Applied Mathematics and Computation 332 (2018) 338–350

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On extremal multiplicative Zagreb indices of trees with given domination number

Shaohui Wang[a], Chunxiang Wang[b], Jia-Bao Liu[c,*]

[a] Department of Mathematics, Savannah State University, Savannah, GA 31404, USA
[b] School of Mathematics and Statistics, Central China Normal University, Wuhan 430079, PR China
[c] School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, PR China

ARTICLE INFO

MSC:
05C05
05C12

Keywords:
Trees
Domination number
Extremal bounds
Multiplicative Zagreb indices

ABSTRACT

For a (molecular) graph, the first multiplicative Zagreb index Π_1 is equal to the product of squares of the vertex degrees, and the second multiplicative Zagreb index Π_2 is equal to the product of the products of degrees of pairs of adjacent vertices. In this paper, we explore the multiplicative Zagreb indices in terms of domination number. Sharp upper and lower bounds of Π_1 and Π_2 are given. In addition, the corresponding extreme graphs are characterized, and our conclusions enrich and extend some known results.

1. Introduction

Molecular descriptors could be helpful for quantitative structure property relationships (QSPR) and quantitative structure–activity relationships (QSAR) studies and for the descriptive purposes of biological and chemical properties, such as toxicity, physico-chemical and biological properties. One of the first topological molecular descriptors is so-called Zagreb indices [1], which are auxiliary quantities in an approximated formula for the total π-electron energy of conjugated molecules. Many interesting results of the applications on Zagreb indices were explored in the area of chemistry and mathematics, see [2–6].

All graphs considered are simple connected graphs. Let $G=(V,E)$ be such a graph, where $V=V(G)$ is its vertex set and $E=E(G)$ is its edge set. For $u\in V(G)$, $G-u$ is an induced subgraph of $V(G)-\{u\}$ in G. A graph G that has n vertices and $n-1$ edges is called a tree. As usual, by P_n and $K_{1,n-1}$ denote the path and the star on n vertices, respectively.

The degree-based graph invariants $M_1(G)$ and $M_2(G)$ [1] are defined as

$$M_1(G)=\sum_{u\in V(G)} d(u)^2,\ \ M_2(G)=\sum_{uv\in E(G)} d(u)d(v). \tag{1}$$

In 2010, Todeschini et al. [7,8] presented the following multiplicative variants of molecular structure descriptors:

$$\Pi_1(G)=\prod_{u\in V(G)} d(u)^2,\ \ \Pi_2(G)=\prod_{uv\in E(G)} d(u)d(v). \tag{2}$$

By the recursive process, we see that $\Pi_2(G)=\prod_{uv\in E(G)} d(u)d(v)=\prod_{u\in V(G)} d(u)^{d(u)}$.

* Corresponding author.
E-mail addresses: shaohuiwang@yahoo.com, wangs@savannahstate.edu (S. Wang), wcxiang@mail.ccnu.edu.cn (C. Wang), liujiabaobaoad@163.com, liujiabao@ahjzu.edu.cn (J.-B. Liu).

https://doi.org/10.1016/j.amc.2018.03.058
0096-3003/

Recently, multiplicative Zagreb indices attracted extensive attention in physics, chemistry, graph theory, etc [15–19]. Xu and Hua [9] proposed a unified approach to characterize extremal (maximal and minimal) trees, unicyclic graphs and bicyclic graphs with respect to multiplicative Zagreb indices, respectively. Iranmanesh et al. [10] investigated these indices the first and the second multiplicative Zagreb indices for a class of dendrimers. Liu and Zhang [11] introduced several sharp upper bounds for π_1-index and π_2-index in terms of graph parameters including the order, size and radius. Wang and Wei [12] studied these indices in k-trees and extremal k-trees were characterized. Ramin Kazemi [13] obtained 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 and Furtula [14] presented upper bounds on Zagreb indices of trees in terms of domination number. Also, 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. For some most recent researches along these lines see [20–22].

Motivated by the above results, in this paper we further investigate the multiplicative Zagreb indices of trees in terms of domination number. The rest of the paper is organized as follows. We first provide some useful lemmas and preliminaries. The lower bounds of first multiplicative Zagreb index and upper bounds of second Zagreb index on trees of given domination number in Section 2. The upper bounds of first multiplicative Zagreb index and lower bounds of second multiplicative Zagreb index on trees of given domination number in Section 3.

Firstly, we provide some propositions and lemmas which are critical in the following proofs.

Proposition 1.1. *The function* $f(x) = \frac{x}{x+m}$ *with* $m > 0$ *is increasing in* $\mathbb{R}$.

Proposition 1.2. *The function* $g(x) = \frac{x^x}{(x+m)^{x+m}}$ *with* $m > 0$ *is decreasing in* $\mathbb{R}$.

Lemma 1.1. *([14]) Let T be a tree with n vertices and domination number* $\frac{n+3}{3} \leq \gamma \leq \frac{n}{2}$*. If the value of max*$\{|d(u) - d(v)|, u, v \in V(T)\}$ *is as small as possible (say* $d(u) \in \{1, 2, 3\}$*), and* n_1 *is the number of vertices of degree 1, then* $n_1 \geq 3\gamma - n$*, where the inequality is strict if there exists a vertex with two pendent neighbors.*

If $\Delta(G) = 1$, G is an edge by the assumption that G is connected, and corresponding results are trivial. We will conisder graphs G with $\Delta(G) \geq 2$ below.

2. Lower bounds of first multiplicative Zagreb index and upper bounds of second Zagreb index on the trees

In this section, we provide sharp lower bounds of first multiplicative Zagreb index and upper bounds of second Zagreb index on trees with n vertices and domination number γ. We start with the following definition.

Definition 2.1. Denoted by $\overline{T}_{n,\gamma}$ the tree obtained from a star graph $K_{1,n-\gamma}$ by attaching a pendant edge to its $\gamma - 1$ pendant vertices.

Let $\mathcal{T}_{n,\gamma}$ be the class of trees $T_{n,\gamma}$. Note that $\gamma = 1$ if and only if $T \cong K_{1,n-1}$. If $\Delta = n - \gamma$ in a tree of order n and domination number γ, then $T \cong \overline{T}_{n,\gamma}$. Then the first multiplicative Zagreb index and second multiplicative Zagreb index of $T_{n,\gamma}$ can be calculated routinely below.

Proposition 2.1. *For the graph* $\overline{T}_{n,\gamma}$*, we have*

$$\Pi_1(\overline{T}_{n,\gamma}) = 4^{\gamma-1}(n-\gamma)^2,\ \ \Pi_2(\overline{T}_{n,\gamma}) = 4^{\gamma-1}(n-\gamma)^{n-\gamma}.$$

2.1. Lower bounds of $\Pi_1(G)$ *on trees with domination number* γ

Theorem 2.1. *Let G be a tree with n vertices and domination number* γ*. Then*

$$\Pi_1(G) \geq 4^{\gamma-1}(n-\gamma)^2, \text{ where the equality holds if and only if } G \cong \overline{T}_{n,\gamma}.$$

Proof. We first consider $\Delta(G) = 2$. Since $n \geq 2$ and G is a connected graph, then $T \cong P_n$. For $n = 2, 3$ or 4, $G \cong T_{2,1}(\equiv P_2)$, $T_{3,1}(\equiv P_3)$ or $T_{4,2}(\equiv P_4)$, respevtively. By the routine caculations of $\Pi_1(G)$, we have that the equality of Theorem 2.1 holds. If $n \geq 5$, then the inequality of Theorem 2.1 holds by direct calculations of $\Pi_1(G)$. Next we will consider trees with $\Delta(G) \geq 3$. Set $P_{d+1} := v_1v_2\ldots v_{d+1}$ to be a longest path in G, where d is the diameter of G. We have $d(v_1) = d(v_{d+1}) = 1$. Let D be a minimal dominating set of G such that $|D| = \gamma$. Then $\triangle \leq n - \gamma$. As one can routinely calculated for $n \leq 5$, Theorem 2.1 is true. Now we will prove it by the induction on $n \geq 6$. Assume that Theorem 2.1 holds for $|G| = n - 1$, and we will show the case of $|G| = n$. There are two possible cases below.

Case 1. Suppose that $\gamma(G - v_1) = \gamma(G)$. Then v_2 is not in the domination set D. By the concept of $\Pi_1(G)$ and $d(v_1) = 1$, we obtain that