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General multiplicative Zagreb indices of trees

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ABSTRACT

We study trees of given order, given number of pendant vertices, segments and branching vertices. We present upper and lower bounds on the general multiplicative Zagreb indices for trees of given order and number of pendant vertices/segments/branching vertices. Bounds on the first and the second multiplicative Zagreb indices are corollaries of the general results. We also characterize trees having the largest and the smallest indices.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in V(G)$, $d_G(v)$, is the number of edges incident with v. We denote by n_i the number of vertices of G having degree i. A tree is a connected graph containing no cycles. Let us denote the star and the path having n vertices by S_n and P_n, respectively.

The neighbourhood $N_G(v)$ of a vertex v is the set of all the vertices adjacent to v in G. The diameter of G is the distance between any two furthest vertices in G. A diametral path is a shortest path in G connecting two vertices whose distance is equal to the diameter. A caterpillar is a tree in which any vertex v belongs to a diametral path D or v is adjacent to a vertex in D.

A vertex of a tree T having degree at least 3 is called a branching vertex and a pendant vertex is a vertex of degree 1. A segment of a tree T is a subtree of T which is a path, its terminal vertices are pendant or branching vertices of T and all internal vertices of a segment have degree 2. It is well-known that a non-increasing sequence $(d_1, d_2, \dots, d_n)$ of n positive integers is a degree sequence of a tree with n vertices (and $n-1$ edges) if and only if

$$\sum_{i=1}^{n} d_i = 2(n-1). \tag{1}$$

Chemical-based experiments indicate that there is strong relationship between the characteristics of chemical compounds and drugs and their molecular structures. Topological indices calculated for these chemical structures help us to understand the physical features, chemical reactivity and biological activity.

The graph based molecular descriptors called Zagreb indices (the first Zagreb index and the second Zagreb index) were introduced by Gutman and Trinajstić in 1972, see [10]. They belong to the oldest topological indices. A lot of research has been done on Zagreb indices due to their chemical importance. Lin [14] and Borovićanin [2] studied bounds on the first and

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the second Zagreb indices for trees. Zagreb indices of trees with given domination number were investigated by Borovićanin and Furtula [3]. Gao et al. [7] gave bounds on the hyper-Zagreb index of trees. The general sum-connectivity index of trees was studied in [5], the general Randić index of trees was considered in [4], the Randić index of trees in [13], the Wiener index of trees in [8] and the Estrada indices for trees in [12,21].

Gutman [9], and Xu and Hua [22] studied the first and the second multiplicative Zagreb indices of trees of given order. Multiplicative Zagreb indices for trees with given number of vertices of maximum degree were investigated in [19], k-trees were studied in [20], molecular graphs in [11], graphs of given order, size and other parameters in [15], bipartite graphs in [18], some derived graphs in [1], graph operations in [6,17].

Let us define the first general multiplicative Zagreb index of a graph G,

$$P_1^a(G) = \prod_{v \in V(G)} d_G(v)^a$$

and the second general multiplicative Zagreb index of G,

$$P_2^a(G) = \prod_{v \in V(G)} d_G(v)^{a d_G(v)},$$

where $a \neq 0$. These indices generalize well-known multiplicative Zagreb indices. If $a = 1$, then $P_1^1(G)$ is the Narumi–Katayama index, see [16], and if $a = 2$, then $P_1^2(G)$ is the first multiplicative Zagreb index

$$\Pi_1(G) = \prod_{v \in V(G)} d_G(v)^2.$$

If $a = 1$, then $P_2^1(G)$ is the second multiplicative Zagreb index

$$\Pi_2(G) = \prod_{v \in V(G)} d_G(v)^{d_G(v)}.$$

Multiplicative and general multiplicative Zagreb indices for trees of given order (number of vertices) in combination with given number of pendant vertices, segments or branching vertices have not been investigated yet. We present upper and lower bounds on the first and the second general multiplicative Zagreb indices for trees of given order and number of pendant vertices/segments/branching vertices. Bounds on the first and the second multiplicative Zagreb indices are corollaries of the general results. We also show that the bounds are best possible.

2. Trees of given order

In this section we give sharp bounds on the general multiplicative Zagreb indices for trees of given order.

Theorem 2.1. *Let T be any tree with $n \geq 4$ vertices. Then for $a > 0$ we have*

$$P_1^a(T) \geq (n-1)^a \text{ and } P_2^a(T) \leq (n-1)^{a(n-1)}$$

with equalities if and only if T is S_n.

Proof. Let T' be a tree having the smallest P_1^a index (having the largest P_2^a index) among trees with n vertices. We prove by contradiction that T' is the star S_n.

Assume that T' is not S_n. Let v be a vertex of T' having the maximum degree. Since T' is not S_n, there is a vertex, say v', in $N_{T'}(v)$ such that $d_{T'}(v') > 1$. Let z be any neighbour of v' other than v. Let T_1 be a tree obtained from T' by removing the edge $v'z$ and adding the edge vz. Note that v, v' are the only vertices whose degree is different in T' and T_1. We have $d_{T'}(v) = q$, $d_{T_1}(v) = q+1$, $d_{T'}(v') = r$ and $d_{T_1}(v') = r-1$, where $2 \leq r \leq q$. Then

$$\frac{P_1^a(T')}{P_1^a(T_1)} = \frac{q^a r^a}{(q+1)^a (r-1)^a} = \left(\frac{qr}{qr+r-q-1}\right)^a > 1$$

since $r-q-1 < 0$. For P_2^a index we have

$$\begin{aligned}\frac{P_2^a(T')}{P_2^a(T_1)} &= \frac{q^{aq} r^{ar}}{(q+1)^{a(q+1)}(r-1)^{a(r-1)}} = \left[\frac{q^q r^r}{(q+1)^{q+1}(r-1)^{r-1}}\right]^a \\ &= \left[\left(1-\frac{1}{q+1}\right)^{q+1}\left(1+\frac{1}{r-1}\right)^{r-1}\frac{r}{q}\right]^a < 1,\end{aligned}$$

since $(1-\frac{1}{q+1})^{q+1} < \frac{1}{e}$, $(1+\frac{1}{r-1})^{r-1} < e$ and $\frac{r}{q} \leq 1$.

Thus $P_1^a(T') > P_1^a(T_1)$ and $P_2^a(T') < P_2^a(T_1)$, which means that T' is not a tree having the smallest P_1^a index (having the largest P_2^a index). A contradiction.

Note that $P_1^a(S_n) = (n-1)^a$ and $P_2^a(S_n) = (n-1)^{a(n-1)}$, so the proof is complete. □

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