) + 2d(u_2) \\
&-d(u)(d(v_{i-1}) + d(v_{i+1}) + 1 + \sum_{j=2}^{d(u)-2} d(u_j)) \\
&= -(d(v_{i-1}) + d(v_{i+1}) + \sum_{j\geq 3} d(u_j)) - (d(u)-2)(d(u_2)-1) < 0
\end{aligned}$$

Thus, $M_2(T') < M_2(BT^2_{min})$, a contradiction to the choice of BT^2_{min} as the tree from $\mathcal{BT}_{n,b}$ with minimal M_2. ■

Consequently, in the tree BT^1_{min} (respectively BT^2_{min}) there exist only vertices of degree 1, 2 or 3. Let n_i be the number of vertices of degree i in BT^1_{min} (respectively in BT^2_{min}). Then, analogously to the proof of Lemma 2.3 (case $n_4 = 0$) we can show that $n_1 = n_3 + 2$. From relation (3), since $n_3 = b$, we obtain $n_1 = b + 2$ and $n_2 = n - 2b - 2$ and conclude that the following result holds.

Theorem 4.1. *Let $T \in \mathcal{BT}_{n,b}$, where $1 \leq b \leq \frac{n}{2} - 1$, then*

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

and the equality holds if and only if $T \in \mathcal{B}^1_{min}(n,b)$, where $\mathcal{B}^1_{min}(n,b)$ is the set of all n-vertex trees with the degree sequence $(\underbrace{3,\ldots,3}_{b}, \underbrace{2,\ldots,2}_{n-2b-2}, \underbrace{1,\ldots,1}_{b+2})$.

Proof. According to previous considerations, the tree which minimizes M_1 belongs to $\mathcal{B}^1_{min}(n,b)$, and for an arbitrary tree T from $\mathcal{B}^1_{min}(n,b)$, one can easily calculate $M_1(T)$ as

$$M_1(T) = b \cdot 3^2 + (n-2b-2) \cdot 2^2 + (b+2) \cdot 1^2 = 2b + 4n - 6\,,$$

by which the proof is completed. ■

Next, we pay attention to the problem of minimizing M_2 among the trees from $\mathcal{BT}_{n,b}$ $(1 \le b \le \frac{n}{2} - 1)$. The vertices of degree 2 should be placed such that $M_2(BT^2_{min})$ is minimum. By Lemma 2.4 (which also holds in this case, since the trees obtained by transformations introduced in Lemma 2.4 still have the prescribed number of branching vertices) we need to place the vertices of degree 2 between the vertices of degree 3 so that there is at least one vertex of degree 2 between any two vertices of degree 3 (if there are enough vertices of degree 2, i.e., $n - 2b - 2 \ge b - 1$ implying $n \ge 3b + 1$), and then the remaining vertices of degree 2 (if they exist) can be placed arbitrarily between two vertices of degree 2 or one vertex of degree 2 and one vertex of degree 3.

Denote by $\mathcal{B}^2_{min}(n, b)$ the set of all n-vertex trees with the degree sequence $(\underbrace{3, \ldots, 3}_{b}, \underbrace{2, \ldots, 2}_{n-2b-2}, \underbrace{1, \ldots, 1}_{b+2})$, whose vertices of degree 2 are placed as described above. Now, we are able to prove

Theorem 4.2. *Let $T \in \mathcal{BT}_{n,b}$, where $1 \le b \le \frac{n}{2} - 1$, then*

$$M_2(T) \ge \begin{cases} 3b + 4n - 10\,, & n \ge 3b + 1 \\ 6b + 3n - 9\,, & n < 3b + 1. \end{cases}$$

and the equality holds if and only if $T \in \mathcal{B}^2_{min}(n, b)$.

Proof. According to previous considerations, the tree from $\mathcal{BT}_{n,b}$ which minimizes M_2 belongs to $\mathcal{B}^2_{min}(n, b)$. The second Zagreb index of an arbitrary tree from $\mathcal{B}^2_{min}(n, b)$ can easily be calculated (taking into account if there are enough vertices of degree 2), which completes the proof. ■

5 On the maximum Zagreb indices of trees with fixed number of branching vertices

We are going to examine the structure of trees that maximize Zagreb indices among all n-vertex trees with fixed number of branching vertices. Let BT^1_{max} (respectively BT^2_{max}) be the tree with maximal first Zagreb index (respectively second Zagreb index) among the trees from $\mathcal{BT}_{n,b}$ $(1 \le b \le \frac{n}{2} - 1)$. Then the following observation hold.

Lemma 5.1. *The tree $BT^1_{max} \in \mathcal{BT}_{n,b}$ (respectively $BT^2_{max} \in \mathcal{BT}_{n,b}$) which maximizes the first Zagreb index (respectively the second Zagreb index) contains only pendent and branching vertices.*

Proof. Suppose, on the contrary, that $V_2(BT^1_{max}) \neq \emptyset$ (respectively $V_2(BT^2_{max}) \neq \emptyset$) . Since $b \geq 1$ (and accordingly the extremal tree is not a path), there must exist a branching vertex, say w, adjacent to a vertex, say u, of degree 2. Let $N_{BT^1_{max}}(u) = \{v, w\}$ (respectively $N_{BT^2_{max}}(u) = \{v, w\}$). Denote by T' the tree obtained from BT^1_{max} (respectively BT^2_{max}) by deleting the edge uv and adding the new edge vw. We notice that $T' \in \mathcal{BT}_{n,b}$. Then, if we denote by $d(x)$ the degree of an arbitrary vertex $x \in BT^1_{max}$ (respectively $x \in BT^2_{max}$), we obtain

$$\begin{aligned}
&M_1(T') - M_1(BT^1_{max})\\
&= (1^2 + (d(w)+1)^2) - (2^2 + d^2(w))\\
&= 2(d(w) - 2) > 0\,,
\end{aligned}$$

a contradiction to the maximality of $M_1(BT^1_{max})$.

Besides, if $N_{BT^2_{max}}(w) = \{u, w_1, \ldots, w_{d(w)-1}\}$, then

$$\begin{aligned}
&M_2(T') - M_2(BT^2_{max})\\
&= (d(w)+1)(\sum_{i=1}^{d(w)-1} d(w_i) + 1 + d(v))\\
&-d(w)(\sum_{i=1}^{d(w)-1} d(w_i) + 2) - 2 \cdot d(v)\\
&= \sum_{i=1}^{d(w)-1} d(w_i) + (d(v)-1)(d(w)-1) > 0\,.
\end{aligned}$$

Hence, we get a contradiction to the choice of BT^2_{max} as the tree with maximal M_2 among the trees from $\mathcal{BT}_{n,b}$. ■

We need also the following result.

Lemma 5.2. *The tree BT^1_{max} (respectively BT^2_{max}) which maximizes the first Zagreb index (respectively the second Zagreb index) among the trees from $\mathcal{BT}_{n,b}$ contains at most one branching vertex of degree greater than 3.*

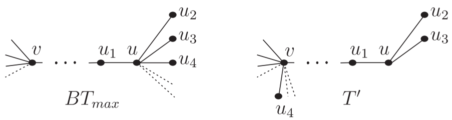


Fig. 6

Proof. We first consider the tree that maximizes M_1. Suppose there exist two vertices u and v with $d(v) \geq d(u) \geq 4$, and let $N_{BT^1_{max}}(u) = \{u_1, u_2, \ldots, u_{d(u)}\}$. Suppose, also, that u is connected to v via u_1 (it may be $u_1 = v$) (Fig. 6). Let $T' = BT^1_{max} - \{uu_i | 4 \leq i \leq d(u)\} + \{vu_i | 4 \leq i \leq d(u)\}$. Then $T' \in \mathcal{B}_{n,b}$ and ,

$$\begin{aligned} & M_1(T') - M_1(BT^1_{max}) \\ &= (3^2 + (d(v) + d(u) - 3)^2) - (d^2(u) + d^2(v)) \\ &= 18 + 2(d(u)d(v) - 3(d(u) + d(v)) > 0 \ . \end{aligned}$$

The last inequality follows from $I = d(u)d(v) - 3(d(u) + d(v)) = d(u)d(v)(1 - 3(\frac{1}{d(u)} + \frac{1}{d(v)}))$ and $d(u), d(v) \geq 4$, implying $1 - 3(\frac{1}{d(u)} + \frac{1}{d(v)}) \geq -\frac{1}{2}$, and $I \geq -8$. So, it holds $M_1(T') > M_1(BT^1_{max})$, a contradiction to the choice of BT^1_{max}.

Next, we consider the tree that maximizes M_2. For this purpose, denote by $\mu(x)$ the sum of the degrees of vertices adjacent to a vertex x in BT^2_{max}. As in previous case, suppose there exist two vertices u and v in BT^2_{max} whose degrees are greater than 3 (here the assumption $d(v) \geq d(u)$ is not necessary). Let $N_{BT^2_{max}}(u) = \{u_1, u_2, \ldots, u_{d(u)}\}$ and $N_{BT^2_{max}}(v) = \{v_1, v_2, \ldots, v_{d(v)}\}$. Suppose also that u is connected to v via u_1 (it may be $u_1 = v$). We examine two possible cases.

Case 1. $uv \notin E(BT^2_{max})$, i.e., $u_1 \neq v$.

Assume, without loss of generality, that $\mu(v) \geq \mu(u)$, and let $T' = BT^2_{max} - \{uu_i | 4 \leq i \leq d(u)\} + \{vu_i | 4 \leq i \leq d(u)\}$. Then $T' \in \mathcal{BT}_{n,b}$ and we have

$$\begin{aligned} & M_2(T') - M_2(BT^2_{max}) \\ &= 3 \sum_{i=1}^{3} d(u_i) \ + (d(v) + d(u) - 3)(\sum_{i=1}^{d(v)} d(v_i) + \sum_{i=4}^{d(u)} d(u_i)) \\ & - d(u) \sum_{i=1}^{d(u)} d(u_i) - d(v) \sum_{i=1}^{d(v)} d(v_i) \\ &= (d(u) - 3)(\sum_{i=1}^{d(v)} d(v_i) - \sum_{i=1}^{3} d(u_i)) + (d(v) - 3) \sum_{i=4}^{d(u)} d(u_i) > 0 \\ & (\text{ since } \mu(v) = \sum_{i=1}^{d(v)} d(v_i) \geq \mu(u) > \sum_{i=1}^{3} d(u_i) \, , d(u) > 3, d(v) > 3 \,), \end{aligned}$$

a contradiction to the maximality of $M_2(BT^2_{max})$.

Case 2. $uv \in E(BT^2_{max})$, i.e., $u_1 = v$ (and also $u = v_1$).

Denote by $\mu_{\neq v}(u)$ (respectively $\mu_{\neq u}(v)$) the sum of the degrees of vertices adjacent to u (respectively v), different from v (respectively u). Then we compare $\mu_{\neq v}(u)$ and $\mu_{\neq u}(v)$. Suppose , without loss of generality, that $\mu_{\neq u}(v) \geq \mu_{\neq v}(u)$. Then, we can transform the tree BT^2_{max} into the tree T', as described in previous case. It follows that

$$M_2(T') - M_2(BT^2_{max})$$
$$= 3(\sum_{i=2}^{3} d(u_i) + d(v) + d(u) - 3) + (d(v) + d(u) - 3)(\sum_{i=2}^{d(v)} d(v_i) + \sum_{i=4}^{d(u)} d(u_i))$$
$$-(d(u)\sum_{i=2}^{d(u)} d(u_i) + d(v)\sum_{i=2}^{d(v)} d(v_i) + d(u)d(v))$$
$$= (d(u) - 3)(\sum_{i=2}^{d(v)} d(v_i) - \sum_{i=2}^{3} d(u_i)) + (d(v) - 3)(\sum_{i=4}^{d(u)} d(u_i) + 3 - d(u)) > 0\,,$$
$$(\text{ since } \sum_{i=2}^{d(v)} d(v_i) = \mu_{\neq u}(v) \geq \mu_{\neq v}(u) > \sum_{i=2}^{3} d(u_i)\,, d(v) > 3,\ d(u) > 3,\ \sum_{i=4}^{d(u)} d(u_i) \geq d(u) - 3\,)$$

a contradiction to the maximality of $M_2(BT^2_{max})$. ■

Consequently, the tree that maximizes M_1 (or M_2) contains at most one branching vertex of degree greater than 3, denoted by v_{max} and it holds that $d(v_{max}) = \Delta$. Hence, the tree BT^1_{max} (or BT^2_{max}), contains $b-1$ branching vertices of degree 3, the branching vertex v_{max} of degree $d(v_{max}) \geq 3$ and $n-b$ pendent vertices. By relation (1) it follows that $\Delta = d(v_{max}) = n - 2b + 1$. Also, $b \leq \frac{n}{2} - 1$ implies $\Delta \geq 3$, whereas $\Delta = 3$ if and only if $b = \frac{n}{2} - 1$.

Since the first Zagreb index is determined by the degrees of vertices, the problem of characterization the extremal trees with maximal first Zagreb index among the n-vertex trees with b branching vertices is solved. Namely, it holds

Theorem 5.1. *Let $T \in \mathcal{BT}_{n,b}$, where $1 \leq b \leq \frac{n}{2} - 1$, then*

$$M_1(T) \leq n^2 + 4b^2 + 4b + 3n - 4bn - 8,$$

and the equality holds if and only if $T \in \mathcal{B}^1_{max}(n,b)$, where $\mathcal{B}^1_{max}(n,b)$ is the set of all n-vertex trees with the degree sequence $(n-2b+1, \underbrace{3,\ldots,3}_{b-1}, \underbrace{1,\ldots,1}_{n-b})$.

Proof. According to previous considerations, the tree which maximizes M_1 belongs to $\mathcal{B}^1_{max}(n,b)$, and for an arbitrary tree T from $\mathcal{B}^1_{max}(n,b)$, one can easily calculate $M_1(T)$ as

$$M_1(T) = (n-2b+1)^2 + (b-1)\cdot 3^2 + (n-b)\cdot 1^2 = n^2 + 4b^2 + 4b + 3n - 4bn - 8\,,$$

by which the proof is completed. ■

In the sequel, we characterize the extremal tree BT^2_{max} with maximal second Zagreb index among the trees from $\mathcal{BT}_{n,b}$.

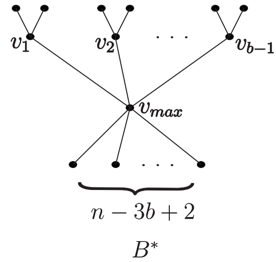


Fig. 7. The tree with maximal M_2 for $1 \leq b \leq \frac{n+2}{3}$

First, we prove that the extremal tree BT^2_{max} is the tree B^*, displayed in Fig. 7, if $\Delta = n - 2b + 1 \geq b - 1$, i.e., $b \leq \frac{n+2}{3}$.

Let $V_3(BT^2_{max}) = \{v_1, \ldots, v_{b-1}, v_{max}\}$ be the set of branching vertices in BT^2_{max}.

Lemma 5.3. *If $1 \leq b \leq \frac{n+2}{3}$ then a branching vertex $v_i \in V_3(BT^2_{max})$ $(1 \leq i \leq b-1)$ is adjacent to the vertex v_{max} of degree Δ.*

Proof. If there exists a branching vertex v_i $(1 \leq i \leq b-1)$ non-adjacent to v_{max}, then, since $\Delta \geq b - 1$, there exists a pendent neighbor w of v_{max}. Let $N(v_i) = \{v_j, z_1, z_2\}$ $(1 \leq j \leq b-1,\ j \neq i)$, where z_1 and z_2 are either pendent or branching vertices different from v_{max}. Denote by T' the tree obtained from BT^2_{max} by deleting the edges $v_j v_i$ and $v_{max} w$ and adding the new edges $v_{max} v_i$ and $v_j w$ (Fig. 8). By this transformation, the degrees of all vertices stay the same, implying that the obtained tree T' belongs to $\mathcal{BT}_{n,b}$.

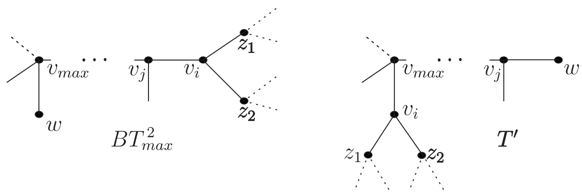


Fig. 8

As it holds

$$
\begin{aligned}
& M_2(T') - M_2(BT^2_{max}) \\
& = \Delta \cdot d(v_i) + d(v_j)d(w) - d(v_j)d(v_i) - \Delta \cdot d(w) \\
& = 2(\Delta - 3) > 0 \ (\text{ since } b \in [1, \tfrac{n+2}{3}]) \,,
\end{aligned}
$$

we get the contradiction to the choice of BT^2_{max} as the tree with maximal M_2 among the trees from $\mathcal{BT}_{n,b}$. Consequently, if $b \in [1, \frac{n+2}{3}]$ the extremal tree BT^2_{max} is the tree B^* displayed in Fig. 7. ■

Remark 5.1. *The last inequality in the proof of Lemma 5.3 reduces to equality if* $\frac{n+2}{3} \geq \frac{n}{2} - 1$ *and* $b = \frac{n}{2} - 1$*, i.e., in the cases* $n = 10$ *and* $b = 4$*,* $n = 8$ *and* $b = 3$*,* $n = 6$ *and* $= 2$*,* $n = 4$ *and* $b = 1$*. By Lemma 5.1, the extremal trees in* $\mathcal{BT}_{8,3}$*,* $\mathcal{BT}_{6,2}$ *and* $\mathcal{BT}_{4,1}$ *are unique and isomorphic to* B^**, and by the proof of Lemma 5.3, there are two trees in* $\mathcal{BT}_{10,4}$ *with maximal* M_2*, one of which is isomorphic to* B^**.*

In the following, we characterize the extremal tree BT^2_{max} for $b \in (\frac{n+2}{3}, \frac{n}{2} - 1]$. For this purpose we need the following result.

Lemma 5.4. *Let* u *be a branching vertex in a tree* $T \in \mathcal{BT}_{n,b}$ *whose neighbor set* $N(u)$ *contain three branching vertices* z, v, w *where* $d(v) \geq 3$, $d(z) = d(w) = 3$, $N(z) = \{u, z_1, z_2\}$ *and* $N(w) = \{u, w_1, w_2\}$*. Let* T' *be a tree obtained from* T *by deleting the edges* uz *and* ww_1 *and adding the new edges* uw_1 *and* wz *(Fig. 9). Then* $T' \in \mathcal{BT}_{n,b}$ *and* $M_2(T') = M_2(T)$*.*

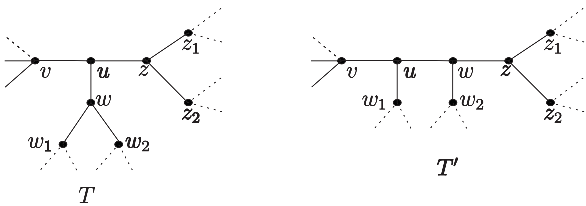


Fig. 9. Trees T and T' from Lemma 5.4

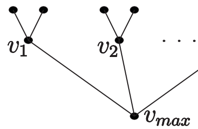
Proof. Obviously, $T' \in \mathcal{BT}_{n,b}$ and it holds

$$
\begin{aligned}
&M_2(T') - M_2(T) \\
&= d(u)d(w_1) + d(z)d(w) - d(u)d(z) - d(w)d(w_1) = 0\,,
\end{aligned}
$$

implying $M_2(T') = M_2(T)$. ■

Remark 5.2. *If* w_1 *and* w_2 *are pendent vertices, according to Lemma 5.4,* M_2 *is the same if there are two branching vertices each of which has two branching neighbors or there exists a branching vertex with three branching neighbors.*

Assume that $3 < \Delta = d(v_{max}) < b-1$, i.e., $b \in (\frac{n+2}{3}, \frac{n}{2}-1)$. Then there exists a branching vertex $v_i \in V_3(BT^2_{max})$ $(1 \le i \le b-1)$ non-adjacent to v_{max}. Besides, the vertex v_{max} has only branching neighbors (in the opposite case, using the transformation of a tree introduced in the proof of Lemma 5.3 we can increase M_2).



T_B

Fig. 10. The base B_T of a tree with maximal M_2 for $\frac{n+2}{3} < b \le \frac{n}{2} - 1$

We construct the tree BT^2_{max} starting from the tree T_B, displayed in Fig. 10, as a base, and then insert a new branching vertex of degree 3 to an arbitrary edge $v_{max}v_i$ $(1 \le i \le \Delta)$. It can easily be proved that M_2 is the same if two branching vertices are inserted on the same edge $v_{max}v_i$ or on different edges $v_{max}v_i$ and $v_{max}v_j$. Also, by Lemma 5.4 (see Remark 5.2), the influence on M_2 is the same if we insert a branching vertex with three branching neighbors or two branching vertices each of which has two branching neighbors. We use the same reasoning when inserting all the remaining branching vertices, and conclude that in this case the extremal tree is determined only by the degrees of vertices, and not by the manner they are connected to each other, except the vertex v_{max} which has only branching neighbors.

If $b = \frac{n}{2} - 1$, i.e., $\Delta = 3$, from Lemma 5.4 it follows that the vertices of degree three may be connected to each other arbitrarily, and so the extremal tree is a tree with $b = \frac{n}{2} - 1$ vertices of degree 3 and $n - b = \frac{n}{2} + 1$ pendent vertices. Thus, we proved

Theorem 5.2. *Let $T \in \mathcal{BT}_{n,b}$, where $1 \le b \le \frac{n}{2} - 1$, then*

$$M_2(T) \le \begin{cases} n^2 - 2bn + 8b - 7\,, & 1 \le b \le \frac{n+2}{3}\,, \\ 3n^2 + 12b^2 - 12bn + 12b - 15\,, & \frac{n+2}{3} < b \le \frac{n}{2} - 1\,, \end{cases}$$

and the equality holds if and only if $T \cong B^*$ for $1 \le b \le \frac{n+2}{3}$, where B^* is the tree displayed in Fig. 7, and $T \in \mathcal{B}^2_{max}(n,b)$, for $\frac{n+2}{3} < b \le \frac{n}{2} - 1$, where $\mathcal{B}^2_{max}(n,b)$ is the set of n-vertex trees with the degree sequence $(n-2b+1, \underbrace{3,\ldots,3}_{b-1}, \underbrace{1,\ldots,1}_{n-b})$ such that the *vertex of degree* $\Delta = n - 2b + 1$ *has only branching neighbors for* $b < \frac{n}{2} - 1$*, and the set* $\mathcal{B}^2_{max}(n, \frac{n}{2} - 1)$ *contains all* n*-vertex trees with the degree sequence* $(\underbrace{3, \ldots, 3}_{\frac{n}{2}-1}, \underbrace{1, \ldots, 1}_{\frac{n}{2}+1})$.

Proof. The first part of Theorem follows immediately from previous considerations. Besides, the second Zagreb index of the tree B^* and of an arbitrary tree $T \in \mathcal{B}^2_{max}(n, b)$ can easily be calculated, which completes the proof. ■

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