South Asian Journal of Mathematics 2012 , Vol. 2 (6) : 578 ∼ 583
www.sajm-online.com ISSN 2251-1512 RESEARCH ARTICLE

A note on multiplicative sum Zagreb index

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This work was supported by NSF of the Higher Education Institutions of Jiangsu Province (No.12KJB110001), P.R. China.

Abstract For a nontrivial (molecular) graph G, its multiplicative sum Zagreb index, denoted by $\pi_1^*(G)$, is defined as the product of the sum $d_G(u) + d_G(v)$ over all edges uv in G, where $d_G(u)$ is the degree of vertex u. In this note, we establish a relationship between $\pi_1^*(G)$ of a graph and the first multiplicative Zagreb index of its total graph. Moreover, we present some bounds for $\pi_1^*(G)$ in terms of some other graph parameters including the second multiplicative Zagreb index, radius, the first Zagreb index.

Key Words distance, Wiener index, the first multiplicative, Zagreb index

MSC 2010 05C12, 05C75

1 Introduction

We only consider finite, undirected and simple graphs throughout this paper. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The *degree* of $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices adjacent to v in G. The *distance* between two vertices u and v in a connected graph G, denoted by $d_G(u, v)$, is the length of the shortest path connecting u and v. For other notations and terminology not defined here, the readers are referred to [2].

A graphical invariant is a number related to a graph, in other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also called the *topological indices*. One of the oldest topological indices is the well-known Zagreb indices firstly introduced in [5], where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structure and elaborated in [6]. For a (molecular) graph G, its *first Zagreb index* $M_1(G)$ and *second Zagreb index* $M_2(G)$ are, respectively, defined as

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

The above two ordinary topological indices (M_1-index and M_2-index) reflect the extent of branching of the molecular carbon-atom skeleton [1, 11]. These two Zagreb indices were well-studied during the past decades, see [3, 4, 8–10] and the references cited therein.

Citation: H. Wang, H. Bao, A note on multiplicative sum Zagreb index, South Asian J Math, 2012, 2(6), 578-583.

Recently, Todeschini et al. [12, 13] have proposed the multiplicative variants of ordinary Zagreb indices, which are defined as

$$\pi_1 = \pi_1(G) = \prod_{v\in V(G)} (d_G(v))^2 \quad \text{and} \quad \pi_2 = \pi_2(G) = \prod_{uv\in E(G)} d_G(u)d_G(v),$$

respectively.

These two topological indices are called *"multiplicative Zagreb indices"* by Gutman [7]. In [7], Gutman characterized that among all trees of order $n \geqslant 4$, the extremal trees with respect to these multiplicative Zagreb indices are the path P_n (with maximal π_1 and minimal π_2) and the star S_n (with maximal π_2 and minimal π_1), resepctively. Xu and Hua [14] provided a unified approach to determine extremal trees, unicyclic graphs and bicyclic graphs with respect to these two multiplicative Zagreb indices.

More recently, Xu and Das [15] proposed the *multiplicative sum Zagreb index*, which is defined as

$$\pi_1^* = \pi_1^*(G) = \prod_{uv\in E(G)} (d_G(u) + d_G(v)).$$

Concerning the multiplicative sum Zagreb index, the authors [15] characterized extremal trees, unicyclic graphs and bicyclic graphs with respect to the multiplicative sum Zagreb index.

In this note, we establish a relationship between $\pi_1^*(G)$ of a graph and the first multiplicative Zagreb index of its total graph. Moreover, we present some bounds for $\pi_1^*(G)$ in terms of some other graph parameters including the second multiplicative Zagreb index, radius, the first Zagreb index.

2 Main results

We divide this section into two subsections. In the first subsection, we establish the relationship between π_1^*-index of a graph and π_1-index of its total graph. In the second subsection, we build some bounds for π_1^*-index of nontrivial graphs in terms of other graph parameters.

Let G be a connected graph composed of s components $G_1, \ldots, G_s$. According to the definition of π_1^*-index , we have $\pi_1^*(G) = \prod\limits_{i=1}^{s} \pi_1^*(G_i)$. So, it suffices to investigate π_1^*-index of connected graphs.

2.1 Relationships between π_1^*-index of a graph and π_1-index of its total graph

Theorem 2.1. *Let G be a nontrivial connected graph, and let $T(G)$ be the total graph of G. Then*

$$\pi_1^*(G) = \frac{1}{2}\sqrt{\frac{\pi_1(T(G))}{\pi_1(G)}}.$$

Proof. By the definition of total graph, $V(T(G)) = V(G) \cup E(G)$. For each vertex v in G, $d_{T(G)}(v) = 2d_G(v)$; For each edge $e = uv$ in G, $d_{T(G)}(e) = d_G(u) + d_G(v)$.

According to the definition of the first multiplicative Zagreb index and the multiplicative sum Zagreb index, we have

$$\begin{aligned}\pi_1(T(G)) &= \prod_{w\in V(T(G))} \left(d_{T(G)}(w)\right)^2\\ &= \prod_{w\in V(G)} (2d_G(w))^2 \cdot \prod_{w=xy\in E(G)} (d_G(x)+d_G(y))^2\\ &= 4\pi_1(G)\cdot\left(\prod_{w=xy\in E(G)} (d_G(x)+d_G(y))\right)^2\\ &= 4\pi_1(G)[\pi_1^*(G)]^2,\end{aligned}$$

implying the expected result. □

2.2 Relationships with other graph parameters

Xu and Das [15] have proposed the problem to find the relationship between the second multiplicative Zagreb index and the multiplicative sum Zagreb index. Here, we present a simple relationship between these two indices.

Theorem 2.2. *Let G be a nontrivial connected graph of size m. Then*

$$\pi_1^*(G) \geqslant 2^m\sqrt{\pi_2(G)}$$

with equality if and only if G is a regular graph.

Proof. By the definition of these two multiplicative Zagreb indices,

$$\begin{aligned}\pi_1^*(G) &\geqslant \prod_{uv\in E(G)} 2\sqrt{d_G(u)d_G(v)} \qquad (1)\\ &= 2^m\sqrt{\prod_{uv\in E(G)} d_G(u)d_G(v)}\\ &= 2^m\sqrt{\pi_2(G)}.\end{aligned}$$

It can be seen that the equality in Ineq. (1) is attained if and only if $d_G(u) = d_G(v)$ for each edge uv in G.

We claim that $\pi_1^*(G) = 2^m\sqrt{\pi_2(G)}$ if and only if G is a regular graph.

If G is a regular graph, then the equality in Ineq. (1) is attained, and thus $\pi_1^*(G) = 2^m\sqrt{\pi_2(G)}$.

Conversely, we assume that $\pi_1^*(G) = 2^m\sqrt{\pi_2(G)}$. Let us prove that G is a regular graph. Suppose to the contrary that there exist two vertices, say u and v, in G, satisfying that $d_G(u) \neq d_G(v)$. Then $uv \notin E(G)$. Because G is connected, there must exist a $v_0v_1\ldots v_s$ path in G, where $v_0 = u$ and $v_s = v$ and $s \geqslant 2$. Note that $d_G(x) = d_G(y)$ for any edge xy in G. Thus, $d_G(u) = d_G(v_1) = \ldots = d_G(v)$, a contradiction to our assumption. Thus, G is a regular graph, as desired. □

The *radius* $R(G)$ of a connected graph G is defined as $R(G) = \min\{\varepsilon_G(u)|u \in V(G)\}$, where $\varepsilon_G(u) = \max\{d_G(u, v)|v \in V(G)\}$.

In the following, we give a result relating multiplicative sum Zagreb index with radius for trees.

Theorem 2.3. *Let G be a nontrivial tree of order n and $R(G)$ be its radius. Then*

$$\pi_1^*(G) \leqslant (n + 1 - R(G))^{\frac{n(n-1)}{2}}$$

with equality if and only if $G \cong P_2$.

Proof. Suppose that G is a nontrivial tree of order n. For any two vertices u and v in G, it holds that

$$d_G(u, v) \leqslant n - (d_G(u) - 1) - (d_G(v) - 1) - 1 = n - d_G(u) - d_G(v) + 1 \qquad (2)$$

with equality if and only if all vertices not belonging to $N_G(u) \cup N_G(v)$ lie within the unique u–v path.

Therefore,

$$\begin{aligned} \pi_1^*(G) &= \prod_{uv \in E(G)} (d_G(u) + d_G(v)) \\ &\leqslant \prod_{\{u, v\} \subseteq V(G)} (d_G(u) + d_G(v)) && (3) \\ &\leqslant \prod_{\{u, v\} \subseteq V(G)} (n - d_G(u, v) + 1) && (4) \\ &\leqslant (n + 1 - R(G))^{\binom{n}{2}}. && (5) \end{aligned}$$

It is easily seen that the equality in Ineq. (3) is attained if and only if $G \cong K_n$. The equality in Ineq. (4) is attained if and only if for any vertex pairs $\{u, v\}$ in G, the equality in Ineq. (2) is attained. Hence, the equality in Ineq. (4) is attained if and only if G is one of the paths P_2, P_3 and P_4. The equality in Ineq. (5) is attained if and only if for any vertex pairs $\{u, v\}$ in G, there exists $d_G(u, v) = R(G)$, that is, G is K_n.

Summarizing above, we obtain

$$\pi_1^*(G) \leqslant (n + 1 - R(G))^{\frac{n(n-1)}{2}}$$

with equality if and only if $G \cong P_2$.

This completes the proof. □

A bipartite graph $G = (X; Y)$ is said to be *semiregular* if there exist two constants a and b such that each vertex in X has degree a and each vertex in Y has degree b; such bipartite graphs are also called $(a; b) - semiregular$.

Theorem 2.4. *Let G be a nontrivial connected graph of size m. Then*

$$\pi_1^*(G) \leqslant (\frac{M_1(G)}{m})^m$$

with equality if and only if G is a regular or semiregular graph.

Proof. According to the definition of multiplicative sum Zagreb index and Geometric-Arithmetic Mean inequality, we obtain

$$\begin{aligned} \pi_1^*(G) &= \prod_{uv\in E(G)} (d_G(u)+d_G(v)) \\ &\leqslant \left(\frac{\sum\limits_{uv\in E(G)} (d_G(u)+d_G(v))}{m}\right)^m \\ &= \left(\frac{\sum\limits_{w\in V(G)} (d_G(w))^2}{m}\right)^m \\ &= (\frac{M_1(G)}{m})^m. \end{aligned} \tag{6}$$

It is obvious that the equality in Ineq. (6) is attained if and only if the value of $d_G(u)+d_G(v)$ is a constant regardless of the choice of edge uv.

We first prove the following claim.

Claim 1. *For each edge $uv \in E(G)$, $d_G(u)+d_G(v)$ is a constant if and only if G is regular or semiregular.*

Proof. The sufficiency is obvious. Now, we check the necessity.

Assume that $d_G(u)+d_G(v)$ is a constant and G is not regular. We shall prove that G is a semiregular graph.

We first verify that G is bipartite. Suppose to the contrary that G is not bipartite. Then G contains an odd cycle, say $C_l = v_1v_2\dots v_lv_1$ (l is odd). As $d_G(u)+d_G(v)$ is a constant and C_l is an odd cycle, one can easily deduce that $d_G(v_1) = d_G(v_2) = \cdots = d_G(v_l)$. Since G is not regular, there exists at least a vertex, say x, lying outside the cycle C_l. Assume that x is adjacent to some v_j ($1 \leqslant j \leqslant l$).

Clearly, for any given vertex u in G, its all neighbors must have equal degrees. Thus, $d_G(x) = d_G(v_1) = \cdots = d_G(v_j) = \cdots = d_G(v_l)$. Obviously, $d_G(x) \geqslant 3$. As above, we can prove that for any vertex $y \in N_G(x) \setminus \{v_j\}$, $d_G(y) = d_G(v_j)$. Now, we actually have proved that for any edge $uv \in E(G) \setminus E(C_l)$, there exists $d_G(u) = d_G(v) = d_G(v_1) = d_G(v_2) = \cdots = d_G(v_l)$. Thus, G is a regular graph, a contradiction to our assumption. So, G must be bipartite.

Assume that G has two partite sets X and Y. Let uv be an edge in G such that $u \in X$ and $v \in Y$, and suppose without loss of generality that $d_G(u) = a$ and $d_G(v) = b$. We further claim that all vertices in X have degree a, and all vertices in Y have degree b. Suppose to the contrary that there exists a vertex, say x, in X whose degree is not equal to a.

Since G is bipartite and connected, there exists an even path connecting u and x. Because $d_G(u) + d_G(v)$ is a constant for any edge uv, we must have $d_G(x) = d_G(u) = a$, a contradiction. Therefore, any vertex in X has degree a. Similarly, any vertex in Y has degree b. Thus, G is semiregular, as claimed. □

By Claim 1, we have

$$\pi_1^*(G) \leqslant (\frac{M_1(G)}{m})^m$$

with equality if and only if G is a regular or semiregular graph.

This completes the proof. □

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