Korean J. Math. **23** (2015), No. 3, pp. 401–408
http://dx.doi.org/10.11568/kjm.2015.23.3.401

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.

Received August 10, 2015. Revised September 4, 2015. Accepted September 7, 2015.

2010 Mathematics Subject Classification: 97K30, 94C15, 05C07.

Key words and phrases: k-apex tree, First Zagreb index, Second Zagreb index.

This work is supported by the Korea Foundation for Advanced Studies' International Scholar Exchange Fellowship for the academic year of 2014–2015.

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*

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

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

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

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

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

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

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

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

$$M_1(G) \le 2n^2 - 6. \tag{2.4}$$

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

$$M_1(G-v) \le k\Big((n-2)^2 + k(n-k-1)\Big). \tag{2.5}$$

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

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

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. □

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

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

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

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

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

$$M_2(G-v) + M_1(G-v) \leq (2n-3)(n-2) \tag{2.8}$$

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

$$M_2(G-v) \leq \frac{1}{2}(n-2)k\Big((k-1)(n-2) + 2k(n-k-1)\Big). \tag{2.9}$$

Also by Theorem 2.5, we have

$$M_1(G-v) \leq k\Big((n-2)^2 + k(n-k-1)\Big). \tag{2.10}$$

From (2.9) and (2.10), we obtain

$$\begin{aligned} M_1(G-v) + M_2(G-v) \leq \frac{1}{2}&(n-2)^2(k+1)k \\ &+ k^2(n-1)(n-k-1). \end{aligned} \tag{2.11}$$

Same as in the proof of Theorem 2.5, we get

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

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

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

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. □

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*

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

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

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