

MAXIMUM ZAGREB INDICES IN THE CLASS OF k -APEX TREES

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ABSTRACT. The first and second Zagreb indices of a graph G are defined as $M_1(G) = \sum_{v \in V} d_G(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$, where $d_G(v)$ is the degree of the vertex v . G is called a k -apex tree if k is the smallest integer for which there exists a subset X of $V(G)$ such that $|X| = k$ and $G - X$ is a tree. In this paper, we determine the maximum Zagreb indices in the class of all k -apex trees of order n and characterize the corresponding extremal graphs.

1. Introduction

Let $G = (V, E)$ be a connected simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v of G is the number of vertices adjacent to v . For a subset X of $V(G)$, the subgraph obtained from G by deleting the vertices in X together with their incident edges is denoted by $G - X$. If $X = \{v\}$ then $G - X$ will be written as $G - v$. For any two nonadjacent vertices u and v in graph G , we use $G + uv$ to denote the graph obtained from adding a new edge uv in G . Denote, as usual, by P_n , S_n and K_n the path, star and complete graph of order n , respectively.

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The first Zagreb index M_1 and the second Zagreb M_2 of graph G are among the oldest and the most famous topological indices and they are defined as:

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

and

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

The Zagreb indices were introduced in [8] and elaborated in [7]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure descriptors [14]. The main mathematical properties of the Zagreb indices were summarized in [2, 5]. Recent studies on the Zagreb indices are reported in [1, 3, 4, 6, 9–13], where also references to the previous mathematical research in this area can be found.

For any positive integer k with $k \geq 1$, a graph G is called a k -apex tree if there exists a subset X of $V(G)$ such that $G - X$ is a tree and $|X| = k$, while for any $Y \subseteq V(G)$ with $|Y| < k$, $G - Y$ is not a tree. A vertex of X is called a k -apex vertex. The join $G \vee H$ of disjoint graphs G and H is the graph obtained from $G + H$ by joining each vertex of G to each vertex of H . The k -apex tree of order n with maximal Harary index were determined in [15] and weighted Harary indices of k -apex trees were studied in [16].

For positive integers $n \geq 3$ and $k \geq 1$, let $\mathbb{T}(n, k)$ denote the class of all k -apex trees of order n . In this paper, we find the maximum Zagreb indices in $\mathbb{T}(n, k)$ and characterize the extremal graphs.

2. Main results

The following lemma easily follows from the definitions of the Zagreb indices.

LEMMA 2.1. *Let G be a non-complete graph. If u and v are nonadjacent vertices in G , then $M_i(G + uv) > M_i(G)$ ($i = 1, 2$).*

We will need the following upper bounds on the Zagreb indices which were obtained in [2, 5].

LEMMA 2.2. *Let T be a tree of order n . Then*

- (i) $M_1(T) \leq n(n - 1)$ with equality if and only if T is isomorphic to S_n .
- (ii) $M_2(T) \leq (n - 1)^2$ with equality if and only if T is isomorphic to S_n .

We now give some preliminary lemmas that are useful for our main theorems.

LEMMA 2.3. *Let $G \in \mathbb{T}(n, k)$ and v be a k -apex vertex of G . If $M_i(G)$ ($i = 1, 2$) is maximum in $\mathbb{T}(n, k)$, then $d_G(v) = n - 1$.*

Proof. Since $G \in \mathbb{T}(n, k)$, we have $|V(G)| = n$. Hence $d_G(u) \leq n - 1$ for all $u \in V(G)$. Suppose that $d_G(v) < n - 1$ for any k -apex vertex v of G . Then there exists a vertex u in G such that $uv \notin E(G)$. Then by Lemma 2.1, we have $M_i(G + uv) > M_i(G)$ ($i = 1, 2$). Clearly $G + uv \in \mathbb{T}(n, k)$ and it contradicts to that $M_i(G)$ ($i = 1, 2$) is maximum in $\mathbb{T}(n, k)$. □

LEMMA 2.4. *Let $G \in \mathbb{T}(n, k)$. If $M_i(G)$ ($i = 1, 2$) is maximum in $\mathbb{T}(n, k)$, then*

$$|E(G)| = \frac{k(2n - k - 3)}{2} + n - 1.$$

Proof. Let X ($|X| = k$) be the set of all k -apex vertices in G . Since $M_i(G)$ ($i = 1, 2$) is maximum in $\mathbb{T}(n, k)$, we have $d_G(u) = n - 1$ for all $u \in X$ by Lemma 2.3. Hence the subgraph induced by X is a complete graph of order k and $G - X$ is a tree of order $n - k$. Thus

$$|E(G)| = \binom{k}{2} + k(n - k) + n - k - 1 = \frac{k(2n - k - 3)}{2} + n - 1.$$

This completes the proof. □

Now we are ready to find the maximum value of the Zagreb indices and give the characterization of extremal graphs.

THEOREM 2.5. *Let $G \in \mathbb{T}(n, k)$. Then*

$$M_1(G) \leq (k + 1) \left((n - 1)^2 + (k + 1)(n - k - 1) \right)$$

with equality if and only if G is isomorphic to $S_{n-k} \vee K_k$.

Proof. Suppose that $M_1(G)$ is maximum in $\mathbb{T}(n, k)$. Let v be a k -apex vertex of G . Then by Lemma 2.3, we have $d_G(v) = n - 1$. Therefore $|E(G - v)| = |E(G)| - n + 1$ and by Lemma 2.4, we get

$$(2.1) \quad |E(G - v)| = k(n - 1) - \frac{k(k + 1)}{2}.$$

Since $d_G(v) = n - 1$, it follows that $d_G(u) = d_{G-v}(u) + 1$ for all $u \in V(G)$ with $u \neq v$. Therefore, we get

$$\begin{aligned} M_1(G) &= \sum_{u \in V(G)} d_G(u)^2 \\ &= \sum_{u \in V(G-v)} (d_{G-v}(u) + 1)^2 + d_G(v)^2 \\ (2.2) \quad &= \sum_{u \in V(G-v)} d_{G-v}(u)^2 + 2 \sum_{u \in V(G-v)} d_{G-v}(u) + n - 1 + d_G(v)^2 \\ &= M_1(G - v) + 4|E(G - v)| + n(n - 1). \end{aligned}$$

We proceed by induction on k . For $k = 1$, $G - v$ is a tree of order $n - 1$. Therefore

$$(2.3) \quad |E(G - v)| = n - 2 \text{ and } M_1(G - v) \leq (n - 1)(n - 2)$$

by Lemma 2.2. Thus from (2.2) and (2.3), one can see easily that

$$(2.4) \quad M_1(G) \leq 2n^2 - 6.$$

By Lemma 2.2, the equality in the inequality (2.3) holds if and only if $G - v$ is isomorphic to S_{n-1} . Therefore since $d_G(v) = n - 1$, we conclude the equality in (2.4) holds if and only if G is isomorphic to $S_{n-1} \vee K_1$.

Now we assume that the result holds for all $(k - 1)$ -apex trees. Clearly $G - v \in \mathbb{T}(n - 1, k - 1)$ since $|V(G - v)| = n - 1$ and v is the k -apex vertex of G . Therefore by induction hypothesis, we have

$$(2.5) \quad M_1(G - v) \leq k \left((n - 2)^2 + k(n - k - 1) \right).$$

By using (2.1) and (2.5) in (2.2), we obtain

$$\begin{aligned}
 M_1(G) &\leq k(n-2)^2 + k^2(n-k-1) \\
 &\quad + n(n-1) + 4k(n-1) - 2k(k+1) \\
 &= kn^2 + k^2(n-k-1) + n(n-1) - 2k(k+1) \\
 (2.6) \quad &= (k+1)(n^2 - k^2 + kn - n) - 2k(k+1) \\
 &= (k+1) \left((n-1)^2 + (k+1)(n-k-1) \right).
 \end{aligned}$$

By induction hypothesis the equality in (2.5) holds if and only if $G-v$ is isomorphic to $S_{n-k} \vee K_{k-1}$. Therefore since $d_G(v) = n-1$, it follows that the equality in (2.6) holds if and only if G is isomorphic to $S_{n-k} \vee K_k$. Thus the proof is complete. \square

THEOREM 2.6. *Let $G \in \mathbb{T}(n, k)$. Then*

$$M_2(G) \leq \frac{1}{2}(n-1)(k+1) \left(k(n-1) + 2(k+1)(n-k-1) \right)$$

with equality if and only if G is isomorphic to $S_{n-k} \vee K_k$.

Proof. Suppose that $M_2(G)$ is maximum in $\mathbb{T}(n, k)$ and v is a k -apex vertex in G . Then $d_G(v) = n-1$ by Lemma 2.3. Thus $d_G(u) = d_{G-v}(u) + 1$ for all $u \in V(G)$ with $u \neq v$. Therefore, we get

$$\begin{aligned}
 M_2(G) &= \sum_{uv \in E(G)} d_G(u)d_G(v) \\
 &= \sum_{uv \in E(G-v)} (d_{G-v}(u) + 1)(d_{G-v}(v) + 1) \\
 (2.7) \quad &\quad + d_G(v) \sum_{u \in V(G-v)} (d_{G-v}(u) + 1) \\
 &= M_2(G-v) + M_1(G-v) + |E(G-v)| \\
 &\quad + (n-1) \left(2|E(G-v)| + (n-1) \right) \\
 &= M_2(G-v) + M_1(G-v) + (2n-1)|E(G-v)| + (n-1)^2.
 \end{aligned}$$

We proceed by induction on k . For $k = 1$, $G-v$ is a tree of order $n-1$. Therefore $|E(G-v)| = n-2$. On the other hand by Lemma 2.2, we get

$$(2.8) \quad M_2(G-v) + M_1(G-v) \leq (2n-3)(n-2)$$

with equality if and only if $G - v$ is isomorphic to S_{n-1} . Thus from (2.7) and (2.8), we conclude that $M_2(G) \leq (n-1)(5n-9)$ with equality if and only if G is isomorphic to $S_{n-1} \vee K_1$.

Now, assume that the result holds for all $(k-1)$ -apex trees. Then clearly $G - v \in \mathbb{T}(n-1, k-1)$. Therefore by induction hypothesis, we have

$$(2.9) \quad M_2(G - v) \leq \frac{1}{2}(n-2)k \left((k-1)(n-2) + 2k(n-k-1) \right).$$

Also by Theorem 2.5, we have

$$(2.10) \quad M_1(G - v) \leq k \left((n-2)^2 + k(n-k-1) \right).$$

From (2.9) and (2.10), we obtain

$$(2.11) \quad M_1(G - v) + M_2(G - v) \leq \frac{1}{2}(n-2)^2(k+1)k + k^2(n-1)(n-k-1).$$

Same as in the proof of Theorem 2.5, we get

$$(2.12) \quad |E(G - v)| = k(n-1) - \frac{k(k+1)}{2}.$$

Therefore by using (2.11) and (2.12) in (2.7), one can see easily that

$$(2.13) \quad \begin{aligned} M_2(G) &\leq \frac{k(k+1)}{2} \left((n-2)^2 - (2n-1) \right) \\ &\quad + (n-1) \left(k^2(n-k-1) + (2n-1)k + n-1 \right) \\ &= \frac{1}{2}k(k+1)(n-1)(n-5) + (n-1)(k+1)(n+kn-k^2-1) \\ &= \frac{1}{2}(n-1)(k+1) \left(k(n-1) + 2(k+1)(n-k-1) \right). \end{aligned}$$

By induction hypothesis and by Theorem 2.5, respectively, the equalities in (2.9) and (2.10) hold if and only if $G - v$ is isomorphic to $S_{n-k} \vee K_{k-1}$. Hence the equality in (2.11) holds if and only if $G - v$ is isomorphic to $S_{n-k} \vee K_{k-1}$. Thus since $d_G(v) = n-1$, it follows that the equality in (2.13) holds if and only if G is isomorphic to $S_{n-k} \vee K_k$. The proof is complete. \square

From Theorem 2.5 and Theorem 2.6, we directly obtain the following sharp upper bound on the sum of Zagreb indices.

COROLLARY 2.7. *Let $G \in \mathbb{T}(n, k)$. Then*

$$M_1(G) + M_2(G) \leq \frac{1}{2}(k+1)\left((n-1)^2(k+2) + 2n(k+1)(n-k-1)\right)$$

with equality if and only if G is isomorphic to $S_{n-k} \vee K_k$.

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