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# Improved Inequality between Zagreb Indices of Trees[1]

**Dragan Stevanović**[2]

*University of Niš, PMF, Višegradska 33, 18000 Niš, Serbia and University of Primorska, UP IAM, Muzejski trg 2, SI6000 Koper, Slovenia*

**Martin Milanič**[3]

*University of Primorska, UP IAM, Muzejski trg 2, SI6000 Koper, Slovenia, and University of Primorska, UP FAMNIT, Glagoljaška 8, SI6000 Koper, Slovenia*

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**Abstract**

For a simple graph $G$ with $n$ vertices and $m$ edges, let $M_1$ and $M_2$ denote the first and the second Zagreb index of $G$. The inequality $M_1/n \leq M_2/m$ in the case of trees has been proved first by Vukičević and Graovac [MATCH Commun. Math. Comput. Chem. 57 (2007), 587–590], and a new proof has been found recently by Andova, Cohen and Škrekovski [Ars Math. Contemp. 5 (2012), 73–76]. Here we improve this inequality by showing that, if $T$ is not a star, then $nM_2 - mM_1 \geq 2(n-3) + (\Delta-1)(\Delta-2)$, where $\Delta$ is the maximum vertex degree in $T$.

## 1 Introduction

Let $G$ be a simple graph with the set of vertices $V(G)$, $n = |V(G)|$, and the set of edges $E(G)$, $m = |E(G)|$. The first and the second Zagreb indices of $G$ are defined as $M_1(G) = \sum_{u \in V(G)} d_G(u)^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$, where $d_G(u)$ denotes the degree of a vertex $u$ in $G$. The Zagreb indices are among the oldest and most famous topological indices—they were introduced by Gutman and Trinajstić in [1] in 1972, while the recent surveys of their chemical importance and mathematical properties appear in [2, 3].

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[2]E-mail: `dragance106@yahoo.com`

[3]E-mail: `martin.milanic@upr.si`

Comparing the values of the Zagreb indices of the same graph, Hansen and Vukičević initially conjectured in [4] that

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}, \tag{1}$$

with equality attained for complete graphs. This conjecture generated a lot of research, and for a survey on its developments the reader is referred to [5]. While the conjecture does not hold in general, it does hold for chemically important classes of trees, unicyclic graphs and graphs with maximum vertex degree four.

In the case of trees, the inequality (1) has been proved first by Vukičević and Graovac [6], and a new proof has been found recently by Andova, Cohen and Škrekovski [7]. Our goal here is to improve the inequality (1) by providing a positive lower bound for the value of $nM_2(T) - mM_1(T)$, when $T$ is not a star.

## 2 The first bound

**Theorem 1** *For a tree $T$ with $n \geq 3$ vertices and $m$ edges, let $w$ denote a vertex of $T$ having the smallest vertex degree larger than one:*

$$d_T(w) = \min\{d_T(v) \mid v \in V(T) \wedge d_T(v) \geq 2\}\,.$$

*Then*

$$nM_2(T) - mM_1(T) \begin{cases} = \ 0, & \text{if } T \text{ is a star;} \\ \geq \ 2\sum_{x \in V(T)\setminus\{w\}} \left(d_T(x) - 1\right), & \text{otherwise.} \end{cases} \tag{2}$$

*Moreover,*

$$M_2(T) - M_1(T) \geq -d_T(w)\,. \tag{3}$$

**Proof** Recall first that $m = n-1$ for every tree with $n$ vertices. We prove (2) and (3) simultaneously by induction on the number of vertices $n$.

If $n = 3$, then $T$ is a star and it is straightforward to verify that (2) and (3) hold.

Suppose now that the theorem holds for all trees with less than $n$ vertices for some $n > 3$, and let $T$ be a tree with $n$ vertices. If $T$ is a star, then

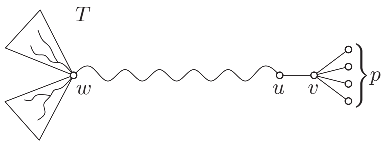
$$M_1(T) = n(n-1), \qquad M_2(T) = (n-1)^2, \qquad d_T(w) = n-1,$$

and, consequently,

$$nM_2(T) - mM_1(T) = 0 \quad \text{and} \quad M_2(T) - M_1(T) = -(n-1) = -d_T(w),$$

showing that (2) and (3) hold in this case.

If $T$ is not a star, let $l$ be a leaf farthest from $w$ in $T$. As $T$ is not a star, $l$ is at distance at least two from $w$. Let $v$ be the unique neighbor of $l$. By the choice of $l$, all neighbors of $v$ are leaves, except for its neighbor $u$ on the unique $(w,v)$-path in $T$ with $d_T(u) \geq 2$. Let $p = d_T(v) - 1$.




Let $T'$ be the tree obtained from $T$ by deleting the $p$ leaves adjacent to $v$. Note that $d_{T'}(w) = d_T(w) \leq d_T(v)$ and $v \neq w$. Denote by $M_1'$ and $M_2'$ the first and the second Zagreb index of $T'$. Since $v$ itself is a leaf in $T'$, we have

$$M_1(T) \;=\; M_1' - 1^2 + (p+1)^2 + p \cdot 1^2 \;=\; M_1' + p^2 + 3p$$

and

$$M_2(T) \;=\; M_2' - 1 \cdot d_T(u) + (p+1) \cdot d_T(u) + p \cdot (p+1) \cdot 1 \;=\; M_2' + p^2 + p \cdot d_T(u) + p\,.$$

Since $T'$ has at least three vertices, it satisfies (2) and (3) by the inductive hypothesis:

$$(n-p)M_2' - (n-p-1)M_1' \begin{cases} = \; 0, & \text{if } T' \text{ is a star;} \\ \geq \; 2\sum_{x \in V(T') \setminus \{w\}} \left(d_{T'}(x) - 1\right), & \text{otherwise.} \end{cases} \tag{4}$$

and

$$M_2' - M_1' \geq -d_{T'}(w)\,. \tag{5}$$

This implies that

$$\begin{aligned} M_2(T) - M_1(T) \;&=\; (M_2' + p^2 + p \cdot d_T(u) + p) - (M_1' + p^2 + 3p) \\ &=\; (M_2' - M_1') + p\,(d_T(u) - 2) \\ &\geq\; -d_{T'}(w) = -d_T(w), \end{aligned}$$

since $d_T(u) \geq 2$, showing that $T$ satisfies (3) as well.

Next,

$$\begin{aligned}
& nM_2(T) - (n-1)M_1(T) \\
= \ & n(M_2' + p^2 + p \cdot d_T(u) + p) - (n-1)(M_1' + p^2 + 3p) \\
= \ & ((n-p)M_2' - (n-p-1)M_1') \\
+ \ & p\,(M_2' - M_1' + np + n \cdot d_T(u) + n - (n-1)p - 3(n-1)) \\
\geq \ & ((n-p)M_2' - (n-p-1)M_1') + p\,(-d_{T'}(w) + p + n \cdot (d_T(u) - 2) + 3) \\
= \ & ((n-p)M_2' - (n-p-1)M_1') + p\,(-d_T(w) + d_T(v) - 1 + n \cdot (d_T(u) - 2) + 3) \\
\geq \ & ((n-p)M_2' - (n-p-1)M_1') + p\,(n \cdot (d_T(u) - 2) + 2) \\
\geq \ & ((n-p)M_2' - (n-p-1)M_1') + 2p \\
= \ & ((n-p)M_2' - (n-p-1)M_1') + 2(d_T(v) - 1)\,.
\end{aligned}$$

Now, if $T'$ is a star, $(n-p)M_2' - (n-p-1)M_1' = 0$ by (4). Further, $u = w$ and $v$ are then the only vertices of $T$ of degree at least two, so that

$$nM_2(T) - (n-1)M_1(T) \ \geq \ 2(d_T(v) - 1) = 2 \sum_{x \in V(T) \setminus \{w\}} (d_T(x) - 1)\,,$$

proving (2) in this case.

In case $T'$ is not a star, we have by (4)

$$(n-p)M_2' - (n-p-1)M_1' \ \geq \ 2 \sum_{x \in V(T') \setminus \{w\}} (d_{T'}(x) - 1)\ ,$$

and consequently,

$$\begin{aligned}
nM_2(T) - (n-1)M_1(T) \ & \geq \ 2 \sum_{x \in V(T') \setminus \{w\}} (d_{T'}(x) - 1) + 2(d_T(v) - 1) \\
& = \ 2 \sum_{x \in V(T) \setminus \{w,v\}} (d_T(x) - 1) + 2(d_T(v) - 1) \\
& = \ 2 \sum_{x \in V(T) \setminus \{w\}} (d_T(x) - 1)\ ,
\end{aligned}$$

proving (2) in this case as well. ∎

**Corollary 2** *Let $T$ be a tree with $n \geq 3$ vertices and $m = n-1$ edges and let $\delta_2$ be the smallest vertex degree of $T$ larger than one. Then*

$$nM_2(T) - mM_1(T) \geq 2(n - 1 - \delta_2)\,, \tag{6}$$

*with equality attained if and only if $T$ is either a star $K_{1,n-1}$ or a path $P_n$.*

**Proof** Since $\sum_{x\in V(T)} d_T(x) = 2m$, we immediately have

$$2\sum_{x\in V(T)\setminus\{w\}} (d_T(x)-1) = 2(2m - d_T(w)) - 2(n-1) = 2(n-1-d_T(w)).$$

Suppose now that equality holds in (6), and that $T$ is not a star. From the proof of Theorem 1, keeping the same notation, we can see that in such case the following equality has to hold as well:

$$nM_2(T) - mM_1(T) = ((n-p)M_2' + (n-p-1)M_1') + 2(d_T(v)-1)$$

at each step at which the leaves adjacent to $v$ are deleted from $T$ to obtain $T'$. In particular, this implies that

$$\begin{aligned} M_2' - M_1' &= -d_{T'}(w), \\ d_T(v) &= d_T(w), \\ d_T(u) &= 2. \end{aligned}$$

Since $d_T(w) \leq d_T(u)$, we have $d_T(w) = 2$ and, consequently, $d_T(v) = 2$. Following the inductive descend towards the case of $T'$ becoming a star, we see that each non-leaf vertex of $T$ has to have degree 2, hence, $T$ has to be a path on $n$ vertices. ■

**Remarks** Similarly as above, from the proof of Theorem 1 we can see that the equality holds in (3) if and only if $d_T(u) = 2$ at each step at which the leaves adjacent to $v$ are deleted from $T$ to obtain $T'$. In particular, this implies $d_T(w) = 2$. Since this does not put additional constraints on the degree of $v$, we can conclude that the equality holds in (3) if and only if $T$ is either a star, a path, a broom (obtained from a star and a path by identifying a leaf of a star and a leaf of a path) or a double comet (obtained from two stars and a path by identifying a leaf of one star with one end vertex of a path and a leaf of another star with another end vertex of a path).

We also note that the inequality (3) has appeared in [6] as well, but proved in a different way. Further, it has been observed in [8] that for a connected triangle-free graph $G$ holds

$$M_2(G) - M_1(G) = p_3(G) - m,$$

where $p_3(G)$ is the number of paths of length three in $G$. ■

# 3 The second bound

After Theorem 1 has been proved, Réti Tamás informed us of Batmend Horoldagva's recent PhD thesis [9] (and accompanying paper [10]), in which many new results on the Zagreb indices of trees, unicyclic and bicyclic graphs have been found. Among other results, Horoldagva proved that, if $T$ is not a star, then

$$nM_2(T) - mM_1(T) \geq 2(n-3), \tag{7}$$

which is better than (6) whenever $\delta_2 \geq 3$. This motivated us to improve (7) and by exploiting computer search for trees extremal with respect to $nM_2(T) - mM_1(T)$, we observed that, if $T$ is not a star, then

$$nM_2(T) - mM_1(T) \geq 2(n-3) + (\Delta-1)(\Delta-2), \tag{8}$$

where $\Delta$ denotes the maximum vertex degree in $T$.

Recall that a *broom* is a tree obtained from a star with at least two leaves by replacing one of its edges with a path having at least two edges. Notice that according to this definition, the only star that is also a broom is the star on three vertices.

**Theorem 3** *Let $T$ be a tree with $n$ vertices, $m = n-1$ edges and maximum degree $\Delta$. Then*

$$nM_2(T) - mM_1(T) \begin{cases} = 0, & \text{if } T \text{ is a star;} \\ \geq 2(n-3) + (\Delta-1)(\Delta-2), & \text{otherwise.} \end{cases} \tag{9}$$

*The equality is attained in (9) if and only if $T$ is a broom.*

**Proof** Let us denote $j(T) = nM_2(T) - mM_1(T)$. A routine calculation shows that $j(T) = 0$ if $T$ is a star, and $j(T) = 2(n-3) + (\Delta-1)(\Delta-2)$ if $T$ is a broom.

Next, suppose that $T$ is not a star. We construct a finite sequence of trees $T_0, T_1, \ldots, T_k$, each with $n$ vertices, $m$ edges, and maximum degree $\Delta$, satisfying the following properties:

(a) $T = T_0$;

(b) $T_k$ is a broom;

(c) for all $i \in \{0, 1, \ldots, k-1\}$, it holds that $j(T_i) \geq j(T_{i+1})$;

Assuming properties (a)–(c), it follows that

$$j(T) = j(T_0) \geq j(T_1) \geq \ldots \geq j(T_k) = 2(n-3) + (\Delta - 1)(\Delta - 2)\,,$$

proving (9).

The sequence $(T_i)_{i=0}^{k}$ is constructed as follows: let $u$ be a maximum degree vertex of $T$, and fix a longest path $P = (u, u_1, \ldots, u_r)$ in $T$ starting at $u$. As $T$ is not a star, $P$ has length at least two and, clearly, $u_r$ is a leaf of $T$. Intuitively, the sequence of trees $T_i$ will be obtained by iteratively applying the following tranformation, until a broom is obtained: *delete a leaf not on $P$ and not adjacent to $u$, and subdivide the first edge of $P$.*

Let us now describe the sequence construction formally. To each tree $T_i$, we will also associate a longest path $P_i$ starting at $u$ in $T_i$, and denote by $w_i$ the neighbor of $u$ on $P_i$. We proceed inductively. For $i = 0$, we set $T_0 := T$ and $P_0 := P$, where $P = (u, u_1, \ldots, u_r)$ is a path defined as above. Denote also $w_0 := u_1$. Suppose that we have already defined $T_i$ and $P_i = (u, w_i, w_{i-1}, \ldots, w_1, w_0 = u_1, \ldots, u_r)$, for some $i \geq 0$. If $T_i$ is a broom, then we set $k := i$ and the sequence construction is complete. Otherwise, let $\ell$ be a leaf of $T_i$ not in $P_i$ and not adjacent to $u$. The existence of such a leaf, if $T_i$ is not a broom, can be established according to the following two cases:

- if there exists an internal vertex $y$ in $P_i$ of degree at least three, we can take $\ell$ to be any leaf of $T_i$ not on $P_i$ and such that $y$ belongs to the $\ell$–$u$ path in $T_i$;
- otherwise (all internal vertices of $P_i$ are of degree exactly two), the graph $T_i - V(P_i)$ has at least one component $T'$ with $|V(T')| \geq 2$, and $\ell$ can be chosen to be any leaf in $T'$ that is also a leaf in $T_i$.

Having chosen leaf $\ell$, let us define $T_{i+1}$ to be the tree obtained from $T_i$ by deleting $\ell$ and subdividing the edge $uw_i$. That is, vertex $\ell$ and edge $uw_i$ are deleted from $T_i$, and a new vertex $w_{i+1}$ is introduced that is made adjacent only to $u$ and $w_i$. Also, set $P_{i+1}$ to be the path $(u, w_{i+1}, w_i, \ldots, w_1, w_0 = u_1, \ldots, u_r)$.

Let us now verify that the above properties are satisfied. Observe that $|V(T_i)| = n$ and $|E(T_i)| = m$ for all $i$. This immediately implies that the sequence is finite: since $|V(P_i)| = |V(P)| + i$ for all $i$ and the number of vertices is unchanged, the procedure must eventually stop.

The transformation mapping $T_i$ to $T_{i+1}$ preserves the maximum degree. Properties (a) and (b) are satisfied by definition. If $\Delta = 2$ then $T$ is a path, which implies $k = 0$

and property (c) is trivially satisfied in this case. Hence, in what follows, we assume that $\Delta > 2$, unless specified otherwise.

Fix $i \geq 0$. Let us write $M_1 := M_1(T_i)$, $M_1' := M_1(T_{i+1})$, $M_2 := M_2(T_i)$, $M_2' := M_2(T_{i+1})$, let $x$ denote the unique neighbor of $\ell$ in $T_i$, and let $N_{T_i}(x) \setminus \{\ell\} = \{x_1, \ldots, x_p\}$. Let us also write $d(y) := d_{T_i}(y)$ for $y \in V(T_i)$, and similarly $d'(y) := d_{T_{i+1}}(y)$ for $y \in V(T_{i+1})$.

First, we analyze the effect of the above transformation on $M_1$. We have

$$M_1' \;=\; M_1 - d(x)^2 - d(\ell)^2 + d'(x)^2 + d'(w_{i+1})^2 \;=\; M_1 - 2d(x) + 4\,,$$

where the last equality follows from relations: $d'(x) = d(x) - 1$, $d(\ell) = 1$ and $d'(w_{i+1}) = 2$.

Further, we have

$$\begin{aligned} M_2' &= M_2 - d(u) \cdot d(w_i) - d(\ell) \cdot d(x) - \sum_{j=1}^{p} d(x) \cdot d(x_j) \\ &+ d'(u) \cdot d'(w_{i+1}) + d'(w_{i+1}) \cdot d'(w_i) + \sum_{j=1}^{p} d'(x) \cdot d'(x_j) \\ &= M_2 - \Delta \cdot d(w_i) - 1 \cdot d(x) - d(x) \cdot \sum_{j=1}^{p} d(x_j) \\ &+ \Delta \cdot 2 + 2 \cdot d(w_i) + (d(x) - 1) \cdot \sum_{j=1}^{p} d(x_j) \\ &= M_2 - (\Delta - 2)\,(d(w_i) - 2) + 4 - d(x) - \sum_{j=1}^{p} d(x_j)\,. \end{aligned}$$

Note that $d(w_i) = 2$ as $P_i$ has length at least 2, and $d(x) \geq 2$. Moreover, $\sum_{j=1}^{p} d(x_j) \geq 2$, since at least one neighbor of $x$ is not a leaf.

Now, let us prove (c) by considering the relation between $j(T_i)$ and $j(T_{i+1})$. We have

$$\begin{aligned} j(T_i) - j(T_{i+1}) &= nM_2 - mM_1 - (nM_2' - mM_1') \\ &= n(M_2 - M_2') - (n-1)(M_1 - M_1') \\ &= n\Big( (\Delta - 2)\,(d(w_i) - 2) - 4 + d(x) + \sum_{j=1}^{p} d(x_j) \Big) \\ &- (n-1)\,(2d(x) - 4) \\ &= n\,(\Delta - 2)\,(d(w_i) - 2) + 2\,(d(x) - 2) + n\Big( \sum_{j=1}^{p} d(x_j) - d(x) \Big)\,. \end{aligned}$$

Notice that $d(w_i) = 2$ and $d(x) \geq 2$. Moreover, since not all of $x_1, \ldots, x_p$ are leaves, we have $\sum_{j=1}^{p} d(x_j) \geq p + 1 = d(x)$ and consequently $\sum_{j=1}^{p} d(x_j) \geq d(x)$. This implies that

$$j(T_i) - j(T_{i+1}) \geq 0, \tag{10}$$

proving (c). Moreover,

$$j(T_{i+1}) = j(T_i) \qquad \Leftrightarrow \qquad d(x) = d(x_1) = 2. \tag{11}$$

It remains to show that $j(T) = 2(n-3) + (\Delta-1)(\Delta-2)$ implies that $T$ is a broom. Suppose that $j(T) = 2(n-3)+(\Delta-1)(\Delta-2)$ holds for a tree $T$. If $T$ is a star, then $j(T) = 0$ and $\Delta = n-1$ imply $n = 3$, hence $T$ is a broom. If $\Delta = 2$, then $T$ is a path, hence a broom. Suppose, therefore, that $T$ is not a broom. Then for the above constructed sequence of trees $T = T_0, T_1, \ldots, T_k$ holds $k \geq 1$. From $j(T) = j(T_k) = 2(n-3) + (\Delta-1)(\Delta-2)$ and inequality (10) we get that $j(T_i) = 2(n-3) + (\Delta-1)(\Delta-2)$ for each $i = 0, 1, \ldots, k$. Let us focus, in particular, on $j(T_{k-1}) = j(T_k)$. From (11) we see that the leaf $\ell$ chosen in $T_{k-1}$ has to be adjacent to a vertex $x$ of degree two, whose other neighbor $x_1$ also has degree two. Since the *broom* $T_k$ is obtained by deleting the leaf $\ell$ from $T_{k-1}$, which is not on $P_{k-1}$, and subdividing an edge incident with the maximum degree vertex $u$, we see that there are only two possibilities for $\ell$:

– $\ell$ is adjacent to an internal vertex $x$ of path $P_{k-1}$, in which case $x$ has degree three;

– $\ell$ is adjacent to a vertex $x$ of degree two, which is adjacent to a vertex $x_1 = u$ which has degree $\Delta > 2$.

In both cases we reach a contradiction to the condition of (11) that both $x$ and $x_1$ have degree two. Thus, $T$ has to be a broom. ■

**Remarks** Using the same transformation and analogous approach as above, it can be further shown that

$$M_1(T) \geq 4n + (\Delta-4)(\Delta+1),$$

with equality if and only if $T$ is a subdivision of a star, and

$$M_2(T) \begin{cases} = \ (n-1)^2, & \text{if } T \text{ is a star;} \\ \geq \ 4(n-2) + (\Delta-1)(\Delta-2), & \text{otherwise.} \end{cases}$$

with equality if and only if $T$ is a broom. These lower bounds, however, have been already obtained by Horoldagva in his PhD thesis [9], so we skip their proofs here. At the end, note that the last two bounds, regardless of the similarity in extremal graphs, cannot be directly used to prove (9) due to opposite signs of $M_1$ and $M_2$ in the expression $nM_2 - mM_1$.

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