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Note

On extremal multiplicative Zagreb indices of trees with given number of vertices of maximum degree

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ABSTRACT

The first multiplicative Zagreb index of a graph G is the product of the square of every vertex degree, while the second multiplicative Zagreb index is the product of the products of degrees of pairs of adjacent vertices. In this paper, we explore the trees in terms of given number of vertices of maximum degree. The maximum and minimum values of $\prod_1(G)$ and $\prod_2(G)$ of trees with arbitrary number of maximum degree are provided. In addition, the corresponding extremal graphs are characterized.

1. Introduction

Throughout this paper, we consider simple, connected and undirected graphs. Denote a graph by $G = (V, E)$, where $V = V(G)$ is called vertex set and $E = E(G)$ is called edge set. For a vertex $v \in V(G)$, the neighborhood of v is the set $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$, and $d_G(v)$ (or $d(v)$) denotes the degree of v with $d_G(v) = |N(v)|$. n_i is the number of vertices of degree $i \geq 0$. If a graph G contains n vertices and $n-1$ edges, then G is called a tree. For a vertex $v \in V(T)$ with $2 \leq d_T(v) \leq \Delta(T) - 1$, its edge rotating capacity is defined to be $d_T(v) - 1$. The total edge rotating capacity of a tree T is equal to the sum of the edge rotating capacities of its vertices that satisfy the condition $2 \leq d_T(v) \leq \Delta(T) - 1$. As usual, denote P_n by the path on n vertices. The maximum vertex degree in the graph G is denoted by $\Delta(G)$.

The degree sequence of G is a sequence of positive integers $\pi = (d_1, d_2, \ldots, d_n)$ if $d_i = d_G(v)(i = 1, \ldots, n)$ holds for $v \in V(G)$. In this work, we assign an order of the vertex degrees as non-increasing, i.e., $d_1 \geq d_2 \geq \cdots \geq d_n$. In addition, a sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called a tree degree sequence if there exists a tree T such that π is its degree sequence. Furthermore, it is well known that the sequence $\pi = (d_1, d_2, \ldots, d_n)$ is a degree sequence of a tree with n vertices if and only if

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

In the interdisciplinary of mathematics, chemistry and physics, molecular invariants/descriptors could be useful for the study of quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) and

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for the descriptive presentations of biological and chemical properties, such as boiling and melting points, toxicity, physico-chemical, and biological properties [4,5,12,14,20,22,25]. One class of the oldest topological molecular descriptors are named as Zagreb indices [7], which are literal quantities in expected formulas for the total π-electron energy of conjugated molecules as follows.

$$M_1(G) = \sum_{u \in V(G)} d(u)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

Based on the successful considerations on these applications of Zagreb indices [6], Todeschini et al. (2010) [17,18,21] presented the following multiplicative variants of molecular structure descriptors:

$$\prod_1(G) = \prod_{u \in V(G)} d(u)^2 \text{ and } \prod_2(G) = \prod_{uv \in E(G)} d(u)d(v) = \prod_{u \in V(G)} d(u)^{d(u)}.$$

Recently, there are lots of articles that explored multiplicative Zagreb indices in the interdisciplinary of chemistry and mathematics [3,8,9,13,16,19,23]. Iranmanesh et al. [10] explored first and second multiplicative Zagreb indices for a class of chemical dendrimers. Xu and Hua [24] provided a unified approach to characterize extremal maximal and minimal trees, unicyclic graphs and bicyclic graphs regarding multiplicative Zagreb indices, respectively. Wang and Wei [21] gave the maximum and minimum indices of these indices in k-trees, and the corresponding extreme graphs are provided. Liu and Zhang [25] investigated some sharp upper bounds for $\prod_1$-index and $\prod_2$-index in terms of graph parameters such as an order, a size and a radius [15]. Kazemi [11] studied the bounds for the moments and the probability generating function of these indices in a randomly chosen molecular graph with tree structure of order n. Borovićanin et al. [1] introduced upper bounds on Zagreb indices of trees, and a lower bound for the first Zagreb index of trees with a given domination number is determined and the extremal trees are characterized as well. Borovićanin and Lampert [2] provided the maximum and minimum Zagreb indices of trees with given number of vertices of maximum degree.

Motivated by above results, in this paper we further investigate the multiplicative Zagreb indices of trees with arbitrary number of vertices of maximum degree. The maximum and minimum values of $\prod_1(G)$ and $\prod_2(G)$ of trees with arbitrary number of maximum degree are provided. In addition, the corresponding extreme graphs are characterized. Our results extend and enrich some known conclusions obtained by [2].

2. Preliminaries

It is known that each tree has at least two minimum degree vertices, named as pendent vertices, and some maximum degree vertices. It is natural to consider the trees with arbitrary number of maximum degree vertices.

Let $\mathcal{T}_{n,k}$ be the class of trees with n vertices, in which there exist k vertices having the maximum degree with $n > k > 0$. Note that the path P_n is the unique element of $\mathcal{T}_{n,n-2}$. So, in the following we consider the class $\mathcal{T}_{n,k}$ with $k \leq n-3$.

We first introduce several facts and tools, which are important in the proofs of following sections.

Proposition 2.1 ([2]). *If $T \in \mathcal{T}_{n,k}$ is a tree with k vertices of maximum degree Δ, then $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$.*

By the routine calculations, one can derive the following propositions.

Proposition 2.2. *Let $f(x) = \frac{x}{x+m}$ be a function with $m > 0$. Then $f(x)$ is increasing in $\mathbb{R}$.*

Proposition 2.3. *Let $g(x) = \frac{x^x}{(x+m)^{x+m}}$ be a function with $m > 0$. Then $g(x)$ is decreasing in $\mathbb{R}$.*

Based on the above algebraic tools, we are ready to provide the sharp upper and lower bounds of first multiplicative Zagreb index of such trees in Section 3, and the sharp upper and lower bounds of second multiplicative Zagreb index of these trees in Section 4. Some of notations and figures are used close to [2].

3. The sharp upper and lower bounds of first multiplicative Zagreb index on the trees

In this section, we obtain the bounds of the first multiplicative Zagreb index in the class $\mathcal{T}_{n,k}$.

3.1. The sharp upper bounds of $\prod_1$ on trees with given number of vertices of maximum degree

The first multiplicative Zagreb index of $\mathcal{T}_{n,k}$ can be routinely calculated if the degree sequence is given.

Lemma 3.1. *Let T^1_{min} be a tree with minimal value of first multiplicative Zagreb index in $\mathcal{T}_{n,k}$. Then $\Delta(T^1_{min}) = \lfloor \frac{n-2}{k} \rfloor + 1$.*