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EXTREMAL FIRST AND SECOND ZAGREB INDICES OF APEX TREES

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Let G be a simple connected graph with edge set $E(G)$ and vertex set $V(G)$. The first and the second Zagreb indices of the graph G are defined as $M_1(G) = \sum_{v \in v(G)} (d(v))^2$ and $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$, respectively, where $d(v)$ is the degree of the vertex v. A graph G is called an apex tree [8] if it contains a vertex x such that $G - x$ is a tree. For any integer $k \geq 1$ the graph G is called k-apex tree if there exists a subset X of $V(G)$ of cardinality k such that $G - X$ is a tree and for any $Y \subset V(G)$ and $|Y| < k$, $G - Y$ is not a tree. In this work we have determined upper and lower bounds of $M_1(G)$ and an upper bound of $M_2(G)$ in k-apex trees. The corresponding extremal k-apex trees are also characterized in each case.

Keyword: first Zagreb index, second Zagreb index, *k*-apex trees

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The first and second Zagreb indices of G are defined as

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{uv \in E(G)} (d(u) + d(v))$$

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$$M_2(G) = \sum_{uv \in V(G)} d(u)d(v),$$

where $d(v)$ is the degree of the vertex v. In the last decade a lot of work was done on these two indices. In [4] a history of these graph parameters as well as their mathematical properties are presented.

All graphs considered in this paper are simple, finite and connected. For a vertex $v \in V(G)$, its degree is denoted by $d_G(v)$ and if G is clear from the context we simplify the notation to $d(v)$. The minimum degree of G is denoted by $\delta(G)$. A vertex in G of degree one is called pendant vertex. For $X \subset V(G)$, $G-X$ is the subgraph of G obtained from G by removing the vertices of X and edges incident with them, in particular $G-\{v\}$ is denoted by $G-v$. The complete bipartite graph $K_{1,n-1}$ is known as n-star and is denoted by S_n. The integers $i_1, i_2, \ldots, i_n$ are called almost equal if $max\{i_1, i_2, \ldots, i_n\} - min\{i_1, i_2, \ldots, i_n\} \leq 1$. The join of two vertex-disjoint graphs G and H is the graph $G+H$ with $V(G+H) = V(G) \cup V(H)$ and the edges of $G+H$ are all edges of graphs G and H and the edges obtained by joining each vertex of G with each vertex of H.

In topological graph theory, graphs that contain a vertex whose removal yields a planar graph play an important role and are called apex graphs [1, 6]. Along these lines a graph G is called an apex tree [8] if it contains a vertex x such that $G-x$ is a tree. The vertex x is called apex vertex of G. Note that a tree is always an apex tree, hence a non-trivial apex tree is an apex tree which itself is not a tree. For any integer $k \geq 1$ the graph G is called *k*-apex tree if there exists a subset X of $V(G)$ of cardinality k such that $G-X$ is a tree and for any $Y \subset V(G)$ and $|Y| < k$, $G-Y$ is not a tree. A vertex in X is called *k*-apex vertex. Clearly, 1-apex trees are precisely non-trivial apex trees. Apex trees and *k*-apex trees were introduced in [7] under the name quasi-tree graphs and *k*-generalized quasi-tree graphs, respectively. Recently in [9] Kinkar Ch. Das et al. determined upper and lower bounds on weighted Harary indices for apex trees and *k*-apex trees.

For any $n \geq 3$ and $k \geq 1$, let

(a) $T(n)$ denotes the set of all non-trivial apex trees of order n.

(b) $T_k(n)$ denotes the set of all *k*-apex trees of order n.

Note that $T_1(n) = T(n)$.

We need the following upper bounds on Zagreb indices:

Lemma 1.1 [2, 3] *If* T *is a tree of order* n*, then*

(a) $M_1(T) \le n(n-1)$; (b) $M_2(T) \le (n-1)^2$

and in both cases equality holds if and only if $T = S_n$, the star graph of order n.

The following Lemma easily follows from definitions.

Lemma 1.2 *If* $u, v \in V(G)$ *are not adjacent, then*

(a) $M_1(G+uv) > M_1(G)$; (b) $M_2(G+uv) > M_2(G)$.

Lemma 1.3 *If* $G \in T(n)$, $M_1(G)$ *and* $M_2(G)$ *are as large as possible and* x *is an apex vertex of* G*, then:*

(a) $\delta(G) = 2$; (b) $d(x) = n-1$.

Proof. (a) Suppose that $\delta(G) = 1$ and $y \in V(G)$ is a pendant vertex, then $xy \notin E(G)$ and $G + xy \in T(n)$. By Lemma 1.2, $M_1(G+xy) > M_1(G)$, which contradicts our hypothesis. Now we will show that $\delta(G) \le 2$. Suppose that all vertices have degree greater or equal to three. Now for any vertex $v \in G$, each vertex in $G - v$ has degree greater or equal to two, which implies that $G - v$ is not a tree for any $v \in V(G)$. Hence $\delta(G) = 2$. The conclusion similarly holds for $M_2(G)$.

(b) Let $G \in T(n)$, $M_1(G)$ is as large as possible and x be an apex vertex of G. Suppose to the contrary that $d(x) < n-1$, then there is a vertex $y \in V(G)$ such that $xy \notin E(G)$. Now $G + xy$ is also in $T(n)$ and $M_1(G+xy) > M_1(G)$, a contradiction, hence $d(x) = n-1$. The conclusion similarly holds for $M_2(G)$.

2. Extremal *k*-Apex Trees for $M_1(G)$

In this section we will find upper and lower bounds of $M_1(G)$ for *k*-apex trees.

Lemma 2.1 [5] *For any two vertex-disjoint graphs* G *and* H*, we have:*

$$\begin{aligned} M_1(G+H) = \; & M_1(G) + M_1(H) + |V(G)|\big(|V(G+H)| - |V(G)|\big)^2 \\ & + |V(H)|\big(|V(G+H)| - |V(H)|\big)^2 \\ & + 4|E(G)|\big(|V(G+H)| - |V(G)|\big) \\ & + 4|E(H)|\big(|V(G+H)| - |V(H)|\big). \end{aligned}$$

Theorem 2.2 *If* $G \in T(n)$ *and* $n \geq 5$, *then*

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

and equality holds if and only if $G = K_1 + S_{n-1}$.

Proof. If $G \in T(n)$ and $M_1(G)$ is as large as possible, then by Lemma 1.3 we have $G = K_1 + T_{n-1}$, where T_{n-1} is a tree of order $n-1$, therefore by using Lemma 2.1, we obtain

$$\begin{aligned} M_1(G) = \;& M_1\left(K_1 + T_{n-1}\right) \\ =\;& M_1\left(K_1\right) + M_1\left(T_{n-1}\right) + \left|V\left(K_1\right)\right|\left(\left|V\left(K_1 + T_{n-1}\right)\right| - \left|V\left(K_1\right)\right|\right)^2 \\ & + |V(T_{n-1})|(|V(K_1 + T_{n-1})| - |V(T_{n-1})|)^2 \\ & +4|E(K_1)|(|V(K_1 + T_{n-1})| - |V(K_1)|) \\ & +4|E(T_{n-1})|(|V(K_1 + T_{n-1})| - |V(T_{n-1})|). \end{aligned}$$

Using Lemma 1.1 yields

$$\begin{aligned} M_1(G) \leq\;& \left(n-1\right)\left(n-2\right) + \left(n-1\right)^2 + \left(n-1\right)\left(n-\left(n-1\right)\right)^2 \\ & +4\left(n-2\right)\left(n-\left(n-1\right)\right) \\ =\;& 2n^2 - 6. \end{aligned}$$

Lemma 1.1 guaranties that equality holds if and only if $G = K_1 + S_{n-1}$.

Theorem 2.3 *If* $k \geq 2$, $n \geq 5$ *and* $G \in T_k(n)$, *then*

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

and equality holds if and only if $G = K_k + S_{n-k}$.

Proof. We will prove it by induction on k. We have already proved this property for $k = 1$ in Theorem 2.2. Now suppose that the result is true for (k -1)-apex trees. Let $G \in T_k(n)$ has the maximum $M_1(G)$. Let $V_k \subset V(G)$ be the set of k-apex vertices. As $M_1(G + uv) > M_1(G)$ for any $uv \notin E(G)$ this implies that V_k forms a complete graph and for any $u \in V_k$, $d(u) = n-1$. So the number m of edges of the graph G is

$$m = \binom{k}{2} + k\left(n-k\right) + n - k - 1$$

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

Let $x\in V_k$ and $V_{k-1}=V_k-x$. Note that $d(x)=n-1$, $G-x$ is a (k-1)-apex tree and

$$M_1(G-x)=\sum_{v\in V(G-x)}\left(d_G(v)-1\right)^2$$

$$M_1(G-x)=\sum_{v\in V(G-x)}d_G^2(v)-2\sum_{v\in V(G-x)}d_G(v)+\sum_{v\in V(G-x)}1$$

$$=\sum_{v\in V(G)}d_G^2(v)-2\sum_{v\in V(G)}d_G(v)+(n-1)-(n-1)^2+2(n-1)$$

$$=M_1(G)-4m-n^2+5n-4,\text{or}$$

$$M_1(G)=M_1(G-x)+4m+n^2-5n+4.$$

By equation (2.1) we have

$$M_1(G)=M_1(G-x)+4\left(\frac{k(k+1)}{2}+(k+1)(n-k-1)\right)+n^2-5n+4.$$

As we have supposed that the result is true for (k-1)-apex trees, we deduce

$$M_1(G)\le\quad k(n-2)^2+(n-k-1)k^2+4\left(\frac{k(k+1)}{2}+(k+1)(n-k-1)\right)$$

$$+n^2-5n+4$$

$$=\quad (k+1)(n-1)^2+(n-k-1)(k+1)^2.$$

Equality holds if and only if $G=K_k+S_{n-k}$.

Theorem 2.4 *If* $G\in T_k(n)$, $k\ge 1$ *and* $n\ge 3k$ *, then*

$$M_1(G)\ge 4n+10k-10$$

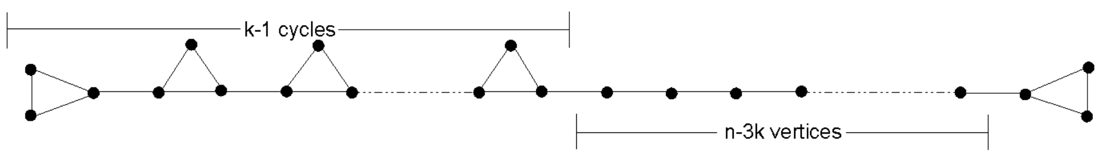
and equality holds if and only if G has $n-2k+2$ vertices of degree 2 and $2k-2$ vertices of degree 3.

Proof. By definition of a k-apex tree, there exists a subset X of $V(G)$ of cardinality k such that $G-X$ is a tree and for any $Y\subset V(G)$ and $|Y|<k$, $G-Y$ is not a tree. It follows that $d(v)\ge 2$ for any vertex $v\in X$. If m denotes the number of edges of

G, it follows that $m \geq 2k+n-k-1=n+k-1$. For given natural numbers n and p, denote $f(x_1,\ldots,x_n;p)=\sum_{i=1}^{n}x_i^2$, where $\sum_{i=1}^{n}x_i=p$. If $\sum_{i=1}^{n}x_i=p$ and p is fixed, it is well known that $f(x_1,\ldots,x_n;p)$ is minimum if and only if $x_1,\ldots,x_n$ are almost equal, or $-1 \leq x_i - x_j \leq 1$ for every $i,j=1,\ldots,n$. Denote this minimum by $f(n,p)$. It is clear that the function $f(n,p)$ is strictly increasing in p. We have $M_1(G) \geq f(n,2m) \geq f(n,2n+2k-2)$ since $m \geq n+k-1$. Equality holds if and only if the degrees of G are almost equal and all vertices in X have the degree equal to two. Suppose that G has exactly the minimum number of edges, equal to $n+k-1$ and denote by n_t and n_{t+1} the number of vertices of G having the degree equal to t and $t+1$, respectively, where $1 \leq n_t \leq n$. It follows that $n_{t+1}=n-n_t$ and $tn_t+(t+1)(n-n_t)=2n+2k-2$, or

$$(t+1)n-n_t=2n+2k-2. \qquad (2.2)$$

If $t=1$ then (2.2) becomes $2n-n_t=2n+2k-2$, which is not possible since



$2n-n_t \leq 2n-1$ and $2n+2k-2 \geq 2n$. Also, if $t \geq 3$ we have

Fig. 1. *k*-apex tree with almost equal degrees

$(t+1)n-n_t \geq 4n-n_t \geq 3n$ but $2n+2k-2 \leq \frac{8n}{3}-2$ since $k \leq \frac{n}{3}$. Consequently, we have $t=2$. From (2.2) we get $n_2=n-2k+2$, hence the minimum of $M_1(G)$ is reached if and only if there exist $n-2k+2$ vertices of degree 2 and $2k-2$ vertices of degree 3. Such a graph is illustrated in Fig. 1.

3. Upper Bound of $M_2(G)$ for *k*-Apex Trees

In this section we will find a sharp upper bound of $M_2(G)$ for *k*-apex trees.

Lemma 3.1 [5] *For any two vertex-disjoint graphs G and H, we have:*

$$\begin{aligned}M_2(G+H) = \;& M_2(G)+\left(\left|V(G+H)\right|-\left|V(G)\right|\right)M_1(G)\\ &+\left(\left|V(G+H)\right|-\left|V(G)\right|\right)\left|E(G)\right|+M_2(H)\\ &+\left(\left|V(G+H)\right|-\left|V(H)\right|\right)M_1(H)+\left(\left|V(G+H)\right|-\left|V(H)\right|\right)\left|E(H)\right|\\ &-12[2\left|E(G)\right|+\left|V(G)\right|\left(\left|V(G+H)\right|-\left|V(G)\right|\right)]^2\\ &-12[2\left|E(H)\right|+\left|V(H)\right|\left(\left|V(G+H)\right|-\left|V(H)\right|\right)]^2\\ &+\frac{1}{2}\begin{bmatrix} 2\left|E(G)\right|+\left|V(G)\right|\left(\left|V(G+H)\right|-\left|V(G)\right|\right)\\ +2\left|E(H)\right|+\left|V(H)\right|\left(\left|V(G+H)\right|-\left|V(H)\right|\right)\end{bmatrix}^2.\end{aligned}$$

Theorem 3.2 *If* $G \in T(n)$ *and* $n \geq 3$*, then*

$$M_2(G) \leq (n-1)(5n-9)$$

and equality holds if and only if $G = K_1 + S_{n-1}$.

Proof. If $G \in T(n)$ and $M_2(G)$ is as large as possible then by Lemma 1.3 $G = K_1 + T_{n-1}$, where T_{n-1} is a tree of order $n-1$. Therefore

$$M_2(G) = M_2(K_1 + T_{n-1})$$

and by using Lemma 3.1, we have

$$\begin{aligned}M_2(K_1+T_{n-1}) = \;& M_2(K_1)+\left(\left|V(K_1+T_{n-1})\right|-\left|V(K_1)\right|\right)M_1(K_1)\\ &+\left(\left|V(K_1+T_{n-1})\right|-\left|V(K_1)\right|\right)E(K_1)\\ &+M_2(T_{n-1})+\left(\left|V(K_1+T_{n-1})\right|-\left|V(T_{n-1})\right|\right)M_1(T_{n-1})\\ &+\left(\left|V(K_1+T_{n-1})\right|-\left|V(T_{n-1})\right|\right)E(T_{n-1})\\ &-12\left[2E(K_1)+\left|V(K_1)\right|\left(\left|V(K_1+T_{n-1})\right|-\left|V(K_1)\right|\right)\right]^2\\ &-12\left[2E(T_{n-1})+\left|V(T_{n-1})\right|\left(\left|V(K_1+T_{n-1})\right|-\left|V(T_{n-1})\right|\right)\right]^2\end{aligned}$$

$$+\frac{1}{2}\left[\begin{array}{l} 2E(K_1)+|V(K_1)|\left(|V(K_1+T_{n-1})|-|V(K_1)|\right) \\ +|V(T_{n-1})|\left(|V(K_1+T_{n-1})|-|V(T_{n-1})|\right) \\ +2E(T_{n-1}) \end{array}\right]^2$$

Using Lemma 1.1 yields

$$M_2(G) \le (n-1)(5n-9).$$

Lemma 1.1 guaranties that equality holds if and only if $G = K_1 + S_{n-1}$.

Theorem 3.3 *If* $k \ge 2$, $n \ge 5$ *and* $G \in T_k(n)$, *then*

$$M_2(G) \le \frac{(n-1)(k+1)(3nk+2n-5k-2k^2-2)}{2}$$

and equality holds if and only if $G = K_k + S_{n-k}$.

Proof. We will prove this theorem by induction on k. We have already proved this property for $k=1$ in Theorem 3.2. Now suppose that the result is true for (k-1)-apex trees. Let $G \in T_k(n)$ has the maximum $M_2(G)$. Let $V_k \subset V(G)$ be the set of k-apex vertices. As $M_2(G+uv) \ge M_2(G)$ for any $uv \notin E(G)$ this property implies that V_k forms a complete graph and for any $u \in V_k$, $d(u) = n-1$. So the number m of edges of graph G is

$$m = \binom{k}{2} + k(n-k) + n-k-1$$
$$= \frac{k(k+1)}{2} + (k+1)(n-k-1). \tag{3.1}$$

Let $x \in V_k$ and $V_{k-1} = V_k - x$. Note that $d(x) = n-1$, $G-x$ is a (k-1)-apex tree and

$$M_2(G-x) = \sum_{uv \in E(G-x)} \left(d_G(u)-1\right)\left(d_G(v)-1\right)$$
$$= \sum_{uv \in E(G-x)} d_G(u) d_G(v) - \sum_{uv \in E(G-x)} \left(d_G(u)+d_G(v)\right) + \sum_{uv \in E(G-x)} 1$$

$$= \sum_{uv\in E(G-x)} d_G(u)d_G(v) + \sum_{xu\in E(G)} (n-1)d_G(u)$$
$$- \sum_{xu\in E(G)} (n-1)d_G(u) - \sum_{uv\in E(G-x)} \left(d_G(u)+d_G(v)\right)$$
$$- \sum_{xu\in E(G)} \left((n-1)+d_G(u)\right) +$$
$$+ \sum_{xu\in E(G)} \left((n-1)+d_G(u)\right) + m-n+1$$
$$= \sum_{uv\in E(G)} d_G(u)d_G(v) - \sum_{uv\in E(G)} \left(d_G(u)+d_G(v)\right)$$
$$- \sum_{xu\in E(G)} (n-1)d_G(u) + \sum_{xu\in E(G)} \left((n-1)+d_G(u)\right) + m-n+1$$
$$= M_2(G) - M_1(G) - (n-1)(2m-n+1) + (n-1)^2$$
$$+2m-n+1+m-n+1, or$$

$$M_2(G) = M_2(G-x) + M_1(G) - 3m + 2n - 2 + (n-1)(2m-n+1) - (n-1)^2.$$

By equation (3.1) and Theorem 2.3, we have

$$M_2(G) \leq M_2(G-x) + (k+1)(n-1)^2 + (n-k-1)(k+1)^2$$
$$-3\left(k(k+1)2 + (k+1)(n-k-1)\right) + 2n-2$$
$$+(n-1)\left(2\left(k(k+1)2 + (k+1)(n-k-1)\right) - n+1\right) - (n-1)^2.$$

As we have supposed that the result is true for (k-1)-apex trees, we get

$$M_2(G) \leq \frac{k(n-2)\left(3(n-1)(k-1) + 2n - 2 - 5k + 5 - 2(k-1)^2 - 2\right)}{2} +$$
$$+(k+1)(n-1)^2 + (n-k-1)(k+1)^2 -$$
$$-3\left(k(k+1)2 + (k+1)(n-k-1)\right) + 2n - 2 +$$
$$+(n-1)\left(2\left(k(k+1)2 + (k+1)(n-k-1)\right) - n + 1\right) - (n-1)^2$$
$$= \frac{1}{2}(5n^2k + 3n^2k^2 - 10nk^2 - 2nk^3 - 12nk + 2n^2 + 7k^2 +$$
$$+ 2k^3 + 7k - 4n + 2)$$

$$=\frac{1}{2}(nk+n-k-1)(2n+3nk-5k-2k^2-2)$$
$$=\frac{(n-1)(k+1)(3nk+2n-5k-2k^2-2)}{2}.$$

Equality holds if and only if $G = K_k + S_{n-k}$.

4. Conclusion

The Zagreb indices have been successfully used in many QSAR/QSPR studies. A study of weighted Harary indices of apex trees and *k*-apex trees has been done in [9]. In this paper we determined the upper and lower bounds for Zagreb indices of *k*-apex trees. We also characterized the extremal graphs for these indices. It would be interesting to derive similar results for other famous indices for example Randić index, sum connectivity index, eccentric connectivity index etc. of *k*-apex trees.

R E F E R E N C E S

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