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Comparing Zagreb Indices and Coindices of Trees

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Abstract

The first (M_1) and the second (M_2) Zagreb indices, as well as the first ($\overline{M}_1$) and the second ($\overline{M}_2$) Zagreb coindices, and the relations between them are examined. An upper bound on $M_1(T)$ and a lower bound on $2M_2(T) + \frac{1}{2}M_1(T)$ of trees is obtained, in terms of the number of vertices (n) and maximum degree (Δ). Moreover, we compare the Zagreb indices and the Zagreb coindices of trees.

1 Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. This graph has n vertices and $m = |E(G)|$ edges. The edge connecting the vertices v_i and v_j will be denoted by $v_i v_j$.

For $v_i \in V(G)$, d_i is the degree of the vertex v_i , $i = 1, 2, \ldots, n$. The maximum vertex degree of the graph G is denoted by Δ .

In the early 1970s Trinajstić and one of the present authors [19] derived a formula for estimating the total π-electron energy of conjugated systems. Within this study, two vertex–degree based invariants were encountered, that eventually were named [6] the first (M_1) and the second (M_2) Zagreb indices. Soon after that, M_1 and M_2 were recognized as measures of the branching of the carbon–atom molecular skeleton [18], and since then these are frequently used for structure–property modeling [28,29]. Details on the chemical applications of the two Zagreb indices can be found in the books [28,29], the reviews [6,26, 30], and elsewhere [27,32]. For details on the mathematical theory of the Zagreb indices see the recent works [1–3,7,9,10,15–17,20,21,23–25,31,35,36]. In the newest time much attention is being paid to the comparison of M_1 and M_2 [1,2,7,9,10,20,21,23–25,31,35].

The first and second Zagreb indices of a graph G are defined as

$$M_1 = M_1(G) = \sum_{v_i \in V(G)} d_i^2 \qquad \text{and} \qquad M_2 = M_2(G) = \sum_{v_i v_j \in E(G)} d_i\, d_j\ .$$

It is easy to show that the first Zagreb index can also be expressed as

$$M_1(G) = \sum_{v_i v_j \in E(G)} [d_i + d_j]\ .$$

The Zagreb indices can be viewed as consisting of the contributions of pairs of adjacent vertices to additively and multiplicatively weighted versions of Wiener numbers and polynomials [22]. Curiously enough, it turns out that similar contributions of non-adjacent pairs of vertices must be taken into account when computing the weighted Wiener polynomials of certain composite graphs [14]. As the sums involved run over the edges of the complement of G, such quantities were called Zagreb coindices. In [4,5], Ashrafi et al. defined the first and second Zagreb coindices of the graph G as

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{v_i v_j \notin E(G)} [d_i + d_j] \qquad \text{and} \qquad \overline{M}_2 = \overline{M}_2(G) = \sum_{v_i v_j \notin E(G)} d_i\, d_j\ .$$

As usual, $K_{1,n-1}$ and P_n denote, respectively, the star and the path on n vertices.

Given a graph G, a subset $S(G)$ of $V(G)$ is called an *independent set* of G if $G[S]$, the subgraph induced by $S(G)$, is a graph with $|S(G)|$ isolated vertices. The *independence number* $\alpha(G)$ of G is the number of vertices in the largest independent set of G. Recall that if T is a tree of order n, then $\lfloor n/2 \rfloor \leq \alpha(T) \leq n-1$ [8].

Let n and α be positive integers, such that $\lfloor n/2 \rfloor \leq \alpha \leq n-1$. Denote by $S_{n,\alpha}$ the tree obtained from the star $K_{1,\alpha}$, by attaching to $n-\alpha-1$ of its pendent vertices a new pendent vertex. Then $S_{n,\alpha}$ is a tree of order n with independence number α. If $\alpha = n-1$, then $S_{n,\alpha} \cong K_{1,n-1}$. If T is a tree of order n, such that $\Delta = \alpha$, then $T \cong S_{n,\alpha}$.

By direct calculation:

$$M_1(S_{n,\alpha}) = \alpha^2 - 3\alpha + 4n - 4 \qquad \text{and} \qquad M_2(S_{n,\alpha}) = n\alpha - 3\alpha + 2n - 2\ .$$

The paper is organized as follows. In Section 2, we present an upper bound on $M_1(T)$ of a tree T in terms of n and Δ. Using this result, we prove that $\overline{M}_1(T) > M_1(T)$ for $T \ncong K_{1,n-1}$. In Section 3, we obtain a lower bound on $2M_2(T) + \frac{1}{2}M_1(T)$ also in terms of n and Δ. In addition, we compare the second Zagreb index and the second Zagreb coindex for trees.

2 Comparing the first Zagreb index and coindex of trees

Theorem 2.1. *Let T be a tree with n vertices and maximum degree Δ. Then*

$$M_1(T) \leq n^2 - 3n + 2(\Delta + 1) \tag{1}$$

with equality holding if and only if $T \cong K_{1,n-1}$ or $T \cong P_4$.

Proof: If $T = K_{1,n-1}$, then $M_1(T) = n^2 - 3n + 2(\Delta+1) = n(n-1)$, the equality holds in (1). If $T = P_n$, then $M_1(T) = 4n - 6 < n^2 - 3n + 2(\Delta+1)$ for $n > 4$ and $M_1(T) = 4n-6 = n^2-3n+2(\Delta+1)$ for $n = 4$. We therefore assume that $T \neq K_{1,n-1}, P_n$, that is, $3 \leq \Delta \leq n-2$.

In this case we have to show that the inequality in (1) is strict. Let v_i be the maximum degree vertex of degree Δ in T. Also let v_k be a vertex of degree one, adjacent to vertex v_j of degree d_j, $j \neq i$ in T. We transform T into another tree T^* by deleting the edge $v_k v_j$, and joining the vertices v_i and v_k by an edge. Let the new degree sequence be $d_1^*, d_2^*, \ldots, d_n^*$. Therefore $d_t^* = d_t$ for $t \neq i, j$ whereas $d_i^* = \Delta + 1$ and $d_j^* = d_j - 1$. Thus

$$M_1(T) - M_1(T^*) = \Delta^2 + d_j^2 - (\Delta+1)^2 - (d_j - 1)^2 = -2(\Delta - d_j + 1) \leq -2$$

because $\Delta - d_j \geq 0$. Therefore we have $M_1(T) \leq M_1(T^*) - 2$, with equality holding if and only if $\Delta = d_j$.

By the above described construction we have increased the value of $M_1(T)$. If T^* is the star, then $T \cong S_{n,n-1}$, $\Delta = n-2$ and hence $M_1(S_{n,n-1}) = n^2 - 3n + 6 < n^2 - n - 2$ as

$n > 4$ ($T \neq K_{1,n-1}$, P_n). Otherwise, we continue the construction as follows. We choose one pendent vertex, which is not adjacent to v_i, from T^*. Repeating the above procedure sufficient number of times, we arrive at a tree in which the vertex v_i is of degree $n-1$, i. e., we arrive at $K_{1,n-1}$. Thus

$$M_1(T) \leq M_1(T^*)-2 < M_1(T^{**})-4 < \cdots < M_1(K_{1,n-1})-2(n-\Delta-1) = n^2-3n+2(\Delta+1)$$

that is,

$$M_1(T) < n^2 - 3n + 2(\Delta + 1) \ .$$

This completes the proof. ■

For the star $K_{1,n-1}$, one can easily see that $M_1(K_{1,n-1}) = n(n-1) > (n-1)(n-2) = \overline{M}_1(K_{1,n-1})$. Also we have $M_1(P_4) = 10 > 8 = \overline{M}_1(P_4)$. For all other tree we have the following:

Theorem 2.2. *Let T be a tree of order n ($n \geq 5$). If $T \ncong K_{1,n-1}$, then*

$$\overline{M}_1(T) > M_1(T) \ .$$

Proof: Since $T \ncong K_{1,n-1}$, we must have $\Delta \leq n-2$. Then there exist a vertex v_i of degree $d_i \geq 2$. Since T is a tree, there are $n(n-1)/2 - (n-1) = (n-1)(n-2)/2$ pairs of non-adjacent vertices. For each such pair (v_i, v_j), the condition $d_i + d_j \geq 2$ is satisfied. Thus we have

$$\overline{M}_1(T) \geq (n-1)(n-2) + (\Delta - 1)(n - \Delta - 1) + (d_i - 1)(n - d_i - 1) \ . \tag{2}$$

For $\Delta = n-2$, it must be $d_i = 2$ and then from (2) and the fact that $n \geq 5$ follows

$$\overline{M}_1(T) \geq n^2 - n - 4 \geq n^2 - 3n + 6 = M_1(T) \ .$$

Otherwise, $\Delta \leq n-3$. Consider the function

$$f(x) = (x-1)(n-x-1) \quad \text{for} \ \ 2 \leq x \leq n-3$$

for which $f'(x) = n - 2x$.

Since $f(x)$ is an increasing function on $[2, n/2]$ and a decreasing function on $[n/2, n-3]$, we have $(x-1)(n-x-1) \geq n-3$ as $n \geq 5$. From (2), in view of Theorem 2.1 and $\Delta \leq n-3$ it follows

$$\overline{M}_1(T) \geq (n-1)(n-2) + 2(n-3) = n^2 - n - 4 \geq n^2 - 3n + 2(\Delta+1) > M_1(T)$$

which completes the proof. ∎

3 Comparing the second Zagreb index and coindex of trees

Denote by $T_{\Delta,n-\Delta-1}$ the tree constructed by joining a pendent vertex of the star $K_{1,\Delta}$ with an end vertex of the path $P_{n-\Delta-1}$. This tree is sometimes referred to as the *broom* [13,33,34]. For this tree,

$$\begin{aligned} M_1(T_{\Delta,n-\Delta-1}) &= \Delta^2 + 4n - 3\Delta - 4 \\ M_2(T_{\Delta,n-\Delta-1}) &= 4n + (\Delta-1)(\Delta-2) - 8 \,. \end{aligned}$$

Therefore

$$2M_2(T_{\Delta,n-\Delta-1}) + \frac{1}{2}M_1(T_{\Delta,n-\Delta-1}) = \frac{5}{2}\Delta^2 - \frac{15}{2}\Delta + 10n - 14 \,.$$

Now we give a lower bound on $2M_2(T) + \frac{1}{2}M_1(T)$ in terms of n and Δ.

Theorem 3.1. *Let T be a tree of order n with maximum degree Δ, different from the star $K_{1,n-1}$. Then*

$$2M_2(T) + \frac{1}{2}M_1(T) \geq \frac{5}{2}\Delta^2 - \frac{15}{2}\Delta + 10n - 14 \tag{3}$$

with equality if and only if $T \cong T_{\Delta,n-\Delta-1}$.

Proof: If $T = T_{\Delta,n-\Delta-1}$, then the equality holds in (3). Therefore we need to consider the trees $T \ncong K_{1,n-1},\ T_{\Delta,n-\Delta-1}$.

Assume that v_i is the maximum degree vertex of degree Δ in T. Now we find the longest path from the vertex v_i and denote it by $P_j:\ v_i v_{i+1} v_{i+2} \dots v_{i+j}$. Its length is j. Let v_k $(k \neq i+j)$ be a vertex of degree one, adjacent to vertex v_ℓ, $\ell \neq i$, that is, $v_k v_\ell \in E$, $v_k v_i \notin E$. We transform T into another tree T^* by deleting the edges $v_k v_\ell$,

$v_i v_{i+1}$, and by joining the vertices v_i and v_{i+1} to v_k, by edges. Let the new degree sequence be $d_1^*, d_2^*, \ldots, d_n^*$. Therefore $d_t^* = d_t$ for $t \neq \ell, k$ whereas $d_\ell^* = d_\ell - 1$ and $d_k^* = 2$. Now,

$$\begin{aligned}
& \left[2M_2(T) + \frac{1}{2}M_1(T)\right] - \left[2M_2(T^*) + \frac{1}{2}M_1(T^*)\right] \\
= \;& 2\left[M_2(T) - M_2(T^*)\right] + \frac{1}{2}\left[M_1(T) - M_1(T^*)\right] \\
= \;& 2\left[d_i d_{i+1} - 2d_i - 2d_{i+1} + d_\ell + \sum_{v_{\ell_r} v_\ell \in E, v_{\ell_r} \neq v_k} d_{\ell_r}\right] + \frac{1}{2}\left[d_\ell^2 + 1 - (d_\ell - 1)^2 - 4\right] \\
= \;& 2\left[(d_i - 2)(d_{i+1} - 2) + d_\ell - 4 + \sum_{v_{\ell_r} v_\ell \in E, v_{\ell_r} \neq v_k} d_{\ell_r}\right] + (d_\ell - 2) \geq 0 \qquad (4)
\end{aligned}$$

as $d_i, d_{i+1}, d_\ell \geq 2$. We thus obtained

$$2M_2(T) + \frac{1}{2}M_1(T) \geq 2M_2(T^*) + \frac{1}{2}M_1(T^*) \ . \qquad (5)$$

If $v_\ell = v_{i+1}$, then one can see easily that relation (5) also holds.

By the above described construction, the value of $2M_2(T) + \frac{1}{2}M_1(T)$ has not increased. If T^* is the tree $T_{\Delta, n-\Delta-1}$, then (5) remains valid. Otherwise, we continue the construction as follows. We choose one pendent vertex from T^*, different from v_{i+j}. Repeating the above procedure sufficient number of times, we arrive at $T_{\Delta, n-\Delta-1}$. Thus

$$\begin{aligned}
& 2M_2(T) + \frac{1}{2}M_1(T) \geq 2M_2(T^*) + \frac{1}{2}M_1(T^*) \geq 2M_2(T^{**}) + \frac{1}{2}M_1(T^{**}) \\
& \geq \cdots > 2M_2(T_{\Delta, n-\Delta-1}) + \frac{1}{2}M_1(T_{\Delta, n-\Delta-1}) = \frac{5}{2}\Delta^2 - \frac{15}{2}\Delta + 10n - 14 \ .
\end{aligned}$$

The inequality in the last step is strict, because in that case the pendent neighbor v_l is adjacent to v_i or the pendent neighbor v_ℓ lies on the longest path from vertex v_i to vertex v_{i+j}. Consequently, the inequality in (4) is strict.

Thus, it is

$$2M_2(T) + \frac{1}{2}M_1(T) = \frac{5}{2}\Delta^2 - \frac{15}{2}\Delta + 10n - 14$$

if and only if $T \cong T_{\Delta, n-\Delta-1}$. This completes the proof. ■

The next result is equivalent to what earlier was obtained in [11] by two of the present authors:

Lemma 3.2. *Let G be a simple graph on n vertices and m edges. Then*

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2} M_1(G) \ .$$

For the path P_n $(n \geq 5)$,

$$\overline{M}_2(P_n) = 2n^2 - 10n + 13 > 4n - 8 = M_2(P_n) \ .$$

Note that $\Delta(P_n) = 2$. For trees with Δ-values greater than 2 we have:

Theorem 3.3. *Let T be a tree of order n with maximum degree Δ. If $\Delta \geq 1.5 + \sqrt{\frac{4}{5}n^2 - \frac{28}{5}n + \frac{173}{20}}$, then*

$$\overline{M}_2(T) \leq M_2(T) \ .$$

Proof: From Lemma 3.2,

$$\begin{aligned} \overline{M}_2(T) - M_2(T) &= 2(n-1)^2 - 2M_2(T) - \frac{1}{2} M_1(T) \\ &\leq 2\Big(n^2 - 2n + 1) - (\frac{5}{2}\Delta^2 - \frac{15}{2}\Delta + 10n - 14\Big) \\ &= 2n^2 - 14n - \frac{5}{2}\Delta^2 + \frac{15}{2}\Delta + 16 \leq 0 \end{aligned}$$

as $\Delta \geq 1.5 + \sqrt{\frac{4}{5}n^2 - \frac{28}{5}n + \frac{173}{20}}$. ■

In the following two results we give upper bounds on the first and second Zagreb indices of trees in terms of n and α.

Lemma 3.4. [12] *Let T be a tree of order n with independence number α. Then*

$$M_1(T) \leq \alpha^2 - 3\alpha + 4n - 4$$

with equality holding if and only if $T \cong S_{n,\alpha}$.

Lemma 3.5. [12] *Let T be a tree of order n with independence number α. Then*

$$M_2(T) \leq n\alpha - 3\alpha + 2n - 2$$

with equality holding if and only if $T \cong S_{n,\alpha}$.

For the star $K_{1,n-1}$,

$$M_2(K_{1,n-1}) = (n-1)^2 > \frac{1}{2}\,(n-1)(n-2) = \overline{M}_2(K_{1,n-1})\ .$$

Also, for $S_{n,\alpha}$,

$$M_2(S_{n,n-2}) = (n-1)(n-2) + 2 > \frac{1}{2}\,(n^2 - 2n - 1) = \overline{M}_2(S_{n,n-2})\ .$$

But we have the following result:

Theorem 3.6. *Let T be a tree of order n with independence number α. If $n \geq \frac{1}{2}\left[\alpha + 5 + \sqrt{2\alpha^2 - 5\alpha + 9}\right]$, then*

$$\overline{M}_2(T) > M_2(T)\ .$$

Proof: By Lemma 3.2,

$$\begin{aligned}
\overline{M}_2(T) - M_2(T) &= 2(n-1)^2 - 2M_2(T) - \frac{1}{2}\,M_1(T) \\
&\geq 2(n-1)^2 - 2(n\alpha - 3\alpha + 2n - 2) - \frac{1}{2}\,(\alpha^2 - 3\alpha + 4n - 4) \\
&= 2n^2 - \frac{1}{2}\alpha^2 - 2n\alpha - 10n + \frac{15}{2}\alpha + 8\ .
\end{aligned}$$

Now we have to show that $\overline{M}_2(T) \geq M_2(T)$, that is,

$$n^2 - n(\alpha+5) - \frac{1}{4}\,\alpha^2 + \frac{15}{4}\,\alpha + 4 \geq 0$$

which, evidently, is always obeyed as $n \geq \frac{1}{2}\left[\alpha + 5 + \sqrt{2\alpha^2 - 5\alpha + 9}\right]$. This completes the proof. ■

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