

ON THE MULTIPLICATIVE ZAGREB COINDEX OF GRAPHS

Kexiang Xu, Kinkar Ch. Das, and Kechao Tang

Communicated by Dalibor Fronček

Abstract. For a (molecular) graph G with vertex set $V(G)$ and edge set $E(G)$, the first and second Zagreb indices of G are defined as $M_1(G) = \sum_{v \in V(G)} d_G(v)^2$ and $M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v)$, respectively, where $d_G(v)$ is the degree of vertex v in G . The alternative expression of $M_1(G)$ is $\sum_{uv \in E(G)} (d_G(u) + d_G(v))$. Recently Ashrafi, Došlić and Hamzeh introduced two related graphical invariants $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v))$ and $\overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u)d_G(v)$ named as first Zagreb coindex and second Zagreb coindex, respectively. Here we define two new graphical invariants $\overline{\Pi}_1(G) = \prod_{uv \notin E(G)} (d_G(u) + d_G(v))$ and $\overline{\Pi}_2(G) = \prod_{uv \notin E(G)} d_G(u)d_G(v)$ as the respective multiplicative versions of \overline{M}_i for $i = 1, 2$. In this paper, we have reported some properties, especially upper and lower bounds, for these two graph invariants of connected (molecular) graphs. Moreover, some corresponding extremal graphs have been characterized with respect to these two indices.

Keywords: vertex degree, tree, upper or lower bound.

Mathematics Subject Classification: 05C05, 05C07, 05C35.

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 in G adjacent to v . For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E' . If $W = \{v\}$ and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v$ and $G - xy$ for short, respectively. For any two nonadjacent vertices x and y of graph G , let $G + xy$ be the graph obtained from G by adding an edge xy . 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. Two of the oldest graph invariants are the well-known Zagreb indices, first introduced in [14], where Gutman and Trinajstić examined the dependence of total π -electron energy on molecular structure, elaborated in [15]. 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:

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

These two classical topological indices (M_1 and M_2) reflect the extent of branching of the molecular carbon-atom skeleton [3, 21]. The first Zagreb index M_1 was also termed as the ‘‘Gutman index’’ by some scholars (see [21]). The main properties of M_1 and M_2 were summarized in [6, 7, 11, 17–19]. In particular, Deng [7] gave a unified approach to determine extremal values of Zagreb indices for trees, unicyclic graphs and bicyclic graphs, respectively. Other recent results on ordinary Zagreb indices can be found in [18, 24] and the references cited therein.

Alternatively the first Zagreb index can be rewritten as

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

Note that contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [8]). Recently, Ashrafi, Došlić and Hamzeh [1, 2] have defined, respectively, the first Zagreb coindex and the second Zagreb coindex as follows:

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

Nowadays several multiplicative versions of Zagreb indices are introduced ([9, 20, 22]) and extensively studied ([10, 26, 27]). In particular, Gutman [10] have determined the extremal tree with respect to multiplicative Zagreb indices, one of the present authors and Hua [27] have provided a unified approach to extremal trees, unicyclic and bicyclic graphs with respect to these multiplicative Zagreb indices. The two present authors [26] have characterized completely extremal trees, unicyclic and bicyclic graphs with respect to this multiplicative sum Zagreb index. Naturally in the following, as the multiplicative versions of Zagreb coindices, we can define the (first and second) multiplicative Zagreb coindices as follows:

$$\overline{\overline{M}}_1(G) = \prod_{uv \notin E(G)} (d_G(u) + d_G(v)), \quad \overline{\overline{M}}_2(G) = \prod_{uv \notin E(G)} d_G(u)d_G(v).$$

Let $\mathcal{T}(n)$ be the set of trees of order n . The paper is organized as follows. In Section 2, we list or prove some lemmas about multiplicative Zagreb coindices of

graphs. In Section 3, we have determined the extremal graphs from $\mathcal{T}(n)$ with respect to multiplicative Zagreb coindices ($\overline{\Pi}_1$ and $\overline{\Pi}_2$). In Section 4, some upper or lower bounds are presented on these two multiplicative Zagreb coindices. And in Section 5, some interesting but open problems are proposed on these two multiplicative Zagreb coindices.

2. PRELIMINARIES

In this section we will list or prove some lemmas as preliminaries, which play an important role in the subsequent proofs.

Lemma 2.1. *For a connected graph G , we have $\overline{\Pi}_2(G) = \prod_{v \in V(G)} d_G(v)^{n-1-d_G(v)}$.*

Proof. By definition, we find that, for each vertex $v \in V(G)$, the factor $d_G(v)$ occurs $n - 1 - d_G(v)$ times in $\overline{\Pi}_2(G)$. Thus this theorem follows immediately. \square

Note that the first and second multiplicative Zagreb indices ([9, 20, 22]) are defined as $\Pi_1(G) = \prod_{u \in V(G)} d_G(u)^2$ and $\Pi_2(G) = \prod_{uv \in E(G)} d_G(u)d_G(v)$, respectively.

Lemma 2.2 ([10]). *For a connected graph G , we have $\Pi_2(G) = \prod_{v \in V(G)} d_G(v)^{d_G(v)}$.*

From Lemmas 2.1 and 2.2 and the definitions of first and second multiplicative Zagreb indices, the following theorem can be easily obtained.

Theorem 2.3. *For a connected graph G , we have $\Pi_2(G)\overline{\Pi}_2(G) = (\Pi_1(G))^{\frac{n-1}{2}}$.*

Lemma 2.4 ([1]). *Let G be a connected graph of order n and with m edges. Then $\overline{M}_1(G) = 2m(n - 1) - M_1(G)$.*

Now we define a new graph invariant which is called the *total multiplicative sum Zagreb index* as follows:

$$\overline{\Pi}(G) = \prod_{u,v \in V(G)} (d_G(u) + d_G(v)).$$

Note that the multiplicative sum Zagreb index ([9, 26]) is defined as $\Pi_1^*(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v))$. From these two definitions ($\Pi_1^*(G)$ and $\overline{\Pi}(G)$), the following lemma is obvious.

Lemma 2.5. *For a connected graph G , we have $\Pi_1^*(G)\overline{\Pi}_1(G) = \overline{\Pi}(G)$.*

Now we consider two graph transformations which increase or decrease the total multiplicative sum Zagreb index of graphs.

Transformation A. Suppose that G is a nontrivial connected graph and v is a given vertex in G . Let G_1 be a graph obtained from G by attaching at v two paths $P : vu_1u_2 \dots u_k$ of length k and $Q : vw_1w_2 \dots w_l$ of length l . We further let $G_2 = G_1 - vw_1 + u_kw_1$. The above referred graphs have been illustrated in Fig. 1.

Lemma 2.6. Let G_1 and G_2 be two graphs as shown in Fig. 1. Then $\prod^T(G_2) > \prod^T(G_1)$.

Proof. Assume that $d_G(v) = x > 0$. Note that only the degrees of vertices v and u_k are changed during the process of Transformation A. Considering the definition of the total multiplicative sum Zagreb index and the fact that $x > 0$, we have

$$\frac{\prod^T(G_2)}{\prod^T(G_1)} = \prod_{y \neq v, u_k} \left[\frac{x + 1 + d(y)}{x + 2 + d(y)} \cdots \frac{2 + d(y)}{1 + d(y)} \right] > 1.$$

It implies that $\prod^T(G_2) > \prod^T(G_1)$, completing the proof of this lemma. □

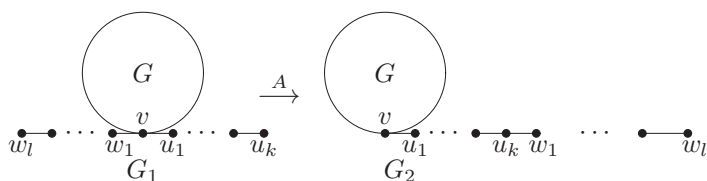


Fig. 1. Transformation A

Remark 2.7. It is easily seen that any tree T of size t attached to a graph G can be changed into a path P_{t+1} by repeating Transformation A. During this process, the total multiplicative sum Zagreb index \prod^T increases by Lemma 2.6.

Transformation B. Let uv be an edge of the connected graph G with $d_G(v) \geq 2$. Suppose that $\{v, w_1, w_2, \dots, w_t\}$ are all the neighbors of vertex u and w_1, w_2, \dots, w_t are pendent vertices. Let $G' = G - \{uw_1, uw_2, \dots, uw_t\} + \{vw_1, vw_2, \dots, vw_t\}$, as shown in Fig. 2.

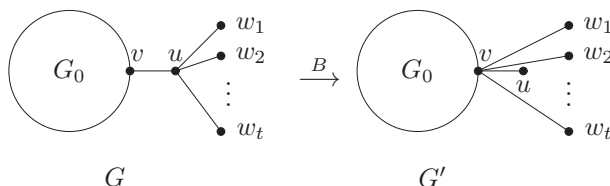


Fig. 2. Transformation B

Lemma 2.8. *Let G and G' be two graphs in Fig. 2. Then we have $\prod^T(G') < \prod^T(G)$.*

Proof. Let $G_0 = G - \{u, w_1, w_2, \dots, w_t\}$. Assume that $d_{G_0}(v) = x > 0$. Similarly to the proof of Lemma 2.6, we have

$$\frac{\prod^T(G)}{\prod^T(G')} = \prod_{y \neq v, u} \left[\frac{x + 1 + d(y)}{x + 1 + t + d(y)} \cdots \frac{t + 1 + d(y)}{1 + d(y)} \right] > 1,$$

finishing the proof of the lemma. □

Remark 2.9. Repeating Transformation B, any tree T of size t attached to a graph G can be changed into a star S_{t+1} . And the total multiplicative sum Zagreb index \prod^T decreases by Lemma 2.8.

3. EXTREMAL GRAPHS IN $\mathcal{T}(N)$ W.R.T. MULTIPLICATIVE ZAGREB COINDICES

In this section we consider the extremal graphs from $\mathcal{T}(n)$ with respect to multiplicative Zagreb coindices $\overline{\prod}_1$ and $\overline{\prod}_2$, respectively. The corresponding extremal graphs are completely characterized.

First we consider the extremal graph from $\mathcal{T}(n)$ with respect to first multiplicative Zagreb coindex $\overline{\prod}_1$. Before doing it, as a necessary tool, the extremal graph from $\mathcal{T}(n)$ is characterized in the following theorem with respect to the total multiplicative sum Zagreb index \prod^T .

Theorem 3.1. *For any graph $G \in \mathcal{T}(n) \setminus \{S_n, P_n\}$, we have $\prod^T(S_n) < \prod^T(G) < \prod^T(P_n)$.*

Proof. For any graph $G \in \mathcal{T}(n) \setminus \{P_n\}$, we can apply Transformation A to G repeatedly until it is changed into path P_n . By Lemma 2.6 and Remark 2.1, we have $\prod^T(G) < \prod^T(P_n)$.

From Lemma 2.8 and Remark 2.9, by a similar reasoning as above, we can obtain that $\prod^T(S_n) < \prod^T(G)$ for any graph $G \in \mathcal{T}(n) \setminus \{S_n\}$, completing the proof of this theorem. □

Lemma 3.2 ([26]). *Let G be a graph in $\mathcal{T}(n)$ different from S_n and P_n . Then we have $\prod_1^*(P_n) < \prod_1(G) < \prod_1^*(S_n)$.*

Theorem 3.3. *For any graph $G \in \mathcal{T}(n) \setminus \{S_n, P_n\}$, we have $\overline{\prod}_1(S_n) < \overline{\prod}_1(G) < \overline{\prod}_1(P_n)$.*

Proof. By Lemma 2.5, we have, for a connected graph G ,

$$\overline{\prod}_1(G) = \frac{\prod^T(G)}{\prod_1^*(G)}.$$

Thus we have

$$\frac{\min_G \prod^T(G)}{\max_G \prod_1^*(G)} \leq \overline{\prod}_1(G) \leq \frac{\max_G \prod^T(G)}{\min_G \prod_1^*(G)}.$$

From Theorem 3.1 and Lemma 3.2, we find that, for any graph from $\mathcal{T}(n)$, the maximal value of $\prod^T(G)$ and the minimal value of $\prod_1^*(G)$ are attained at P_n simultaneously, and the minimal value of $\prod^T(G)$ and the maximal value of $\prod_1^*(G)$ are attained at S_n simultaneously. So the result in this theorem follows immediately. \square

Now we consider the extremal graph from $\mathcal{T}(n)$ with respect to the second multiplicative Zagreb coindex $\overline{\prod}_2$.

Lemma 3.4 ([10, 27]). *Let T be a tree in $\mathcal{T}(n)$ with $n \geq 5$ different from S_n and P_n . Then:*

- (1) $\prod_1(S_n) < \prod_1(T) < \prod_1(P_n)$,
- (2) $\prod_2(P_n) < \prod_2(T) < \prod_2(S_n)$.

Theorem 3.5. *For any graph $G \in \mathcal{T}(n) \setminus \{S_n, P_n\}$, we have $\overline{\prod}_2(S_n) < \overline{\prod}_2(G) < \overline{\prod}_2(P_n)$.*

Proof. From Lemma 2.3, for a connected graph G , we have

$$\overline{\prod}_2(G) = \frac{(\prod_1(G))^{\frac{n-1}{2}}}{\prod_2(G)}.$$

Thus we have

$$\frac{(\min_G \prod_1(G))^{\frac{n-1}{2}}}{\max_G \prod_2(G)} \leq \overline{\prod}_2(G) \leq \frac{(\max_G \prod_1(G))^{\frac{n-1}{2}}}{\min_G \prod_2(G)}.$$

From Lemma 3.4, we find that the extremal graph from $\mathcal{T}(n)$ with minimal (or maximal) $\overline{\prod}_2$ is just the one with maximal (or minimal) \prod_1 . Therefore, this theorem follows immediately. \square

4. SOME BOUNDS ON MULTIPLICATIVE ZAGREB COINDICES

In this section we will present some upper and lower bounds on multiplicative Zagreb coindices ($\overline{\prod}_1$ and $\overline{\prod}_2$) of graphs.

Theorem 4.1. *For a connected graph G of order n and with m edges, we have*

$$\overline{\prod}_2(G) \leq \left(\frac{2(n-1)m - M_1(G)}{n(n-1) - 2m} \right)^{n(n-1)-2m}$$

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

Proof. Assume that $V(G) = \{v_1, v_2, \dots, v_n\}$ with $d_G(v_i) = d_i$ for $i = 1, 2, \dots, n$. Taking into account that the geometric mean of n positive integers is not greater than the arithmetic mean of them (AM-GM inequality), by the definition of M_1 and Lemma 2.1, we have

$$\begin{aligned} \overline{\Pi}_2(G) &= \prod_{i=1}^n d_i^{m-1-d_i} \leq \left(\frac{\sum_{i=1}^n (n-1-d_i)d_i}{(n-1)n - \sum_{i=1}^n d_i} \right)^{(n-1)n - \sum_{i=1}^n d_i} = \\ &= \left(\frac{2(n-1)m - M_1(G)}{n(n-1) - 2m} \right)^{n(n-1) - 2m} \end{aligned}$$

with equality holding if and only if $d_1 = d_2 = \dots = d_n$, i.e., G is $\frac{2m}{n}$ -regular. This completes the proof of this theorem. \square

Based on Lemma 2.4, the following corollary can be obtained easily.

Corollary 4.2. *For a connected graph G of order n and with m edges, we have*

$$\overline{\Pi}_2(G) \leq \left(\frac{\overline{M}_1(G)}{n(n-1) - 2m} \right)^{n(n-1) - 2m}$$

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

In graph theory, the well-known *Moore graph* is a r -regular graph with diameter k whose order attains the upper bound

$$1 + r \sum_{i=0}^{k-1} (r-1)^i.$$

Hoffman and Singleton ([16]) proved that every r -regular Moore graph G with diameter 2 must have $r \in \{2, 3, 7, 57\}$. They pointed out that $G \cong C_5$ if $r = 2$, G is just a Petersen graph for $r = 3$; G is called a Hoffman-Singleton graph for $r = 7$ and when $r = 57$ we do not know whether such a graph G exists or not.

Lemma 4.3 ([28]). *Let G be a connected graph of order n and with m edges and $n_2(v)$ be the number of vertices at a distance 2 to vertex $v \in V(G)$.*

- (1) *Then $M_1(G) \geq 2m + \sum_{v \in V(G)} n_2(v)$ with equality holding if and only if G is a triangle- and quadrangle-free graph.*
- (2) *If G is a triangle- and quadrangle-free graph with radius R . Then $M_2(G) \leq m(n+1-R)$ with equalities holding if and only if G is a Moore graph of diameter 2 or $G = C_6$.*

Corollary 4.4. *For a connected graph G of order n and with m edges, we have*

$$\overline{\Pi}_2(G) \leq \left(\frac{2(n-2)m - \sum_{v \in V(G)} n_2(v)}{n(n-1) - 2m} \right)^{n(n-1) - 2m}$$

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

Lemma 4.5. *Let G be a connected graph of order n and with m edges. Then*

$$\prod_2(G) \leq \left(\frac{M_2(G)}{m}\right)^m$$

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

Proof. In view of AM-GM inequality, we have

$$\prod_2(G) = \prod_{v_i v_j \in E(G)} d_i d_j \leq \left(\frac{\sum_{v_i v_j \in E(G)} d_i d_j}{m}\right)^m = \left(\frac{M_2(G)}{m}\right)^m$$

with equality holding if and only if $d_1 = d_2 = \dots = d_n$, i.e., G is $\frac{2m}{n}$ -regular. This completes the proof of this lemma. \square

Corollary 4.6. *Let G be a triangle- and quadrangle-free graph of order n and with m edges and radius R . Then we have*

$$\overline{\prod}_2(G) \geq \frac{(\prod_1(G))^{\frac{n-1}{2}}}{(n+1-R)^m}$$

with equality holding if and only if $G \cong C_6$ or G is one of the following four graphs: (i) C_5 , (ii) Petersen graph, (iii) Hoffman-Singleton graph, (iv) a possibly existing 57-regular graph of order 3250 and with diameter 2.

Proof. By Lemma 2.3 and Lemmas 4.3 and 4.5, we have

$$\overline{\prod}_2(G) = \frac{(\prod_1(G))^{\frac{n-1}{2}}}{\prod_2(G)} \geq \frac{(\prod_1(G))^{\frac{n-1}{2}}}{\left(\frac{M_2(G)}{m}\right)^m} \geq \frac{(\prod_1(G))^{\frac{n-1}{2}}}{(n+1-R)^m}$$

with equalities holding if and only if G is a Moore graph of diameter 2 or $G = C_6$. Thanks to the excellent results by Hoffman and Singleton ([16]), this corollary follows immediately. \square

Theorem 4.7. *For a connected graph G of order n and with m edges, we have*

$$\overline{\prod}_1(G) \geq 2^{\frac{n(n-1)}{2}-m} \overline{\prod}_2(G)^{\frac{1}{2}}$$

with equality holding if and only if G is a $(n-1, a)$ -biregular, or a $\frac{2m}{n}$ -regular graph.

Proof. By definition, we have

$$\begin{aligned} \overline{\prod}_1(G) &= \prod_{uv \notin E(G)} (d_G(u) + d_G(v)) \geq \\ &\geq \prod_{uv \notin E(G)} (2\sqrt{d_G(u)d_G(v)}) = 2^{\frac{n(n-1)}{2}-m} \overline{\prod}_2(G)^{\frac{1}{2}}. \end{aligned}$$

The above equality holds if and only if $d_G(u) = d_G(v)$ for any two nonadjacent vertices $u, v \in V(G)$. Now we only need to consider the following two cases:

Case 1. $\Delta(G) = n - 1$.

In this case, the vertices of degree $n - 1$ are not counted in the product of the first multiplicative Zagreb coindex. So we claim that the vertices adjacent to the vertices of degree $n - 1$ must have the same degree, which will be denoted by a . So G is a $(n - 1, a)$ -biregular graph. If the degrees of every vertices are all $n - 1$, then $G \cong K_n$ is obviously $\frac{2m}{n}$ -regular.

Case 2. $\Delta(G) < n - 1$.

In this case, all vertices are counted in the product of the first multiplicative Zagreb coindex. So we have $d_G(u) = d_G(v)$ for any two vertices u and v . It implies that G is $\frac{2m}{n}$ -regular.

Combining these two cases, this theorem follows immediately. □

Theorem 4.8. For a connected graph G of order n and with m edges, we have

$$\overline{\Pi}_1(G) \leq \left(\frac{4m(n - 1) - 2M_1(G)}{n(n - 1) - 2m} \right)^{\binom{n}{2} - m}$$

with equality holding if and only if G is a $(n - 1, a)$ -biregular, or a $\frac{2m}{n}$ -regular graph.

Proof. Again assume that $V(G) = \{v_1, v_2, \dots, v_n\}$ with $d_G(v_i) = d_i$ for $i = 1, 2, \dots, n$. By definition and the AM-GM inequality, we have

$$\begin{aligned} \overline{\Pi}_1(G) &= \prod_{uv \notin E(G)} (d_G(u) + d_G(v)) \leq \\ &\leq \left(\frac{\sum_{i=1}^n (n - 1 - d_i)d_i}{\binom{n}{2} - m} \right)^{\binom{n}{2} - m} = \left(\frac{4m(n - 1) - 2M_1(G)}{n(n - 1) - 2m} \right)^{\binom{n}{2} - m}. \end{aligned}$$

The above equality holds if and only if for any two nonadjacent vertices v_i and v_j , $d_i = d_j$. By a similar reasoning as that in the proof of Theorem 4.7, we find that G is a $(n - 1, a)$ -biregular, or a $\frac{2m}{n}$ -regular graph, which completes the proof of this theorem. □

Based on Lemma 2.4, the following corollary is easily obtained.

Corollary 4.9. For a connected graph G of order n and with m edges, we have

$$\overline{\Pi}_1(G) \leq \left(\frac{2\overline{M}_1(G)}{n(n - 1) - 2m} \right)^{\binom{n}{2} - m}$$

with equality holding if and only if G is a $(n - 1, a)$ -biregular, or a $\frac{2m}{n}$ -regular graph.

Next we will give the Multiplicative Nordhaus-Gaddum-type result for multiplicative Zagreb coindices $(\overline{\Pi}_1$ and $\overline{\Pi}_2)$, in which the (upper and lower) bounds on $\overline{\Pi}_i(G)\overline{\Pi}_i(\overline{G})$ are considered for $i = 1, 2$.

Theorem 4.10. For a connected graph G of order n and with m edges, we have:

- (1) $0 \leq \overline{\Pi}_1(G)\overline{\Pi}_1(\overline{G}) \leq \frac{\overline{M}_1(G)\binom{n}{2}}{m^m \left[\binom{n}{2}-m\right]\binom{n}{2}^{-m}}$ with the left equality if and only if G has at least two vertices of degree $n-1$, and the right equality if and only if G is $\frac{2m}{n}$ -regular.
- (2) $0 \leq \overline{\Pi}_2(G)\overline{\Pi}_2(\overline{G}) \leq \left(\frac{n-1}{2}\right)^{(n-1)n}$ with the left equality if and only if G has at least one vertex of degree $n-1$, and the right equality if and only if G is a regular self-complementary graph.

Proof. Let G be a connected graph with vertex set $\{v_1, v_2, \dots, v_n\}$ such that $d_G(v_i) = d_i$.

(1) For the definition of the first multiplicative Zagreb coindex ($\overline{\Pi}_1$), considering Lemma 2.4, we have

$$\begin{aligned} \overline{\Pi}_1(G)\overline{\Pi}_1(\overline{G}) &= \prod_{v_i v_j \notin E(G)} (d_i + d_j) \cdot \prod_{v_i v_j \in E(G)} (n-1-d_i + n-1-d_j) \leq \\ &\leq \left(\frac{\sum_{v_i v_j \notin E(G)} (d_i + d_j)}{\binom{n}{2} - m} \right)^{\binom{n}{2} - m} \cdot \left(\frac{\sum_{v_i v_j \in E(G)} [2n-2-(d_i + d_j)]}{m} \right)^m = \\ &= \left[\frac{\overline{M}_1(G)}{\binom{n}{2} - m} \right]^{\binom{n}{2} - m} \cdot \left[\frac{2(n-1)m - M_1(G)}{m} \right]^m = \\ &= \frac{\overline{M}_1(G)\binom{n}{2}}{m^m \left[\binom{n}{2}-m\right]\binom{n}{2}^{-m}} \end{aligned}$$

with equality holding if and only if $d_1 = d_2 = \dots = d_n$, i.e., G is $\frac{2m}{n}$ -regular, finishing the right part of (1).

For the left part, we can easily obtain $\overline{\Pi}_1(G)\overline{\Pi}_1(\overline{G}) \geq 0$ with equality holding if and only if G has at least two vertices of degree $n-1$. Thus the proof of (1) is complete.

(2) By Lemma 2.1, we have

$$\begin{aligned} \overline{\Pi}_2(G)\overline{\Pi}_2(\overline{G}) &= \prod_{i=1}^n d_i^{n-1-d_i} (n-1-d_i)^{d_i} \leq \left(\frac{\sum_{i=1}^n d_i^{n-1-d_i} (n-1-d_i)^{d_i}}{n} \right)^n \leq \\ &\leq \left[\frac{\sum_{i=1}^n \left(\frac{2(n-1-d_i)d_i}{n-1} \right)^{n-1}}{n} \right]^n \leq \left[\frac{\sum_{i=1}^n \left(\frac{\binom{n-1}{2}}{n-1} \right)^{n-1}}{n} \right]^n = \\ &= \left[\frac{n\left(\frac{n-1}{2}\right)^{n-1}}{n} \right]^n = \left(\frac{n-1}{2} \right)^{(n-1)n} \end{aligned}$$

with three equalities holding if and only if $d_1 = d_2 = \dots = d_n$ and $d_i = n - 1 - d_i$ for $i = 1, 2, \dots, n$, which implies that G is a regular self-complementary graph. Thus the proof of the right part is over.

For the left part, clearly, we have

$$\overline{\overline{\Pi}}_2(G)\overline{\overline{\Pi}}_2(\overline{G}) = \prod_{i=1}^n d_i^{n-1-d_i}(n-1-d_i)^{d_i} \geq 0. \tag{4.1}$$

The above equality holds if and only if there is at least one vertex v_i of degree $d_i = n - 1$. This completes the proof of this theorem. \square

5. SOME OPEN PROBLEMS

In this section we will propose some interesting but open problems on these two multiplicative Zagreb coindices ($\overline{\overline{\Pi}}_1$ and $\overline{\overline{\Pi}}_2$).

From the definitions of $\overline{\overline{\Pi}}_1$ and $\overline{\overline{\Pi}}_2$, obviously, we have $\overline{\overline{\Pi}}_1(K_n) = \overline{\overline{\Pi}}_1(\overline{K}_n) = 0 = \overline{\overline{\Pi}}_2(\overline{K}_n) = \overline{\overline{\Pi}}_2(K_n)$ where \overline{K}_n is the complement of K_n . Therefore, K_n is the unique graph with minimal multiplicative Zagreb coindex ($\overline{\overline{\Pi}}_1$ or $\overline{\overline{\Pi}}_2$) among all connected graphs of order n .

Remark 5.1. For a connected graph G with two nonadjacent vertices $u, v \in V(G)$, we DO NOT always have $\overline{\overline{\Pi}}_i(G) < \overline{\overline{\Pi}}_i(G + uv)$ for $i = 1, 2$.

For example, by choosing $G = S_4$ with v_1, v_2 as its two pendent vertices, we have $\overline{\overline{\Pi}}_1(S_4 + v_1v_2) = 9 > 8 = \overline{\overline{\Pi}}_1(S_4)$ and $\overline{\overline{\Pi}}_2(S_4 + v_1v_2) = 4 > 1 = \overline{\overline{\Pi}}_2(S_4)$. But if $G = P_4$ with u_1, u_2 as its two pendent vertices, we have $\overline{\overline{\Pi}}_1(P_4 + u_1u_2) = 16 < 18 = \overline{\overline{\Pi}}_1(P_4)$; while $G = C_4$ with w_1, w_2 as its two nonadjacent vertices, we have $\overline{\overline{\Pi}}_2(C_4 + w_1w_2) = 4 < 16 = \overline{\overline{\Pi}}_2(C_4)$. So we have the following problem:

Problem 5.2. Which graph has the largest multiplicative Zagreb coindex $\overline{\overline{\Pi}}_i$ for $i = 1, 2$ among all connected graphs of order n ?

Now we start to reconsider the lower bound on the Multiplicative Nordhaus-Gaddum-type result for multiplicative Zagreb coindices ($\overline{\overline{\Pi}}_1$ and $\overline{\overline{\Pi}}_2$), which is presented in Theorem 4.10. If we add one more condition that \overline{G} , i.e., the complement of G , is also connected, it seems to be a bit difficult to find the corresponding extremal graph.

Problem 5.3. Which graph makes $\overline{\overline{\Pi}}_1(G)\overline{\overline{\Pi}}_1(\overline{G})$ achieve its minimal value for $i = 1, 2$ among all connected graphs of order n with their complements being also connected?

Let $\mathcal{X}^k(n)$ be the set of connected graphs of order n and with chromatic number k such that $2 \leq k < n$. The following problem seems to be more difficult to us even in the case when $k = 2$.

Problem 5.4. Which graph from $\mathcal{X}^k(n)$ with $2 \leq k < n$ has the maximal first multiplicative Zagreb coindex ($\overline{\Pi}_1$ or $\overline{\Pi}_2$)?

Acknowledgments

The authors are grateful to two anonymous referees for some valuable comments and corrections, which have considerably improved the presentation of this paper.

The first author is supported by NUAA Research Funding, No. NN2012080.

The second author is supported by BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea.

REFERENCES

- [1] A.R. Ashrafi, T. Došlić, A. Hamzeh, *The Zagreb coindices of graph operations*, Discrete Appl. Math. **158** (2010), 1571–1578.
- [2] A.R. Ashrafi, T. Došlić, A. Hamzeh, *Extremal graphs with respect to the Zagreb coindices*, MATCH Commun. Math. Comput. Chem. **65** (2011), 85–92.
- [3] A.T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, *Topological indices for structure-activity corrections*, Topics Curr. Chem. **114** (1983), 21–55.
- [4] J.A. Bondy, U.S.R. Murty, *Graph Theory with Applications*, Macmillan Press, New York, 1976.
- [5] K.C. Das, I. Gutman, B. Zhou, *New upper bounds on Zagreb indices*, J. Math. Chem. **46** (2009), 514–521.
- [6] K.C. Das, I. Gutman, *Some properties of the second Zagreb index*, MATCH Commun. Math. Comput. Chem. **52** (2004), 103–112.
- [7] H. Deng, *A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs*, MATCH Commun. Math. Comput. Chem. **57** (2007), 597–616.
- [8] T. Došlić, *Vertex-weighted Wiener polynomials for composite graphs*, Ars Math. Contemp. **1** (2008), 66–80.
- [9] M. Eliasi, A. Iranmanesh, I. Gutman, *Multiplicative versions of first Zagreb index*, MATCH Commun. Math. Comput. Chem. **68** (2012), 217–230.
- [10] I. Gutman, *Multiplicative Zagreb indices of trees*, Bulletin of Society of Mathematicians Banja Luka **18** (2011), 17–23.
- [11] I. Gutman, K.C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), 83–92.
- [12] I. Gutman, M. Ghorbani, *Some properties of the Narumi-Katayama index*, Appl. Math. Lett. **25** (2012), 1435–1438.
- [13] I. Gutman, O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [14] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. III. Total π -electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535–538.

- [15] I. Gutman, B. Ruščić, N. Trinajstić, C.F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), 3399–3405.
- [16] A.J. Hoffman, R.R. Singleton, *On Moore graphs with diameters 2 and 3*, IBM J. Res. Develop. **4** (1960), 497–504.
- [17] A. Ilić, D. Stevanović, *On comparing Zagreb indices*, MATCH Commun. Math. Comput. Chem. **62** (2009), 681–687.
- [18] B. Liu, Z. You, *A survey on comparing Zagreb indices*, MATCH Commun. Math. Comput. Chem. **65** (2011), 581–593.
- [19] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003) 113–124.
- [20] R. Todeschini, D. Ballabio, V. Consonni, *Novel molecular descriptors based on functions of new vertex degrees* [in:] Novel molecular structure descriptors – Theory and applications I, I. Gutman, B. Furtula, (eds.), pp. 73–100. Univ. Kragujevac, Kragujevac, 2010.
- [21] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [22] R. Todeschini, V. Consonni, *New local vertex invariants and molecular descriptors based on functions of the vertex degrees*, MATCH Commun. Math. Comput. Chem. **64** (2010), 359–372.
- [23] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, 1992.
- [24] K. Xu, *The Zagreb indices of graphs with a given clique number*, Appl. Math. Lett. **24** (2011), 1026–1030.
- [25] K. Xu, I. Gutman, *The largest Hosoya index of bicyclic graphs with given maximum degree*, MATCH Commun. Math. Comput. Chem. **66** (2011), 795–824.
- [26] K. Xu, K.C. Das, *Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index*, MATCH Commun. Math. Comput. Chem. **68** (2012), 257–272.
- [27] K. Xu, H. Hua, *A unified approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs*, MATCH Commun. Math. Comput. Chem. **68** (2012), 241–256.
- [28] S. Yamaguchi, *Estimating the Zagreb indices and the spectral radius of triangle- and quadrangle-free connected graphs*, Chem. Phys. Lett. **458** (2008), 396–398.

Kexiang Xu
kexxu1221@126.com

Nanjing University of Aeronautics and Astronautics
College of Science
Nanjing, Jiangsu 210016, PR China

Kinkar Ch. Das
kinkardas2003@googlemail.com

Sungyunkwan University
Department of Mathematics
Suwon 440-746, Republic of Korea

Kechao Tang

Nanjing University of Aeronautics and Astronautics
College of Science
Nanjing, Jiangsu 210016, PR China

Received: March 29, 2012.

Revised: June 8, 2012.

Accepted: June 11, 2012.