MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 231-240

ISSN 0340 - 6253

Sharp Upper Bounds for Multiplicative Zagreb Indices

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(Received October 24, 2011)

Abstract

For a (molecular) graph, the multiplicative Zagreb indices $\prod_1$-index and $\prod_2$-index are multiplicative versions of the ordinary Zagreb indices (M_1-index and M_2-index). In this note we report several sharp upper bounds for $\prod_1$-index in terms of graph parameters including the order, size, radius, Wiener index and eccentric distance sum, and upper bounds for $\prod_2$-index in terms of graph parameters including the order, size, the first Zagreb index, the first Zagreb coindex and degree distance.

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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 is the length of a shortest path connecting u and v. Other undefined notations and terminology from graph theory can be found in [4].

A graphical invariant is a number related to a graph which is a structural invariant, in other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also known as the topological indices. One of the oldest graph invariants is the well-known Zagreb indices first introduced in [8] where Gutman and Trinajstić examined the dependence of total $\prod$-electron energy on molecular structure and elaborated in [9]. For a (molecular) graph G, the **first Zagreb index** $M_1(G)$ and the **second Zagreb index** $M_2(G)$ are, respectively, defined as follows:

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

These two classical topological indices (M_1-index and M_2-index) reflect the extent of branching of the molecular carbon-atom skeleton [3, 23]. These two Zagreb indices were well-studied during the past decades, see [5, 6, 12, 20, 21, 29, 30] for instance.

Recently, Todeschini et al. [24,25] have proposed the multiplicative variants of ordinary Zagreb indices, which are defined as follows:

$$\prod_1 = \pi_1(G) = \prod_{v\in V(G)} (d_G(v))^2, \qquad \prod_2 = \pi_2(G) = \prod_{uv\in E(G)} d_G(u)d_G(v).$$

These two graph invariants are called “ **multiplicative Zagreb indices** ” by Gutman [10]. In the same paper, Gutman determined that among all trees of order $n \geq 4$, the extremal trees with respect to these multiplicative Zagreb indices are path P_n (with maximal $\prod_1$ and minimal $\prod_2$) and star S_n (with maximal $\prod_2$ and minimal $\prod_1$). More recently, Xu and Hua [28] provided a unified approach to determine extremal trees and unicyclic graphs with respect to these two Multiplicative Zagreb indices. The readers can also refer to [11] for properties of these new indices.

In this note we report further properties of multiplicative Zagreb indices. In Section 2, we report several sharp upper bounds for $\prod_1$-index in terms of graph parameters including the order, size, radius, Wiener index and eccentric distance sum. In Section 3, we report some upper bounds for $\prod_2$-index in terms of graph parameters including the order, size, the first Zagreb index, the first Zagreb coindex and degree distance.

2 Bounds for $\prod_1$-index of connected graphs

Let G be a connected graph composed of m components $G_1, \ldots, G_m$. According to the definition of $\prod_j$-index, we clearly have $\prod_j(G) = \prod_{i=1}^{m} \prod_j(G_i)$ $(j = 1, 2)$. So, it suffices to investigate $\prod_j$-index of connected graphs.

The **Arithmetic Mean** of $a_1, \cdots, a_n$ is

$$AM(a_1, \cdots, a_n) = \frac{a_1 + \cdots + a_n}{n}$$

and the **Geometric Mean** of $a_1, \cdots, a_n$ is

$$GM(a_1, \cdots, a_n) = \sqrt[n]{a_1 \cdots a_n}.$$

Regarding these two means, we have the following well-known inequality.

Lemma 2.1 *(Arithmetic–Geometric Mean Inequality) Let $a_1, \cdots, a_n$ be positive numbers. Then*

$$AM(a_1, \cdots, a_n) \geq GM(a_1, \cdots, a_n)$$

with equality if and only if all $a_i^{'}s$ are equal.

In the following, we shall present some upper bounds for π_1-index of connected graphs.

Theorem 2.1 *Let G be a nontrivial connected graph of order n and size m. Then*

$$\prod{}_1(G) \leq \left(\frac{2m}{n}\right)^{2n}$$

with equality if and only if G is a $\frac{2m}{n}$-regular graph.

Proof. For brevity, we label vertices of G as $v_1, \ldots, v_n$ and let $d_i = d_G(v_i)$. By the definition of π_1-index, Lemma 2.1 and the fact that $\sum_{i=1}^{n} d_i = 2m$,

$$\begin{aligned}
\prod{}_1(G) &= (d_1 d_2 \cdots d_n)^2 \\
&= [(2m - d_2 - \cdots - d_n) d_2 \cdots d_n]^2 \\
&\leq \left\{ \left[\frac{(2m - d_2 - \cdots - d_n) + d_2 + \cdots + d_n}{n} \right]^n \right\}^2 \\
&= \left[(\frac{2m}{n})^n \right]^2 = (\frac{2m}{n})^{2n}.
\end{aligned}$$

The above equality holds if and only if $2m - d_2 - \cdots - d_n = d_2 = \cdots = d_n$, that is, $d_2 = \cdots = d_n = \frac{2m}{n}$ and then $d_1 = 2m - (n-1) \cdot \frac{2m}{n} = \frac{2m}{n}$.

So, $\prod_1(G) \leq (\frac{2m}{n})^{2n}$ with equality if and only if G is a $\frac{2m}{n}$-regular graph, as claimed. ∎

A connected graph is called a unicyclic graph if it possesses equal number of vertices and edges. Note that C_n is the unique 2-regular graph ($\frac{2m}{n} = 2$) among all connected unicyclic graphs of order n. By Theorem 2.1, we immediately obtain the following result.

Corollary 2.1 ([28]) *Let G be a unicyclic graph of order n. Then*

$$\prod{}_1(G) \leq 4^n$$

with equality if and only if G is the n-vertex cycle C_n.

Corollary 2.2 *Let G be a connected bipartite graph of order $2n$. Then*

$$\prod{}_1(G) \leq n^{4n}$$

with equality if and only if G is the balanced bipartite graph $K_{n,n}$.

Proof. Let $m(G)$ denote the number of edges in G. By Theorem 2.1,

$$\prod{}_1(G) \leq (\frac{2m(G)}{2n})^{4n} = (\frac{m(G)}{n})^{4n}$$

with equality if and only if G is a connected $\frac{m(G)}{n}$-regular bipartite graph of order $2n$. Note that $m(G) \leq n^2$. Thus, $\prod_1(G) \leq (\frac{m(G)}{n})^{4n} \leq n^{4n}$ with equality if and only if G is a connected n-regular bipartite graph of order $2n$, that is, $G \cong K_{n,n}$. ∎

For a vertex u in a nontrivial connected graph G, we let $ecc_G(u) = \max\{d_G(u, v)|v \in V(G)\}$ denote the **eccentricity** of u. The **radius** $r(G)$ of G is defined as $r(G) = \min\{ecc_G(u)|u \in V(G)\}$.

The **Wiener index** of a connected graph G (see [22, 26, 27]), denoted by $W(G)$, is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} D_G(u) \tag{1}$$

and the **eccentric distance sum** of G (see [15–17]), denoted by $\xi^d(G)$, is defined as

$$\xi^d(G) = \sum_{u \in V(G)} ecc_G(u) D_G(u) \tag{2}$$

where $D_G(u)$ is the sum of distances between u and all other vertices in G.

Theorem 2.2 *Let G be a nontrivial connected graph of order n. Then*

$$\prod{}_1(G) \leq (\frac{2W(G)}{n})^{2n}$$

with equality if and only if G is the complete graph K_n.

Proof. As done in the previous theorem, we label vertices of G as $v_1, \ldots, v_n$ and let $d_i = d_G(v_i)$. Moreover, we write $D_i = D_G(v_i)$ and $ecc_i = ecc_G(v_i)$. It is obvious that

$$D_i = d_i + \sum_{v_j \in V(G)\setminus N_G[v_i]} d_G(v_i, v_j) \geq d_i \tag{3}$$

with equality if and only if $ecc_i = 1$, that is, $d_i = n-1$, for any $i = 1, \ldots, n$.

By the definition of π_1-index, Lemma 2.1, and the equations (1) and (3),

$$\begin{aligned}\prod{}_1(G) &= (d_1 d_2 \ldots d_n)^2 \\ &\leq (D_1 D_2 \ldots D_n)^2 \\ &= [(2W(G) - D_2 - \cdots - D_n)D_2 \cdots D_n]^2 \\ &\leq \left[(\frac{2W(G)}{n})^n\right]^2 = (\frac{2W(G)}{n})^{2n}.\end{aligned}$$

The above first equality holds if and only if $ecc_i = 1$, that is, $d_i = n-1$, for any $i = 1, \ldots, n$. The above second equality holds if and only if $2W(G) - D_2 - \cdots - D_n = D_2 = \cdots = D_n$, that is, $D_2 = \cdots = D_n = \frac{2W(G)}{n}$ and $D_1 = 2W(G) - (n-1) \cdot \frac{2W(G)}{n} = \frac{2W(G)}{n}$.

So, $\prod_1(G) \leq (\frac{2W(G)}{n})^{2n}$ with equality if and only if $d_1 = \cdots = d_n = n-1$ and $D_1 = \cdots = D_n$, i.e., G is the complete graph K_n. ∎

Corollary 2.3 *Let G be a nontrivial connected graph of order n. Then*

$$\prod{}_1(G) \leq (\frac{\xi^d(G)}{n})^{2n}$$

with equality if and only if G is the complete graph K_n.

Proof. As $ecc_G(u) \geq 1$ for any u in G, by the equations (1) and (2), we have $\xi^d(G) \geq 2W(G)$ with equality if and only if $ecc_G(u) = 1$ for each u, that is, $G \cong K_n$. According to Theorem 2.2, we have $\prod_1(G) \leq (\frac{\xi^d(G)}{n})^{2n}$ with equality if and only if G is the complete graph K_n. ∎

In the following, we shall give a sharp upper bound for $\prod_1$-index of connected graphs in terms of its order and radius.

We first summarize here a result of [17] as the following lemma.

Lemma 2.2 *Let G be a nontrivial connected graph of order n. For each vertex v in G, it holds*

$$ecc_G(v) \leq n - d_G(v). \tag{4}$$

Moreover, all equalities hold together if and only if $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$, where $K_n - iK_2$ denotes the graph obtained by removing i independent edges from G.

Theorem 2.3 *Let G be a nontrivial connected graph of order n. Then*

$$\prod{}_1(G) \leq (n - r(G))^{2n}$$

with equality if and only if $G \cong K_n$, or the graph obtained from K_n by removing a perfect matching.

Proof. As before, we label vertices of G as $v_1, \ldots, v_n$, and let $d_i = d_G(v_i)$ and $ecc_i = ecc_G(v_i)$.

By the definition of π_1-index and the equation (4),

$$\begin{aligned}\prod{}_1(G) &= (d_1 d_2 \ldots d_n)^2 \\ &\leq [(n - ecc_1)(n - ecc_2) \ldots (n - ecc_n)]^2 \\ &\leq [(n - r(G))^n]^2 = (n - r(G))^{2n}.\end{aligned}$$

By Lemma 2.2, the above first equality holds if and only if $d_i = n - ecc_i$ for each i, that is, $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor \frac{n}{2} \rfloor)$. The above second equality holds if and only if $r(G) = ecc_i$ for each i.

So, $\prod_1(G) \leq (n - r(G))^{2n}$ with equality if and only if $G \cong K_n$, or the graph obtained from K_n by removing a perfect matching. ∎

3 Bounds for $\prod_2$-index of connected graphs

In this section, we give some bounds for $\prod_2$-index of connected graphs in terms of other graph invariants including the first Zagreb index, the first Zagreb coindex and the degree distance.

Theorem 3.1 *Let G be a nontrivial connected graph of order n and size m. Then*

$$\prod{}_2(G) \leq \left(\frac{M_1(G)}{2m}\right)^{2m}$$

with equality if and only if G is a $\frac{2m}{n}$-regular graph.

Proof. For convenience, we label vertices of G as $v_1, \ldots, v_n$ and let $d_i = d_G(v_i)$. By the definition of π_2-index, Lemma 2.1 and the fact that $\sum_{i=1}^{n} d_i = 2m$,

$$\begin{aligned}
\prod{}_2(G) &= d_1^{d_1} d_2^{d_2} \cdots d_n^{d_n} \\
&\le \left[\frac{\underbrace{(d_1 + \cdots + d_1)}_{d_1 times} + \underbrace{(d_2 + \cdots + d_2)}_{d_2 times} + \cdots + \underbrace{(d_n + \cdots + d_n)}_{d_n times}}{2m} \right]^{2m} \\
&= \left(\frac{d_1^2 + d_2^2 + \cdots + d_n^2}{2m} \right)^{2m} \\
&= (\frac{M_1(G)}{2m})^{2m}.
\end{aligned}$$

The above equality holds if and only if $d_1 = d_2 = \cdots = d_n$, that is, G is a regular graph. So, $\prod_2(G) \le (\frac{M_1(G)}{2m})^{2m}$ with equality if and only if G is a $\frac{2m}{n}$-regular graph, as claimed. ∎

Let $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_u + d_v)$ denote the **first Zagreb coindex** (see [1, 2, 13]).

Lemma 3.1 **([1])** *Let G be a simple graph with n vertices and m edges. Then $\overline{M}_1(G) = 2m(n-1) - M_1(G)$.*

It then follows from Theorem 3.1 and Lemma 3.1 the following consequence.

Corollary 3.1 *Let G be a nontrivial connected graph of order n and size m. Then*

$$\prod{}_2(G) \le \left[\frac{2m(n-1) - \overline{M}_1(G)}{2m} \right]^{2m}$$

with equality if and only if G is a $\frac{2m}{n}$-regular graph.

The **degree distance** of a nontrivial connected graph G (see [18, 19, 31]), denoted by $D^{'}(G)$, is defined as

$$D^{'}(G) = \sum_{u \in V(G)} d_G(u) D_G(u)$$

where $D_G(u)$ is defined as before.

Theorem 3.2 *Let G be a nontrivial connected graph of order n and size m. Then*

$$\prod{}_2(G) \le (\frac{D^{'}(G)}{2m})^{2m}$$

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

Proof. For convenience, we label vertices of G as $v_1, \ldots, v_n$ and let $d_i = d_G(v_i)$. By the definition of $\prod_2$-index, Lemma 2.1, the equation (3) and the fact that $\sum_{i=1}^{n} d_i = 2m$,

$$\begin{aligned}
\prod{}_2(G) &= d_1^{d_1} d_2^{d_2} \cdots d_n^{d_n} \\
&\leq D_1^{d_1} D_2^{d_2} \cdots D_n^{d_n} \\
&\leq \left[\frac{(\underbrace{D_1 + \cdots + D_1}_{d_1 times}) + (\underbrace{D_2 + \cdots + D_2}_{d_2 times}) + \cdots + (\underbrace{D_n + \cdots + D_n}_{d_n times})}{2m} \right]^{2m} \\
&= \left(\frac{d_1 D_1 + d_2 D_2 + \cdots + d_n D_n}{2m} \right)^{2m} \\
&= (\frac{D'(G)}{2m})^{2m}.
\end{aligned}$$

The above first equality holds if and only if $d_i = D_i$ for each i, that is, $d_i = n-1$ for each i. The above second equality holds if and only if $D_1 = D_2 = \cdots = D_n$. So, $\prod_2(G) \leq (\frac{D'(G)}{2m})^{2m}$ with equality if and only if $G \cong K_n$, as claimed. ∎

4 Concluding remarks

In this paper, we have established sharp upper bounds for $\prod_1$-index in terms of graph parameters including the order, size, radius, Wiener index and eccentric distance sum, and upper bounds for $\prod_2$-index in terms of graph parameters including the order, size, the first Zagreb index, the first Zagreb coindex and degree distance. It may be interesting to give the bounds for $\prod_1$-index and $\prod_2$-index in terms of other graph invariants.

Acknowledgment: The authors are grateful to the referee and the editors for helpful suggestions which improved considerably the presentation of this paper.

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