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COMPARING THE SECOND MULTIPLICATIVE ZAGREB COINDEX WITH SOME GRAPH INVARIANTS

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ABSTRACT. The second multiplicative Zagreb coindex of a simple graph G is defined as:

$$\bar{\Pi}_2(G) = \prod_{uv \notin E(G)} d_G(u) d_G(v),$$

where $d_G(u)$ denotes the degree of the vertex u of G . In this paper, we compare $\bar{\Pi}_2$ -index with some well-known graph invariants such as the Wiener index, Schultz index, eccentric connectivity index, total eccentricity, eccentric-distance sum, the first Zagreb index and coindex and the first multiplicative Zagreb index and coindex.

1. Introduction

Throughout the paper, we consider connected finite graphs without any loops or multiple edges. Let G be such a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $u \in V(G)$, we denote by $N_G(u)$ the set of all first neighbors of u in G . The cardinality of $N_G(u)$ is called the *degree of u* in G and denoted by $d_G(u)$. We denote by $\delta(G)$ and $\Delta(G)$, the minimum and maximum degree of G , respectively. For vertices $u, v \in V(G)$, the *distance* $d_G(u, v)$ is defined as the length of any shortest path in G connecting u and v and $D_G(u)$ denotes the sum of distances between u and all other vertices of G . The *eccentricity* $\varepsilon_G(u)$ is the largest distance between u and any other vertex of G . The minimum eccentricity of any vertex of G is called *radius* of G and denoted by $r(G)$. A *topological index* $Top(G)$ of G is a real number with the property that for every graph H isomorphic to G , $Top(H) = Top(G)$. In organic chemistry, topological indices have been found to

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be useful in chemical documentation, isomer discrimination, structure-property relationships (SPR), structure-activity relationships (SAR) and pharmaceutical drug design [14].

The *Wiener index* is the first reported distance-based topological index introduced in 1947 by Wiener [23, 24], who used it for modeling the shape of organic molecules and for calculating several of their physico-chemical properties. The Wiener index $W(G)$ of G is defined as the sum of distances between all pairs of vertices of G :

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

The *molecular topological index* or *Schultz index* was introduced by Harry Schultz in 1989. Schultz index $S(G)$ of a graph G is defined as [20]:

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} [d_G(u) + d_G(v)]d_G(u,v) = \sum_{u \in V(G)} d_G(u)D_G(u).$$

The *eccentric connectivity index* was introduced by Sharma et al. in 1997 [21]. The eccentric connectivity index $\xi^c(G)$ of a graph G is defined as:

$$\xi^c(G) = \sum_{u \in V(G)} d_G(u)\varepsilon_G(u) = \sum_{uv \in E(G)} [\varepsilon_G(u) + \varepsilon_G(v)].$$

The *total eccentricity* $\xi(G)$ of G [7] is defined as the sum of eccentricities of all vertices of G :

$$\xi(G) = \sum_{u \in V(G)} \varepsilon_G(u).$$

In 2002, Gupta et al. introduced another eccentricity-based invariant called the *eccentric-distance sum* (EDS) [12]. The eccentric-distance sum $\xi^d(G)$ of G is defined as:

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V(G)} [\varepsilon_G(u) + \varepsilon_G(v)]d_G(u,v) = \sum_{u \in V(G)} \varepsilon_G(u)D_G(u).$$

For more information on the vertex-eccentricity-based invariants see [1, 5, 16].

The *Zagreb indices* are among the oldest topological indices, and were introduced as early as in 1972 [15]. These indices have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. For details on their theory and applications see [4, 17, 18, 27]. The first and second Zagreb indices of G are denoted by $M_1(G)$ and $M_2(G)$, respectively, and defined as:

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

The first Zagreb index can also be expressed as a sum over edges of G :

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

As the sums involved run over the edges of the complement of G , such quantities are called *Zagreb coindices* [2]. More formally, the first and second Zagreb coindices of G are denoted by $\overline{M}_1(G)$ and

$\overline{M}_2(G)$, respectively, and defined as:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v).$$

The multiplicative versions of Zagreb indices were introduced by Todeschini et al. in 2010 [22]. The first and second *multiplicative Zagreb indices* of G are denoted by $\Pi_1(G)$ and $\Pi_2(G)$, respectively, and defined as:

$$\Pi_1(G) = \prod_{u \in V(G)} d_G(u)^2 \quad \text{and} \quad \Pi_2(G) = \prod_{uv \in E(G)} d_G(u)d_G(v).$$

The second multiplicative Zagreb index can also be expressed as a product over vertices of G [13]:

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

In 2012, Eliasi et al. introduced another multiplicative version of the first Zagreb index called *multiplicative sum Zagreb index* [9]. The multiplicative sum Zagreb index $\Pi_1^*(G)$ of G is defined as:

$$\Pi_1^*(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(v)].$$

We refer the reader to [3, 6, 8, 10, 11, 19, 26] for mathematical properties and applications of the multiplicative Zagreb indices and multiplicative sum Zagreb index.

Recently, Xu et al. introduced the multiplicative versions of Zagreb coindices [25]. The first and second *multiplicative Zagreb coindices* of G are denoted by $\overline{\Pi}_1(G)$ and $\overline{\Pi}_2(G)$, respectively, and defined as:

$$\overline{\Pi}_1(G) = \prod_{uv \notin E(G)} [d_G(u) + d_G(v)] \quad \text{and} \quad \overline{\Pi}_2(G) = \prod_{uv \notin E(G)} d_G(u)d_G(v).$$

The second multiplicative Zagreb coindex $\overline{\Pi}_2(G)$ of n vertex graph G can also be expressed as [25]:

$$\overline{\Pi}_2(G) = \prod_{u \in V(G)} d_G(u)^{n-1-d_G(u)}.$$

In this paper, we compare $\overline{\Pi}_2$ -index with some well-known graph invariants.

2. Preliminaries

In this section, we list some results as preliminaries. We begin by recalling the Arithmetic-Geometric Mean inequality.

Lemma 2.1. *Let x_1, x_2, \dots, x_n be nonnegative numbers. Then*

$$\frac{x_1 + x_2 + \dots + x_n}{n} \geq \sqrt[n]{x_1 x_2 \cdots x_n},$$

with equality if and only if $x_1 = x_2 = \dots = x_n$.

Theorem 2.2. [2] *Let G be a graph of order n and size m . Then*

$$\overline{M}_1(G) = 2m(n - 1) - M_1(G).$$

Theorem 2.3. [16] Let G be a nontrivial connected graph of order n . For each vertex $u \in V(G)$, $\varepsilon_G(u) \leq n - d_G(u)$, with equality if and only if $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$, where $K_n - iK_2$ denotes the graph obtained from the complete graph K_n by removing i independent edges.

Lemma 2.4. Let G be a nontrivial connected graph of order n . For each vertex $u \in V(G)$, $D_G(u) \geq d_G(u)$, with equality if and only if $\varepsilon_G(u) = 1$.

Proof. By definition of $D_G(u)$,

$$D_G(u) = d_G(u) + \sum_{v \in V(G) \setminus N_G(u)} d_G(u, v) \geq d_G(u).$$

The above equality holds if and only if $d_G(u, v) = 0$, for every $v \in V(G) \setminus N_G(u)$. That is $d_G(u) = n - 1$ or equivalently $\varepsilon_G(u) = 1$. \square

Lemma 2.5. Let G be a nontrivial connected graph of order n . For each vertex $u \in V(G)$, $D_G(u) \leq (n - 1)\varepsilon_G(u)$, with equality if and only if $\varepsilon_G(u) = 1$.

Proof. By definition of $D_G(u)$,

$$D_G(u) = \sum_{v \in V(G) \setminus \{u\}} d_G(u, v) \leq \sum_{v \in V(G) \setminus \{u\}} \varepsilon_G(u) = (n - 1)\varepsilon_G(u).$$

The above equality holds if and only if $d_G(u, v) = \varepsilon_G(u)$, for every $v \in V(G) \setminus \{u\}$. That is $\varepsilon_G(u) = 1$. \square

As two direct consequences of Lemma 2.5, we obtain the following Corollaries.

Corollary 2.6. Let G be a nontrivial connected graph of order n . Then

$$2W(G) \leq (n - 1)\xi(G),$$

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

Corollary 2.7. Let G be a nontrivial connected graph of order n . Then

$$S(G) \leq (n - 1)\xi^c(G),$$

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

Theorem 2.8. Let G be a nontrivial connected graph of order n . Then

$$2W(G) \leq \xi^d(G),$$

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

Proof. Using the fact that $\varepsilon_G(u) \geq 1$ for each vertex $u \in V(G)$, we can easily get the desired result. \square

3. Results and Discussion

In this section, we present several sharp lower bounds on $\bar{\Pi}_2$ -index in terms of some graph parameters such as the order, size, radius, minimum and maximum degree and some graph invariants such as the Wiener index, Schultz index, eccentric connectivity index, total eccentricity, eccentric-distance sum, the first Zagreb index and coindex and the first multiplicative Zagreb index and coindex.

Throughout this section, let G be a nontrivial connected graph of order n and size m . For convenience, we label the vertices of G as v_1, v_2, \dots, v_n and let $d_i = d_G(v_i)$, $D_i = D_G(v_i)$ and $\varepsilon_i = \varepsilon_G(v_i)$, for $i = 1, 2, \dots, n$. Remind that if G is regular, then by using the fact that $\sum_{i=1}^n d_i = 2m$, we have $nd_i = 2m$, for $i = 1, 2, \dots, n$. So $d_1 = d_2 = \dots = d_n = \frac{2m}{n}$ and G is a $\frac{2m}{n}$ -regular graph.

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

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n-1-\Delta}{2}}.$$

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

Proof. Using the definition of $\bar{\Pi}_2$ -index, we obtain:

$$\bar{\Pi}_2 = \prod_{i=1}^n d_i^{n-1-d_i} \geq \prod_{i=1}^n d_i^{n-1-\Delta} = \left(\prod_{i=1}^n d_i\right)^{n-1-\Delta} = \Pi_1(G)^{\frac{n-1-\Delta}{2}}.$$

The equality holds if and only if $d_1 = d_2 = \dots = d_n = \Delta$. So $\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n-1-\Delta}{2}}$, with equality if and only if G is a $\frac{2m}{n}$ -regular graph. □

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

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{r(G)-1}{2}},$$

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

Proof. Using the definition of $\bar{\Pi}_2$ -index and Theorem 2.3,

$$\begin{aligned} \bar{\Pi}_2(G) &= \prod_{i=1}^n d_i^{n-1-d_i} \\ &= \prod_{i=1}^n d_i^{(n-d_i)-1} \\ &\geq \prod_{i=1}^n d_i^{\varepsilon_i-1} \\ &\geq \prod_{i=1}^n d_i^{r(G)-1} \\ &= \left(\prod_{i=1}^n d_i\right)^{r(G)-1} = \Pi_1(G)^{\frac{r(G)-1}{2}}. \end{aligned}$$

The above first equality holds if and only if $d_i = n - \varepsilon_i$, for $i = 1, 2, \dots, n$. This by Theorem 2.3 implies that $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$ and the above second equality holds if and only if

$r(G) = \varepsilon_i$, for $i = 1, 2, \dots, n$. So $\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{r(G)-1}{2}}$, with equality if and only if $G \cong K_n$ or the graph obtained from K_n by removing a perfect matching. \square

Theorem 3.3. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \left(\frac{\delta}{2\Delta}\right)^{n(n-1)-2m} \bar{\Pi}_1(G)^2,$$

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

Proof. By definitions of $\bar{\Pi}_1$ -index and $\bar{\Pi}_2$ -index, we have:

$$\frac{\bar{\Pi}_2(G)}{\bar{\Pi}_1(G)^2} = \prod_{v_i v_j \notin E(G)} \frac{d_i d_j}{(d_i + d_j)^2} \geq \prod_{v_i v_j \notin E(G)} \frac{\delta^2}{4\Delta^2} = \left(\frac{\delta^2}{4\Delta^2}\right)^{\binom{n}{2}-m} = \left(\frac{\delta}{2\Delta}\right)^{n(n-1)-2m}.$$

The above equality holds if and only if for any two nonadjacent vertices v_i and v_j of G , $d_i = d_j = \delta = \Delta$. So G is a $\frac{2m}{n}$ -regular graph. \square

Theorem 3.4. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2m+M_1(G)} \right]^{n+2m},$$

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

Proof. By definition of $\bar{\Pi}_2$ -index and Lemma 2.1, we have:

$$\begin{aligned} \bar{\Pi}_2(G) &= \prod_{i=1}^n d_i^{n-1-d_i} \\ &= \frac{\prod_{i=1}^n d_i^n}{\prod_{i=1}^n d_i^{1+d_i}} \\ &= \frac{\Pi_1(G)^{\frac{n}{2}}}{\prod_{i=1}^n d_i^{1+d_i}} \\ &\geq \frac{\Pi_1(G)^{\frac{n}{2}}}{\left[\frac{\sum_{i=1}^n d_i(1+d_i)}{\sum_{i=1}^n (1+d_i)} \right]^{\sum_{i=1}^n (1+d_i)}} \\ &= \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2m+M_1(G)} \right]^{n+2m}. \end{aligned}$$

The equality holds if and only if $d_1 = d_2 = \dots = d_n$. So G is a $\frac{2m}{n}$ -regular graph. \square

Using Theorem 3.4 and Theorem 2.2, we easily arrive at:

Corollary 3.5. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2mn - \bar{M}_1(G)} \right]^{n+2m},$$

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

Theorem 3.6. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \delta^{\xi(G)-n},$$

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

Proof. Using the definition of $\bar{\Pi}_2$ -index and Theorem 2.3,

$$\begin{aligned} \bar{\Pi}_2(G) &= \prod_{i=1}^n d_i^{n-1-d_i} \\ &\geq \prod_{i=1}^n \delta^{n-1-d_i} \\ &= \prod_{i=1}^n \delta^{(n-d_i)-1} \\ &\geq \prod_{i=1}^n \delta^{\varepsilon_i-1} \\ &= \delta^{\sum_{i=1}^n (\varepsilon_i-1)} = \delta^{\xi(G)-n}. \end{aligned}$$

The above first equality holds if and only if $d_1 = d_2 = \dots = d_n = \delta$, which implies that G is a $\frac{2m}{n}$ -regular graph. The above second equality holds if and only if $d_i = n - \varepsilon_i$, for $i = 1, 2, \dots, n$, which by Theorem 2.3 implies that $G \cong P_4$ or $G \cong K_n - iK_2$, $0 \leq i \leq \lfloor \frac{n}{2} \rfloor$. So $\bar{\Pi}_2(G) \geq \delta^{\xi(G)-n}$, with equality if and only if $G \cong K_n$ or the graph obtained from K_n by removing a perfect matching. \square

Corollary 3.7. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \delta^{n(r(G)-1)},$$

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

Proof. It is easy to see that $\xi(G) \geq nr(G)$, with equality if and only if $r(G) = \varepsilon_i$, for $i = 1, 2, \dots, n$. Now by Theorem 3.6, we can get the desired result. \square

Using Theorem 3.6 and Corollary 2.6, we easily arrive at:

Corollary 3.8. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \delta^{\frac{2W(G)}{n-1}-n},$$

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

Theorem 3.9. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2W(G)+S(G)} \right]^{n+2m},$$

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

Proof. By definition of $\bar{\Pi}_2$ -index, Lemma 2.1 and Lemma 2.4, we have:

$$\begin{aligned} \bar{\Pi}_2(G) &= \prod_{i=1}^n d_i^{n-1-d_i} \\ &= \frac{\prod_{i=1}^n d_i^n}{\prod_{i=1}^n d_i^{1+d_i}} \\ &= \frac{\Pi_1(G)^{\frac{n}{2}}}{\prod_{i=1}^n d_i^{1+d_i}} \\ &\geq \frac{\Pi_1(G)^{\frac{n}{2}}}{\prod_{i=1}^n D_i^{1+d_i}} \\ &\geq \frac{\Pi_1(G)^{\frac{n}{2}}}{\left[\frac{\sum_{i=1}^n D_i(1+d_i)}{\sum_{i=1}^n (1+d_i)} \right]^{\sum_{i=1}^n (1+d_i)}} \\ &= \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2W(G)+S(G)} \right]^{n+2m}. \end{aligned}$$

The above first equality holds if and only if $d_i = D_i$, for $i = 1, 2, \dots, n$, which by Lemma 2.4 implies that $\varepsilon_i = 1$, for $i = 1, 2, \dots, n$. So $G \cong K_n$. By Lemma 2.1, the above second equality holds if and only if $D_1 = D_2 = \dots = D_n$. So $\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{2W(G)+S(G)} \right]^{n+2m}$, with equality if and only if $G \cong K_n$. \square

Corollary 3.10. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{(n-1)(\xi(G) + \xi^c(G))} \right]^{n+2m},$$

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

Proof. Using Corollaries 2.6 and 2.7, we obtain:

$$2W(G) + S(G) \leq (n-1)(\xi(G) + \xi^c(G)),$$

with equality if and only if $G \cong K_n$. Now by Theorem 3.9, the result is obvious. \square

Corollary 3.11. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{n+2m}{\xi^d(G) + (n-1)\xi^c(G)} \right]^{n+2m},$$

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

Proof. Using Theorem 2.8 and Corollary 2.7, we have:

$$2W(G) + S(G) \leq \xi^d(G) + (n-1)\xi^c(G),$$

with equality if and only if $G \cong K_n$. Now by Theorem 3.9, the result is obvious. \square

Theorem 3.12. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{2W(G) + n}{S(G) + 2m} \right]^{2W(G)+n},$$

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

Proof. By Lemma 2.1 and Lemma 2.4, we have:

$$\begin{aligned} \bar{\Pi}_2(G) &= \prod_{i=1}^n d_i^{n-1-d_i} \\ &= \frac{\prod_{i=1}^n d_i^n}{\prod_{i=1}^n d_i^{1+d_i}} \\ &= \frac{\Pi_1(G)^{\frac{n}{2}}}{\prod_{i=1}^n d_i^{1+d_i}} \\ &\geq \frac{\Pi_1(G)^{\frac{n}{2}}}{\prod_{i=1}^n d_i^{1+D_i}} \\ &\geq \frac{\Pi_1(G)^{\frac{n}{2}}}{\left[\frac{\sum_{i=1}^n (1+D_i)d_i}{\sum_{i=1}^n (1+D_i)} \right]^{\sum_{i=1}^n (1+D_i)}} \\ &= \Pi_1(G)^{\frac{n}{2}} \left[\frac{2W(G) + n}{S(G) + 2m} \right]^{2W(G)+n}. \end{aligned}$$

The above first equality holds if and only if $d_i = D_i$, for $i = 1, 2, \dots, n$, which by Lemma 2.4 implies that $\varepsilon_i = 1$, for $i = 1, 2, \dots, n$. So $G \cong K_n$. By Lemma 2.1, the above second equality holds if and only if $d_1 = d_2 = \dots = d_n$, which implies that G is a regular graph. So $\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{2W(G)+n}{S(G)+2m} \right]^{2W(G)+n}$, with equality if and only if $G \cong K_n$. \square

Using Theorem 3.12 and Corollary 2.7, we easily arrive at:

Corollary 3.13. *Let G be a nontrivial connected graph of order n and size m . Then*

$$\bar{\Pi}_2(G) \geq \Pi_1(G)^{\frac{n}{2}} \left[\frac{2W(G) + n}{(n-1)\xi^c(G) + 2m} \right]^{2W(G)+n},$$

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

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