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A Unified Approach to Extremal Multiplicative Zagreb Indices for Trees, Unicyclic and Bicyclic Graphs^{*}

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Abstract

For a (molecular) graph, the (first or second) multiplicative Zagreb index \prod_1 or \prod_2 is a multiplicative variant of ordinary Zagreb index $(M_1 \text{ or } M_2)$. Gutman [6] determined that among all trees of order $n \ge 4$, the extremal trees with respect to these multiplicative Zagreb indices are *n*-vertex path (with maximal \prod_1 and with minimal \prod_2) and *n*-vertex star (with maximal \prod_2 and with minimal \prod_1). Regarding these new topological indices, there is no further results reported so far. In this paper we investigate extremal properties of these indices along the same line of [6]. We first introduce some graph transformations which increase or decrease these two indices. As an application, we obtain a unified approach to characterize extremal (maximal and minimal) trees, unicyclic graphs and bicyclic graphs with respect to multiplicative Zagreb indices, respectively.

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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 in G adjacent to v. For a subset W of V(G), let G - Wbe 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 [2].

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 [10] where Gutman and Trinajstić examined the dependence of total π -electron energy on molecular structure and elaborated in [11]. 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 $(M_1 \text{ and } M_2)$ reflect the extent of branching of the molecular carbon-atom skeleton [1, 17]. The first Zagreb index M_1 was also termed as "Gutman index" by some scholars (see [17]). The main properties of M_1 and M_2 were summarized in [4, 5, 7, 13, 14]. In particular, Deng [5] 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 [12, 20] and the references cited therein.

Recently, Todeschini et al. [16, 18] have proposed the multiplicative variants of ordinary Zagreb indices, which are defined as follows:

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

These two graph invariants are called "multiplicative Zagreb indices" by Gutman [6].

In the same paper, Gutman determined that among all trees of order $n \ge 4$, the extremal trees with respect to these multiplicative Zagreb indices are path P_n (with maximal \prod_1 and with minimal \prod_2) and star S_n (with maximal \prod_2 and with minimal \prod_1). More recently, Gutman and Ghorbani [8] have obtained some properties of Narumi-Katayama index whose definition is $NK(G) = \prod_{v \in V(G)} d_G(v)$ for a graph G. A molecular graph which models the skeleton of a molecule ([19]) is a connected graph of maximum degree at most 4. The bounds of a molecular topological descriptor are important information of a (molecular) graph in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters.

Let $\mathcal{T}(n)$ and $\mathcal{U}(n)$ be the set of trees of order n, and the set of connected unicyclic graphs of order n, respectively. Denote by $\mathcal{B}(n)$ the set of connected bicyclic graph of order n. The paper is organized as follows. In Section 2, we introduce some graph transformations which increase or decrease the multiplicative Zagreb index of graphs. In Section 3, using a unified approach based on these graph transformations in Section 2, we have determined the extremal multiplicative Zagreb indices of graphs from $\mathcal{T}(n)$, $\mathcal{U}(n)$ and $\mathcal{B}(n)$, respectively. Moreover, we completely characterize the extremal graph from these three sets at which maximal or minimal multiplicative Zagreb index is attained. Finally we pose a related problem as a researching topic in the future.

2 Some graph transformations

In this section we will introduce some graph transformations, which increase or decrease the multiplicative Zagreb index of graphs. And these graph transformations play an important role in determining the extremal graphs from $\mathcal{T}(n)$, $\mathcal{U}(n)$ and $\mathcal{B}(n)$ with respect to multiplicative Zagreb indices.

Now we introduce a graph transformation which increases the first multiplicative Zagreb index \prod_1 and simultaneously decreases the second multiplicative Zagreb index \prod_2 .

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 $P : vu_1u_2\cdots u_k$ of length k and $Q : vw_1w_2\cdots w_l$ of length l. We further let $G_2 =$



Fig. 1. Transformation A

Lemma 2.1. Let G_1 and G_2 be two graphs as shown in Fig. 1. Then we have

- (1) $\prod_1(G_2) > \prod_1(G_1);$
- (2) $\prod_2(G_2) < \prod_2(G_1).$

Proof. Assume that $d_G(v) = x > 0$. By the definitions of multiplicative Zagreb indices $(\prod_1 \text{ and } \prod_2)$, we have

$$\begin{split} \prod_1(G_2) &- \prod_1(G_1) \geq 4^{k+l-1}(x+1)^2 - 4^{k-1}4^{l-1}(x+2)^2 \\ &= 4^{k+l-2}(3x^2+4x) > 0; \\ \prod_2(G_1) &- \prod_2(G_2) \geq [2(x+2)]^2 4^{k+l-3} - 2(x+1)4^{k+l-2} \times 2 \\ &= 4^{k+l-3} \times 4x^2 > 0. \end{split}$$

Thus we complete the proof of the lemma.

Remark 2.1. 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 first multiplicative Zagreb index \prod_1 increases, while the second multiplicative Zagreb index \prod_2 decreases by Lemma 2.1.

Here we define a function $f(x) = x^x$ where x are positive integers.

Lemma 2.2. Assume that f(x) is a function defined as above. Then we have

$$f(x) > f(x_1)f(x+1-x_1)$$

for any positive integer x_1 such that $1 < x_1 < x$.

Proof. Note that f(x) > 0 for any positive integer x. Therefore it suffices to prove that $lnf(x) > lnf(x_1) + lnf(x + 1 - x_1)$. Now we define another function $g(x) = lnf(x) - lnf(x_1) - ln(x + 1 - x_1)$ where x > 0 is a variant.

Clearly, $g'(x) = lnx - ln(x + 1 - x_1) > 0$. Therefore, the function g(x) is strictly increasing when x > 0. So we have $g(x) > g(x_1)$ when $x > x_1$. It is equivalent that

- $lnf(x) lnf(x_1) lnf(x+1-x_1) > 0$, i.e., that
- $f(x) > f(x_1)f(x+1-x_1),$

finishing the proof of this lemma.

Transformation B. Let uv be an edge of 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 $G' = G - \{uw_1, uw_2, \dots, uw_t\} + \{vw_1, vw_2, \dots, vw_t\}$, see Fig. 2 for these graphs.



Fig. 2. Transformation B

Lemma 2.3. Let G and G' be two graphs in Fig. 2. Then we have

- (1) $\prod_1(G) > \prod_1(G');$
- (2) $\prod_2(G) < \prod_2(G').$

Proof. Assume that $G_0 = G - \{u, w_1, w_2, \dots, w_t\}$. Let $d_{G_0}(v) = k > 0$. Similar to the proof of Lemma 2.1, we have

$$\begin{split} \prod_1(G) &- \prod_1(G') \geq (t+1)^2 (k+1)^2 - (k+t+1)^2 \\ &> kt > 0, \\ \prod_1(G') &- \prod_1(G) \geq (k+t+1)^{k+t+1} - (t+1)^{t+1} (k+1)^{k+1} \\ &> 0 \quad (\text{ by setting } x = t+k+1, \ x_1 = t+1 \text{ in Lemma 2.2) }, \end{split}$$

ending the proof.

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Remark 2.2. 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 first multiplicative Zagreb index \prod_1 decreases, while the second multiplicative Zagreb index \prod_2 increases.

Transformation C. Given a nontrivial connected graph G and its two vertices u and v. Let u_1, u_2, \dots, u_k be pendent vertices adjacent to u and v_1, v_2, \dots, v_l be pendent vertices adjacent to v. Further, we let $G' = G - \{uu1, uu2, \dots, uu_k\} + \{vu_1, vu_2, \dots, vu_k\}$ and $G'' = G - \{vv_1, vv_2, \dots, vv_l\} + \{uv_1, uv2, \dots, uv_l\}$, see Fig. 3 for these graphs.



Fig. 3. Transformation C

Lemma 2.4. Let G, G' and G'' be graphs as shown in Fig. 3. Then we have

- (1) either $\prod_{1}(G) > \prod_{1}(G')$ or $\prod_{1}(G) > \prod_{1}(G'');$
- (2) either $\prod_2(G) < \prod_2(G')$ or $\prod_2(G) < \prod_2(G'')$.

Proof. Assume that $G_0 = G - \{u_1, u_2, \dots, u_k, v_1, v_2, \dots, v_l\}$. Let $d_{G_0}(v) = x > 0$ and $d_{G_0}(u) = y > 0$. Then we have

$$\begin{split} \prod_1(G) &- \prod_1(G') \geq (x+k)^2(y+l)^2 - (x+k+l)^2y^2 \\ &> (x+k)(y+l) - (x+k+l)y > 0, \quad if \ x-y \geq 0, \\ \prod_1(G) &- \prod_1(G'') \geq (x+k)^2(y+l)^2 - (y+k+l)^2x^2 \\ &> (x+k)(y+l) - (y+k+l)x > 0, \quad if \ x-y < 0. \end{split}$$

Therefore the result in (1) follows immediately. Set $\Delta_1 = \prod_2 (G') - \prod_2 (G)$ and $\Delta_2 = \prod_2 (G'') - \prod_2 (G)$. Then we have

$$\begin{aligned} \Delta_1 &\geq (x+k+l)^{x+k+l} - (x+k)^{x+k} - (y+l)^{y+l}, \\ \Delta_2 &\geq (y+k+l)^{y+k+l} - (x+k)^{x+k} - (y+l)^{y+l}. \end{aligned}$$
Note that $k \geq 1$ and $l \geq 1$. Thus, from Lemma 2.1, we have
$$\begin{aligned} \Delta_1 + \Delta_2 &\geq (x+k+l)^{x+k+l} + (y+k+l)^{y+k+l} - 2(x+k)^{x+k} - 2(y+l)^{y+l} \\ &> (x+k)^{x+k}(l+1)^{l+1} - 2(x+k)^{x+k} + (y+l)^{y+l}(k+1)^{k+1} - 2(y+l)^{y+l} \geq 0. \end{aligned}$$
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Thus we complete the proof of this lemma.

Remark 2.3. Repeating Transformations B and C, any unicyclic or bicyclic graph can be changed into a unicyclic or bicyclic graph such that all the pendant edges are attached to the same vertex. And the obtained unicyclic or bicyclic graph has a smaller first multiplicative Zagreb index \prod_1 and a larger second multiplicative Zagreb index \prod_2 .

Transformation D. Assume that a pendent path $P = v_1 v_2 \cdots v_{t-1} v_t$ is attached at v_1 in graph G and there are two neighbors x and y of v_1 different from x_2 . Let $G' = G - xv_1 + xv_t$, see Fig. 4.



Lemma 2.5. Let G and G' be two graphs as shown in Fig. 4. Then we have

- (1) $\prod_1(G) < \prod_1(G');$
- (2) $\prod_{2}(G) > \prod_{2}(G').$

Proof. By definition, we have

$$\begin{split} &\prod_1(G') - \prod_1(G) \ge 4^{t-1}4 - 3^2 4^{t-2} = 7 \times 4^{t-2} > 0, \\ &\prod_2(G) - \prod_2(G') \ge (2 \times 3)(3d_G(x))(3d_G(y))4^{t-3} \times 2 - (2d_G(x))(2d_G(y))4^{t-1} \\ &= 11d_G(x)d_G(y)4^{t-2} > 0. \end{split}$$

This completes the proof of this lemma.

3 Main results

In this section we turn to determine the extremal multiplicative Zagreb indices of graphs from $\mathcal{T}(n)$, $\mathcal{U}(n)$ and $\mathcal{B}(n)$, respectively. And the corresponding extremal graphs from these three sets are completely characterized.

3.1 Extremal graphs in T(n) and U(n) w.r.t. multiplicative Zagreb indices

Bearing in mind that Remarks 2.1 and 2.2, and using Lemmas 2.1 and 2.3, one can easily obtain the following result.

Theorem 3.1. [6] 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) $\prod_1(P_n) < \prod_2(G) < \prod_2(S_n).$

Let C_n^k be a graph obtained by attaching n - k pendent edges to a vertex of C_k . From Lemmas 2.3 and 2.4, considering Remark 2.3, we have the following lemma.

Lemma 3.1. Let G be a unicyclic graph in $\mathcal{U}(n)$ with girth k different from C_n^3 . Then

- (1) $\prod_1 (C_n^k) < \prod_1 (G);$
- (2) $\prod_2(G) < \prod_2(C_n^k).$

By definition, we have $\prod_1 (C_n^k) = (n-k+2)^2 4^{k-1}$ and $\prod_2 (C_n^k) = (n-k+2)^{n-k+2} 4^{k-1}$. By calculating their derivatives, we find that function $h_1(x) = (n-x+2)^2 4^{x-1}$ is strictly increasing while $h_2(x) = (n-x+2)^{n-x+2} 4^{x-1}$ is strictly decreasing when x is a real number in the interval (3, n). Therefore we can obtain

$$\begin{split} &\prod_1 (C_n^k) - \prod_1 (C_n^3) = (n-k+2)^2 4^{k-1} - (n-1)^2 4^2 > 0 \text{ if } 3 < k < n; \\ &\prod_2 (C_n^3) - \prod_1 (C_n^k) = (n-1)^2 4^2 - (n-k+2)^{n-k+2} 4^{k-1} > 0 \text{ if } 3 < k < n. \end{split}$$

Thus the following theorem holds immediately.

Theorem 3.2. Let G be a graph in $\mathcal{U}(n)$ different from C_n^3 . Then we have

(1)
$$\prod_{1} (C_n^3) < \prod_{1} (G);$$

(2) $\prod_2(G) < \prod_2(C_n^3).$

A unicyclic graph G is said to be a sun graph ([15]) if cycle vertices have degree at most three and remaining vertices have degree at most two. The extremal graph in $\mathcal{U}(n)$ with maximal \prod_1 and minimal \prod_2 is presented in the following theorem.

Theorem 3.3. Let G be a graph in $\mathcal{U}(n)$ different from C_n . Then we have

- (1) $\prod_{1}(G) < \prod_{1}(C_n);$
- (2) $\prod_2 (C_n) < \prod_2 (G).$

Proof. Since the proof of (2) is similar to that of (1), we only give the proof of (1).

By Lemma 2.1, considering Remark 2.1, we find that any unicyclic graph G can be changed into a sun graph with a larger first multiplicative Zagreb index \prod_1 . We can apply repeatedly Lemma 2.5 to any sun graph as long as it is not the cycle C_n , increasing its first multiplicative Zagreb index \prod_1 . Thus the result in (1) follows immediately. \Box

Combining Theorems 3.2 and 3.3, we list the following theorem, in which extremal graph from $\mathcal{U}(n)$ is characterized completely with respect to multiplicative Zagreb indices $(\prod_1 \text{ and } \prod_2).$

Theorem 3.4. Let G be a graph in $\mathcal{U}(n)$ different from C_n^3 and C_n . Then we have

- (1) $\prod_1 (C_n^3) < \prod_1 (G) < \prod_1 (C_n);$
- (2) $\prod_2(C_n) < \prod_2(G) < \prod_2(C_n^3).$

3.2 Extremal graphs in $\mathcal{B}(n)$ w.r.t. multiplicative Zagreb indices

Now we start to deal with the extremal graphs in $\mathcal{B}(n)$ with respect to multiplicative Zagreb indices (\prod_1 and \prod_2). To do it, we first introduce necessary definitions.

As in [21], for any graph $G \in \mathcal{B}(n)$, there are at least two cycles in G. The structure of cycles in $G \in \mathcal{B}(n)$ can be divided into the following three cases:

- (I) The two cycles C_p and C_q in G have only one common vertex v;
- (II) The two cycles C_p and C_q in G are linked by a path of length l > 0;

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(III) The two cycles C_{l+k} and C_{l+m} in G have a common path of length l > 0.

The graphs $C_{p,q}$, $C_{p,l,q}$ and $\theta_{k,l,m}$ (where $1 \leq l \leq min\{k,m\}$) corresponding to the cases above shown in Fig. 5 are called main subgraphs of $G \in \mathcal{B}(n)$ of type (I), (II) and (III), respectively.



Fig. 5. The graphs $C_{p,q}$, $C_{p,l,q}$ and $\theta_{k,l,m}$

Based on Transformations D and B, we can deduce the following transformation.

Transformation E. Let $P = xv_1v_2\cdots v_ty$ be an internal path in G, i.e., $d_G(v_i) = 2$ for $i = 1, 2, \cdots, t$, $d_G(x) \ge 2$ and $d_G(y) \ge 2$. $G' = G - \{v_2v_3, v_3v_4, \cdots, v_{t-1}v_t, v_ty\} + \{v_1v_3, v_1v_4, \cdots, v_1v_t, v_1y\}$ as shown in Fig. 6.

$$\begin{array}{c} \vdots \\ x \quad v_1 \quad v_2 \\ G \\ \end{array} \xrightarrow{v_1 \quad v_2} \cdots \xrightarrow{v_t \quad y} \vdots \xrightarrow{E} \xrightarrow{v_2 \quad v_3 \\ x \quad v_1 \quad y} \vdots \xrightarrow{v_t \quad v_t \quad y} \vdots$$

Fig. 6. Transformation E

From Lemmas 2.5 and 2.3 it follows immediately the following lemma.

Lemma 3.2. Let G and G' be two graphs shown in Fig. 6. Then we have

- (1) $\prod_{1}(G) > \prod_{1}(G');$
- (2) $\prod_2(G) < \prod_2(G').$

Lemma 3.3. [6] For any graph G, we have $\prod_2(G) = \prod_{x \in V(G)} d_G(x)^{d_G(x)}$.

Let B'_n be a graph as shown in Fig. 7 obtained by attaching two adjacent edges in S_n among its three pendent vertices.



Fig. 7 The graph B'_n

When n = 4, $\mathcal{B}(n)$ contains only graph, which is obtained by deleting an edge of complete graph K_4 . If n = 5, there are 5 graphs in $\mathcal{B}(n)$. It is easy to check that B'_n has the minimal first multiplicative Zagreb index \prod_1 and the maximal second multiplicative Zagreb index \prod_2 among these five graphs. By the following theorem we determine the extremal graph from $\mathcal{B}(n)$ for $n \ge 6$ with respect to multiplicative Zagreb indices.

Theorem 3.5. Let G be a graph in $\mathcal{B}(n)$ with $n \ge 6$ different from B'_n . Then we have

- (1) $\prod_1 (B'_n) < \prod_1 (G);$
- (2) $\prod_{2} (G) < \prod_{2} (B'_{n}).$

Proof. (1) Let G_0 be a graph from $\mathcal{B}(n)$ with minimum first multiplicative Zagreb index \prod_1 and B_0 be its main subgraph. Then B_0 is of one of types I, II and III. By Remark 2.3, we find that G_0 must be a graph obtained by attaching some pendent edges to one vertex of the graph B_0 . Next we will prove the following claim.

Claim 1. The length of any cycle in B_0 is less than 5.

Proof of Claim 1. Otherwise, if B_0 is of type I or II, applying Transformation E, by Lemma 3.2, we can easily obtain another graph G'_0 with a smaller first multiplicative Zagreb index \prod_1 . It contradicts to the choice of G_0 .

Now we consider the case when B_0 is of type *III*. Assume that $B_0 \cong \theta_{k,l,m}$ with $1 \leq l \leq min\{k,m\}$ and k+m > 5. Then one of two integers k and m, say k, is not less than 3. Considering the structure of G_0 , we conclude that there is an internal path of length not less than 2 in B_0 of G_0 . By Lemmas 3.2 and 2.4, we can construct a new graph G_0'' in $\mathcal{B}(n)$ with a smaller first multiplicative Zagreb index \prod_1 . This is also a contradiction to the choice of G_0 , which completes the proof of this claim.

From Claim 1, we find that the length of cycle in B_0 of G_0 is 3 or 4. Clearly, we have $B_0 \cong C_{3,3}$ if B_0 is of type I, $B_0 \cong C_{3,l,3}$ if B_0 is of type II and $B_0 \cong \theta_{2,1,2}$ when it is of type III. Now we claim that l = 1 in $B_0 \cong C_{3,l,3}$ when it is of type II. If not, based on Lemmas 3.2 and 2.4, we can get a new graph from $\mathcal{B}(n)$ with a smaller first multiplicative Zagreb index \prod_1 . This is impossible because of the minimality of $\prod_1(G_0)$.

Let $C'_{3,3}$ be the graph obtained by attaching n-5 pendent edges to a vertex in $C_{3,3}$ of degree 2 and $C''_{3,3}$ the graph obtained by attaching n-5 pendent edges to a vertex in $C_{3,3}$ of degree 4. Denote by $C'_{3,1,3}$ the graph obtained by attaching n-6 pendent edges to a vertex in $C_{3,1,3}$ of degree 2, and by $C''_{3,1,3}$ obtained by attaching n-6 pendent edges to a vertex in $C_{3,1,3}$ of degree 3. And the graph obtained by attaching n-4 pendent edges to one vertex in $\theta_{2,1,2}$ of degree 2 is denoted by $\theta'_{2,1,2}$. By definition, we have

$$\begin{split} &\prod_1 (C'_{3,3}) = 4^5 (n-3)^2, \\ &\prod_1 (C'_{3,3}) = 4^4 (n-1)^2, \\ &\prod_1 (C'_{3,1,3}) = 4^3 9^2 (n-4)^2, \\ &\prod_1 (C''_{3,1,3}) = 4^4 9 (n-3)^2, \\ &\prod_1 (\theta'_{2,1,2}) = 4 \times 9^2 (n-2)^2 \\ &\prod_1 (B'_n) = 4^2 9 (n-1)^2. \end{split}$$

By a simple comparison of above values, our result in (1) holds immediately.

(2) Set $S = \{C'_{3,3}, C''_{3,3}, C'_{3,1,3}, C''_{3,1,3}, \theta'_{2,1,2}, B'_n\}$. By a very similar reasoning to that in the proof of (1), we find that the maximum of $\prod_2(G)$ with $G \in \mathcal{B}(n)$ is attained at one of graphs in the set S. From Lemma 3.3, we have

$$\begin{split} &\prod_2(C'_{3,3})=4^7(n-3)^{n-3},\\ &\prod_2(C'_{3,3})=4^4(n-1)^{n-1},\\ &\prod_2(C'_{3,1,3})=4^{3}9^3(n-4)^{n-4},\\ &\prod_2(C''_{3,1,3})=4^43^3(n-3)^{n-3},\\ &\prod_2(\theta'_{2,1,2})=4\times9^3(n-2)^{n-2},\\ &\prod_2(B'_n)=4^23^3(n-1)^{n-1}. \end{split}$$

Obviously, $\prod_2(B'_n) > \prod_2(C''_{3,3})$, and $\prod_2(C'_{3,3}) > \prod_2(C''_{3,1,3})$. Therefore, the remaining is to prove that $\prod_2(B'_n) > \prod_2(C'_{3,3})$, $\prod_2(B'_n) > \prod_2(\theta'_{2,1,2})$ and $\prod_2(B'_n) > \prod_2(C'_{3,1,3})$. For convenience, set $A_1 = \prod_2(B'_n) - \prod_2(C'_{3,3})$, $A_2 = \prod_2(B'_n) - \prod_2(\theta'_{2,1,2})$ and $A_3 = \prod_2(B'_n) - \prod_2(B'_n)$

$$\begin{split} \prod_2 (B'_n) &- \prod_2 (C'_{3,1,3}). \text{ Then we have} \\ A_1 &= 4^2 3^3 (n-1)^{n-1} - 4^7 (n-3)^{n-3} \\ &= 4^2 [3^3 (n-1)^{n-1} - 4^5 (n-3)^{n-3}]; \\ A_2 &= 4^2 3^3 (n-1)^{n-1} - 4 \times 9^3 (n-2)^{n-2} \\ &= 4 \times 3^3 [4(n-1)^{n-1} - 3^3 (n-2)^{n-2}]; \\ A_3 &= 4^2 3^3 (n-1)^{n-1} - 4^3 9^3 (n-4)^{n-4} \\ &= 4^2 3^3 [(n-1)^{n-1} - 4 \times 3^3 (n-4)^{n-4}] \end{split}$$

To prove $A_i > 0$ for i = 1, 2, 3, we only need to prove that, for $n \ge 6$,

$$\begin{split} & 3ln3+(n-1)ln(n-1)-5ln4-(n-3)ln(n-3)>0,\\ & ln4+(n-1)ln(n-1)-3ln3-(n-2)ln(n-2)>0,\\ & (n-1)ln(n-1)-ln4-3ln3-(n-4)ln(n-4)>0. \end{split}$$

By calculating their derivatives, we find that functions $f_1(x) = 3ln3 + (x-1)ln(x-1) - 5ln4 - (x-3)ln(x-3)$, $f_2(x) = ln4 + (x-1)ln(x-1) - 3ln3 - (x-2)ln(x-2)$ and $f_3(x) = (x-1)ln(x-1) - ln4 - 3ln3 - (x-4)ln(x-4)$ are all strictly increasing for $x \ge 6$. And $f_i(6) > 0$ for i = 1, 2, 3. Thus the above three inequalities all hold for $n \ge 6$. This finishes the proof of this lemma.

Now we introduce three subsets of the set $\mathcal{B}(n)$ as follows:

$$\begin{split} \mathcal{B}_1(n) &= \{C_{p,q}: p+q-1=n\};\\ \mathcal{B}_2(n) &= \{C_{p,l,q}: p+q+l-1=n\};\\ \mathcal{B}_3(n) &= \{\theta_{k,l,m}: k+l+m-1=n\},\\ \text{Let } G_i \text{ be any graph from } \mathcal{B}_i(n) \text{ for } i=1,2,3. \text{ We have }\\ \prod_1(G_1) &= 4^{n+1} \text{ and } \prod_2(G_1) = 4^{n+3};\\ \prod_1(G_2) &= 3^4 4^{n-2} \text{ and } \prod_2(G_2) = 9^3 4^{n-2};\\ \prod_1(G_3) &= 3^4 4^{n-2} \text{ and } \prod_2(G_3) = 9^3 4^{n-2}. \end{split}$$

Theorem 3.6. Let G be a graph in $\mathcal{B}(n) \setminus \mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ with $n \ge 6$ and H be a graph in $\mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$. Then we have

(1)
$$\prod_1(G) < \prod_1(H);$$

(2) $\prod_{2}(H) < \prod_{2}(G).$

Proof. Here we only give the proof of (2) because of the similarity of the proof of (1) to that of (2).

Using Lemmas 2.1 and 2.5, and noting Remark 2.1, we conclude that the extremal graph from $\mathcal{B}(n)$ with minimal second multiplicative Zagreb index \prod_2 must be graph from the set $\mathcal{B}_1(n) \bigcup \mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$.

From the above calculation of graph G_i in $\mathcal{B}_i(n)$ with i = 1, 2, 3, we have

$$\begin{split} \prod_2(G_1) - \prod_2(G_2) &= \prod_2(G_1) - \prod_2(G_3) \\ &= 4^{n+3} - 9^3 4^{n-2} > 0. \end{split}$$

This completes the proof.

Now we present the following theorem in which the extremal from $\mathcal{B}(n)$ are completely determined with respect to multiplicative Zagreb indices $(\prod_1 \text{ and } \prod_2)$.

Theorem 3.7. Assume that H is any graph from $\mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$. Let G be a graph in $\mathcal{B}(n) \setminus \mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ different from B'_n . Then we have

- (1) $\prod_1(B'_n) < \prod_1(G) < \prod_1(H);$
- (2) $\prod_2(H) < \prod_2(G) < \prod_2(B'_n).$

Based on our results obtained in Theorems 3.1, 3.4 and 3.7, we shall end the paper by posing the following problem.

Problem 3.1. Within any given set of nontrivial connected graphs, is the graph with maximal first multiplicative Zagreb index \prod_1 (or minimal first multiplicative Zagreb index \prod_1 , resp.) just the one with minimal second multiplicative Zagreb index \prod_2 (or maximal second multiplicative Zagreb index \prod_2 , resp.)?

Obviously, the answer to this problem is positive for the sets $\mathcal{T}(n)$, $\mathcal{U}(n)$ and $\mathcal{B}(n)$, respectively, without considering the non-uniqueness of extremal graph from $\mathcal{B}(n)$ with maximal first multiplicative Zagreb index \prod_1 (or minimal second multiplicative Zagreb index \prod_2). But for other general given sets of graphs, the answer to it is still unknown. Maybe it will be an interesting topic for the further research in the future.

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