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Trees, Unicyclic, and Bicyclic Graphs Extremal with Respect to Multiplicative Sum Zagreb Index*

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Abstract

For a (molecular) graph G with vertex set $V(G)$ and edge set $E(G)$, the first Zagreb index of G is defined as $M_1(G) = \sum_{v \in V(G)} d_G(v)^2$ where $d_G(v)$ is the degree of vertex v in G. The alternative expression for $M_1(G)$ is $\sum_{uv \in E(G)}(d_G(u)+d_G(v))$. Very recently, Eliasi, Iranmanesh and Gutman [7] introduced a new graphical invariant $\prod_1^*(G) = \prod_{uv \in E(G)}(d_G(u) + d_G(v))$ as the multiplicative version of M_1. Here we call this new index the *multiplicative sum Zagreb index*. We characterize the trees, unicylcic, and bicyclic graphs extremal (maximal and minimal) with respect to the multiplicative sum Zagreb index. Moreover, we use a method different but shorter than that in [7] for determining the minimal multiplicative sum Zagreb index of trees.

1 Introduction

Throughout this paper we consider finite, undirected and simple graphs. 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

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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 [3].

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 [13] where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structure and elaborated in [14]. 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 and M_2) reflect the extent of branching of the molecular carbon-atom skeleton [1, 19]. The first Zagreb index M_1 was also termed as "Gutman index" by some scholars (see [19]). The main properties of M_1 and M_2 were summarized in [5, 6, 10, 15, 16]. In particular, Deng [6] 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 [15, 22] and the references cited therein.

Recently, Todeschini et al. [18, 20] 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 [9]. In the same paper, Gutman showed that among all trees of order $n \geq 4$, the trees extremal with respect to these multiplicative Zagreb indices are the path P_n (with maximal $\prod_1$ and with minimal $\prod_2$), and the star S_n (with maximal $\prod_2$ and with minimal $\prod_1$). More recently, Gutman and Ghorbani [11] obtained some properties of the Narumi–Katayama index, whose definition is $NK(G) = \prod_{v\in V(G)} d_G(v)$ for a graph G. By using a unified approach, one of the present authors and Hua [24] determined the trees, unicylcic, and bicyclic graphs extremal with respect to $\prod_1$ and $\prod_2$. A molecular graph which models the skeleton of a molecule ([21]) 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.

Very recently, Eliasi, Iranmanesh and Gutman [7] introduced a new graphical invariant as the multiplicative version of ordinary first Zagreb index M_1, which is defined as:

$$\prod_1^*(G) = \prod_{uv\in E(G)}(d_G(u) + d_G(v)).$$

According to its definition, we call $\prod_1^*(G)$ the *multiplicative sum Zagreb index*. As pointed out in [7], the multiplicative sum Zagreb index $\prod_1^*$ is not equal to the first multiplicative Zagreb index $\prod_1$. For example, we have $\prod_1^*(P_3) = 9$ while $\prod_1(P_3) = 4$.

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 graphs of order n.

The paper is organized as follows. In Section 2, we introduce some graph transformations that increase or decrease the multiplicative sum Zagreb index of graphs. In Section 3, based on these graph transformations, we determine the extremal multiplicative sum Zagreb indices of graphs from $\mathcal{T}(n)$, $\mathcal{U}(n)$, and $\mathcal{B}(n)$, respectively. Moreover, we completely characterize the extremal graphs from these three sets at which the maximal or minimal value of the multiplicative sum Zagreb index is attained.

2 Some graph transformations

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

Now we introduce a graph transformation that decreases the multiplicative sum Zagreb index $\prod_1^*$.

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 $G_2 = G_1 - vw_1 + u_kw_1$. The above referred graphs are illustrated in Fig. 1.

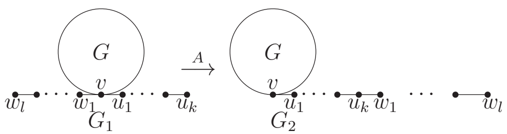

Fig. 1. Transformation A

Lemma 2.1. *Let G_1 and G_2 be two graphs as shown in Fig. 1. Then $\prod_1^*(G_2) < \prod_1^*(G_1)$.*

Proof. Assume that $d_G(v) = x > 0$ and the degrees of neighbors of v in G are $d^{(1)}, d^{(2)}, \ldots, d^{(x)}$, respectively. For $k, l \geq 2$, by the definition of multiplicative sum Zagreb index, we have

$$\begin{aligned}\prod\nolimits_1^*(G_1) - \prod\nolimits_1^*(G_2) &\geq 9 \times (x+4)^2 4^{k+l-4} \prod_{i=1}^{x} (d^{(i)}+x+2) - 3 \times 4^{k+l-2}(x+3) \prod_{i=1}^{x} (d^{(i)}+x+1) \\ &> 4^{k+l-4}[9(x+4)^2 - 48(x+3)] \\ &\geq 9x^2 + 24x > 0.\end{aligned}$$

When $k = l = 1$ or $k = 1$ and $l = 2$, or $k = 2$ and $l = 1$, simple calculation shows the validity of $\prod_1^*(G_2) < \prod_1^*(G_1)$.

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 multiplicative sum Zagreb index $\prod_1^*$ decreases by Lemma 2.1.*

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

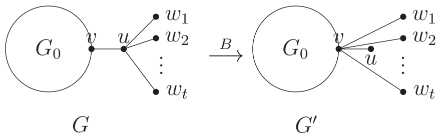

Fig. 2. Transformation B

Lemma 2.2. *Let G and G' be two graphs in Fig. 2. Then $\prod_1^*(G) < \prod_1^*(G')$.*

Proof. Let $G_0 = G - \{u, w_1, w_2, \cdots, w_t\}$. Assume that $d_{G_0}(v) = x > 0$ and the degrees of neighbors of v in G_0 are $d^{(1)}, d^{(2)}, \ldots, d^{(x)}$, respectively. Similar to the proof of Lemma 2.1, we have

$$\begin{aligned}\prod\nolimits_1^*(G') - \prod\nolimits_1^*(G) &\geq (x+t+2)^{t+1} \prod_{i=1}^{x} (d^{(i)}+x+t+1) - (x+t+1)(t+2)^t \prod_{i=1}^{x} (d^{(i)}+x+1) \\ &> (x+t+2)^{t+1} - (x+t+1)(t+2)^t > 0\ ,\end{aligned}$$

ending the proof. □

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 multiplicative sum Zagreb index $\prod_1^*$ increases by Lemma 2.2.*

Transformation C. Given a nontrivial connected graph G with two non-pendent adjacent vertices u and v where u and v have no common neighbor in G. Further, we construct a new graph G' which is obtained by identifying the vertices u and v to a new vertex w and attaching a pendent vertex w_0 to the vertex w, see Fig. 3 for these graphs.

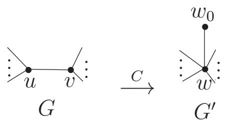

Fig. 3. Transformation C

Lemma 2.3. *Let G, G' be graphs as shown in Fig. 3. Then* $\prod_1^*(G') > \prod_1^*(G)$.

Proof. Assume that the neighbors of u except v are $u_1, \ldots, u_x$ with degrees $d_u^{(1)}, \ldots, d_u^{(x)}$, respectively, and the neighbors of v except u are $v_1, \ldots, v_y$ with degrees $d_v^{(1)}, \ldots, d_v^{(y)}$, respectively. Set $A = \prod_1^*(G') - \prod_1^*(G)$, then

$$\begin{aligned}
A \geq\ & (x+y+2)\prod_{i=1}^{x}(d_u^{(i)}+x+y+1)\prod_{j=1}^{y}(d_v^{(j)}+x+y+1) \\
& -(x+y+2)\prod_{i=1}^{x}(d_u^{(i)}+x+1)\prod_{j=1}^{y}(d_v^{(j)}+y+1) \\
> & \prod_{i=1}^{x}(d_u^{(i)}+x+y+1)\prod_{j=1}^{y}(d_v^{(j)}+x+y+1)-\prod_{i=1}^{x}(d_u^{(i)}+x+1)\prod_{j=1}^{y}(d_v^{(j)}+y+1) > 0.
\end{aligned}$$

Therefore the result in this lemma follows immediately. □

Transformation D. Assume that a pendent path $P = v_1v_2\cdots v_{t-1}v_t$ is attached at v_1 in graph G and there are two neighbors u and w of v_1 different from v_2. Let $G' = G - uv_1 + uv_t$, see Fig. 4.

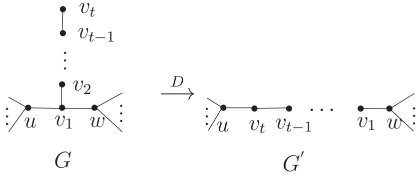

Fig. 4. Transformation D

Lemma 2.4. *Let G and G' be two graphs as shown in Fig. 4. Then* $\prod_1^*(G') < \prod_1^*(G)$.

Proof. Assume that $d_G(u) = x > 1$ and $d_G(w) = y > 1$. When $t \geq 2$, by the definition of multiplicative sum Zagreb index, we have

$$\begin{aligned}\prod_1^*(G) - \prod_1^*(G') &\geq (x+3)(y+3)(3+2)4^{t-2} \times 3 - (x+2)(y+2)4^t \\ &= 4^{t-2}[18(x+3)(y+3) - 16(x+2)(y+2)] > 0.\end{aligned}$$

Similarly, if $t = 1$, then

$$\begin{aligned}\prod_1^*(G) - \prod_1^*(G') &\geq (x+3)(y+3) \times 4 - (x+2)(y+2) \times 4 \\ &> (x+3)(y+3) - (x+2)(y+2) > 0.\end{aligned}$$

This completes the proof of this lemma. □

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 $i = 1, 2, \cdots, t$, $d_G(x) \geq 2$ and $d_G(y) \geq 2$. $G' = G - \{v_2v_3, v_3v_4, \cdots, v_{t-1}v_t, v_ty\} + \{v_1v_3, v_1v_4, \cdots, v_1v_t, v_1y\}$ as shown in Fig. 5.

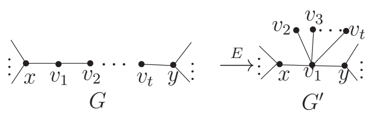

Fig. 5. Transformation E

From Lemmas 2.4 and 2.2 the lemma below follows immediately.

Lemma 2.5. *Let G and G' be two graphs shown in Fig. 5. Then* $\prod_1^*(G) < \prod_1^*(G')$.

Let $d^{(1)}, d^{(2)}, \ldots, d^{(m)}$ be m nonnegative integers. Now we define a function

$$f(x) = (x+m+1)^x \prod_{i=1}^{m}(d^{(i)} + x + m)$$

where $x > 0$ is a variant.

Lemma 2.6. *Let $f(x)$ be a function defined as above. Then, for any two positive integers s and t, we have $f(s+t)f(0) > f(s)f(t)$.*

Proof. Note that $f(x) > 0$ for any variant $x > 0$. Therefore, to obtain the result, it suffices to prove that $lnf(s+t) + lnf(0) > lnf(s) + lnf(t)$.

Now we consider a new function $g(x) = lnf(x) + lnf(0) - lnf(x_1) - lnf(x - x_1)$ where $0 < x_1 < x$ is an invariant. Setting another new function $h(x) = ln(x+m+1) + \frac{x}{x+m+1} + \sum_{i=1}^{m} \frac{1}{d^{(i)}+x+m}$, then we have

$$h'(x) = \frac{1}{x+m+1} - \frac{m+1}{(x+m+1)^2} + \sum_{i=1}^{m} \frac{1}{(d^{(i)}+x+m)^2}$$
$$= \frac{x}{(x+m+1)^2} + \sum_{i=1}^{m} \frac{1}{(d^{(i)}+x+m)^2} > 0.$$

Therefore we claim that $h(x)$ is strictly increasing when $x > 0$. Thus we have

$$g'(x) = ln(x+m+1) + \frac{x}{x+m+1} + \sum_{i=1}^{m} \frac{1}{d^{(i)}+x+m}$$
$$- [ln(x-x_1+m+1) + \frac{x-x_1}{x-x_1+m+1} + \sum_{i=1}^{m} \frac{1}{d^{(i)}+x-x_1+m}]$$
$$= h(x) - h(x-x_1) > 0.$$

Again $g(x)$ is also strictly increasing when $x > 0$. Obviously we have $g(x) > g(x_1) = 0$. By choosing $x = s+t$ and $x_1 = s$, it follows that $g(s+t) > g(s) = 0$, i.e., that $lnf(s+t) + lnf(0) - lnf(s) - lnf(t) > 0$, which completes the proof of this theorem. $\square$

Now we introduce a new graph transformation as follows:

Transformation F. Given a connected graph G with $u, v \in V(G)$, let $u_1, u_2, \ldots, u_s$ be pendent vertices adjacent to u and $v_1, v_2, \ldots, v_t$ be pendent vertices adjacent to v. Set $G_0 = G - \{u_1, u_2, \ldots, u_k, v_1, v_2, \ldots, v_l\}$. In G_0, vertex u has m neighbors $u_1^0, \ldots, u_m^0$ and v has also m neighbors $v_1^0, \ldots, v_m^0$ with $d_{G_0}(u_i^0) = d_{G_0}(v_i^0) = d^{(i)}$ for $i = 1, 2, \ldots, m$. Further, we let $G' = G - \{uu_1, uu_2, \ldots, uu_s\} + \{vu_1, vu_2, \ldots, vu_s\}$ and $G'' = G - \{vv_1, vv_2, \ldots, vv_t\} + \{uv_1, uv_2, \cdots, uv_t\}$, see Fig. 6 for these graphs.

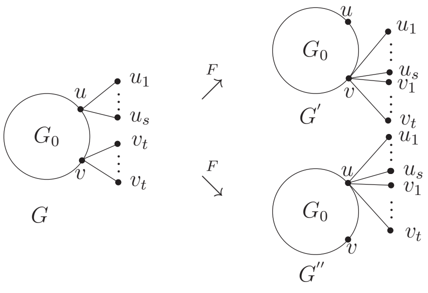

Fig. 6. Transformation F

Lemma 2.7. *Let G, G' and G'' be graphs as shown in Fig. 6. Then* $\prod_1^*(G) < \prod_1^*(G') = \prod_1^*(G'')$.

Proof. By definition, we have

$$\prod\nolimits_1^*(G') - \prod\nolimits_1^*(G) = \prod\nolimits_1^*(G'') - \prod\nolimits_1^*(G)$$
$$\geq (s+t+m+1)^{s+t} \prod_{i=1}^{m}(d^{(i)}+s+t+m) \prod_{i=1}^{m}(d^{(i)}+m)$$

$$- (s + +m + 1)^s (t + +m + 1)^t \prod_{i=1}^{m} (d^{(i)} + s + m) \prod_{i=1}^{m} (d^{(i)} + t + m)$$
$$> 0 \ \ by \ \ Lemma \ \ 2.6.$$

Therefore we complete the proof of this lemma. □

3 Main results

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

3.1 Graphs in $\mathcal{T}(n)$ and $\mathcal{U}(n)$ extremal w.r.t. multiplicative sum Zagreb index

By the definition of multiplicative sum Zagreb index, the following corollary can be easily obtained.

Lemma 3.1. *Let G be a graph with two nonadjacent vertices $u, v \in V(G)$ and $e \in E(G)$. Then*

(1) $\prod_1^*(G + uv) > \prod_1^*(G)$;

(2) $\prod_1^*(G - e) < \prod_1^*(G)$.

Theorem 3.1. [7] *Among all connected graphs of order $n > 1$, the path P_n has the minimal multiplicative sum Zagreb index.*

Combining Lemma 3.1 (2) with Theorem 3.1, we can obtain the following theorem, in which the minimal multiplicative sum Zagreb index of trees from $\mathcal{T}(n)$ is determined.

Theorem 3.2. *Let T be a tree in $\mathcal{T}(n)$ with $n \geq 4$ different from P_n. Then $\prod_1^*(P_n) < \prod_1^*(T)$.*

In fact, taking Remark 2.1 into account, and using Lemma 2.1 repeatedly, one can easily obtain the above result.

A *caterpillar* is a tree if deleting all its pendent vertices will reduce it to a path. Note that caterpillar is also called as *Gutman tree* (see [2, 8]). Now we consider the maximal multiplicative sum Zagreb index of trees from $\mathcal{T}(n)$.

Theorem 3.3. *Let T be a tree in $\mathcal{T}(n)$ with $n \geq 4$ different from S_n. Then $\prod_1^*(T) < \prod_1^*(S_n)$.*

Proof. By Lemma 2.2 and Remark 2.2, we find that the tree from $\mathcal{T}(n)$ with maximal multiplicative sum Zagreb index must be a caterpillar. Considering Transformations C and E, from Lemmas 2.3 and 2.5, we conclude that any caterpillar can be changed into star S_n with a larger multiplicative sum Zagreb index. Thus the result in this theorem follows immediately. □

Combining Theorems 3.2 and 3.3, we list the following theorem, in which the graph from $\mathcal{T}(n)$ extremal with respect to multiplicative sum Zagreb index $\prod_1^*$ is completely characterized.

Theorem 3.4. *Let G be a graph in $\mathcal{T}(n)$ different from S_n and P_n. Then we have $\prod_1^*(P_n) < \prod_1(G) < \prod_1^*(S_n)$.*

Denote by $\mathcal{T}^0(n)$ the set of all trees of order n and with a unique vertex of maximum degree 3. Let S_n^0 be a tree obtained by attaching a pendent edge to a pendent vertex of S_{n-1}. In [7], Eliasi, Iranmanesh and Gutman have proved that any tree from $\mathcal{T}^0(n)$ has the second minimal multiplicative sum Zagreb index among all connected graphs of order n. In the following theorem the graph from $\mathcal{T}(n)$ is characterized having second minimal or second maximal multiplicative sum Zagreb index.

Theorem 3.5. *Let G be a tree in $\mathcal{T}(n)$ different from S_n, P_n, S_n^0 and any tree T_n^0 from $\mathcal{T}^0(n)$. Then we have $\prod_1^*(T_n^0) < \prod_1(G) < \prod_1^*(S_n^0)$.*

Proof. For any tree $T \in \mathcal{T}(n)$ different from S_n, P_n, S_n^0 and any tree T_n^0 from $\mathcal{T}^0(n)$, T can be changed into a tree of order n and with a unique vertex of maximum degree 3 which has a smaller multiplicative sum Zagreb index from Remark 2.1 and Lemma 2.1. Therefore the result in left side holds immediately.

Similarly, for the above tree T, it can be changed into a caterpillar with diameter 3 which has a larger multiplicative sum Zagreb index. Any caterpillar with diameter 3 is just a double star, denoted by S_{n_1,n_2}, with $1 \leq n_1 \leq n_2$ and $n_1 + n_2 = n - 2$, which is obtained by attaching n_1 pendent vertices to one pendent vertex of P_2 and n_2 pendent vertices to the other. Now we claim that $\prod_1^*(S_{n_1,n_2})$ reaches its maximum value when $n_1 = 1$ and $n_2 = n - 3$. Otherwise, $n_1 \geq 2$. Using Transformation F, by Lemma 2.7, we can get the graph $S_{1,n-3}$ with $\prod_1^*(S_{1,n-3}) > \prod_1^*(S_{n_1,n_2})$. Note that $S_{1,n-3} \cong S_n^0$ defined as above. By now we finish the proof of this theorem. □

A unicyclic graph G is said to be a *sun graph* ([17]) if the vertices belonging to the cycle have degree at most three and the remaining vertices have degree at most two. The graph in $\mathcal{U}(n)$ with minimal $\prod_1^*$ is specified in the following theorem.

Theorem 3.6. *Let G be a graph in $\mathcal{U}(n)$ different from C_n. Then $\prod_1^*(C_n) < \prod_1^*(G)$.*

Proof. By Lemma 2.1, considering Remark 2.1, we find that any unicyclic graph G can be changed into a sun graph with a smaller multiplicative sum Zagreb index $\prod_1^*$. We can apply repeatedly Lemma 2.4 to any sun graph as long as it is not the cycle C_n, decreasing its multiplicative sum Zagreb index $\prod_1^*$. Thus the result in this theorem follows immediately. □

A unicyclic graph is called as *cycle-caterpillar* if deleting all its pendent vertices will reduce it to a cycle. If a cycle-caterpillar has girth k, then we say that this cycle-caterpillar is on the cycle C_k. Let C_n^k be a graph obtained by attaching $n-k$ pendent edges to a vertex of C_k. By the following theorem we determine the graph from $\mathcal{U}(n)$ with maximal multiplicative sum Zagreb index $\prod_1^*$.

Theorem 3.7. *Let G be a unicyclic graph in $\mathcal{U}(n)$ different from C_n^3. Then $\prod_1^*(G) < \prod_1^*(C_n^3)$.*

Proof. Considering Remark 2.2, by Lemma 2.2, we claim that the graph from $\mathcal{U}(n)$ with maximal multiplicative sum Zagreb index must be a cycle–caterpillar.

Applying Transformations E and C, from Lemma 2.5 and 2.3, we conclude that any cycle-caterpillar can be changed into a cycle-caterpillar on triangle $C_3 = v_1v_2v_3v_1$ with a larger multiplicative sum Zagreb index. Denote by $C_3(n_1, n_2, n_3)$ the cycle-caterpillar of order n obtained by attaching n_i pendent vertices to vertex v_i for $i = 1, 2, 3$. Using Transformation F at most twice, by Lemma 2.7, we can obtain the graph C_n^3 with $\prod_1^*(C_n^3) > \prod_1^*(C_3(n_1, n_2, n_3))$, ending the proof of this theorem. □

Combining Theorems 3.6 and 3.7, we list the following theorem, in which the graph from $\mathcal{U}(n)$ extremal with respect to the multiplicative sum Zagreb index is completely characterized.

Theorem 3.8. *Let G be a graph in $\mathcal{U}(n)$ different from C_n^3 and C_n. Then we have $\prod_1^*(C_n) < \prod_1^*(G) < \prod_1^*(C_n^3)$.*

3.2 Graphs in $\mathcal{B}(n)$ extremal w.r.t. multiplicative sum Zagreb index

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

As in [23], 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 $l > 0$;

(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. 7 are called main subgraphs of $G \in \mathcal{B}(n)$ of type (I), (II) and (III), respectively.

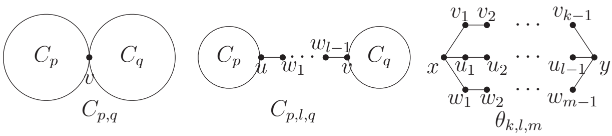

Fig. 7. The graphs $C_{p,q}$, $C_{p,l,q}$ and $\theta_{k,l,m}$

Let B'_n be a graph as shown in Fig. 8 obtained by attaching two adjacent edges in S_n among its three pendent vertices.

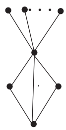

Fig. 8 The graph B'_n

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 maximal multiplicative sum Zagreb index $\prod_1^*$ among these five graphs. In what follows, we only consider the extremal graph from $\mathcal{B}(n)$ with $n \geq 6$. By the following theorem we determine the extremal graph from $\mathcal{B}(n)$.

Theorem 3.9. *Let G be a graph in $\mathcal{B}(n)$ with $n \geq 6$ different from B'_n. Then we have $\prod_1^*(G) < \prod_1^*(B'_n)$.*

Proof. Let G_0 be a graph from $\mathcal{B}(n)$ with maximum multiplicative sum 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

2.2, we find that G_0 must be a graph obtained by attaching some pendent edges to some vertices of the graph B_0. Owing to Transformations C and E, in view of Lemmas 2.3 and 2.5, any graph G from $\mathcal{B}(n)$ with main subgraph of type II can be changed into another graph G' with main subgraph of type I with a larger multiplicative sum Zagreb index. Therefore we only need to consider the graphs from $\mathcal{B}(n)$ with main subgraph of type I or III. 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, applying Transformations C and E, by Lemmas 2.3 and 2.5, we can easily obtain another graph G_0' with two shorter cycles than those in G_0 and $\prod_1^*(G_0') > \prod_1^*(G_0)$. 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 $k + m \geq 5$. Then one of two integers k and m, say k, is not less than 3. Considering the structure of G_0, we apply Transformation C or Transformation E to B_0 in G_0 and obtain a new graph G_0'' in $\mathcal{B}(n)$ with a smaller multiplicative sum Zagreb index by Lemma 2.3 or 2.5. This is also a contradiction to the choice of G_0, which completes the proof of this claim.

By Claim 1, we found that the length of any cycle in B_0 is 3 or 4. Furthermore, we conclude that $B_0 \cong C_{3,3}$ when it is of type I, $B_0 \cong \theta_{2,1,2}$ if it is of type III.

Let $C_{3,3}(n_1, n_2)$ be a graph obtained by attaching n_1 pendent vertices to one vertex of degree 2 in $C_{3,3}$ and n_2 pendent vertices to one vertex of degree 4 in it. Denote by $\theta_{2,1,2}(n_1, n_2)$ a graph obtained by attaching n_1 pendent vertices to one vertex of degree 2 in $C_{3,3}$ and n_2 pendent vertices to one vertex of degree 3 in it. Noticing the symmetry of $C_{3,3}$ and $\theta_{2,1,2}$, in view of Transformation F and Lemma 2.7, we find that G_0 must be of the form $C_{3,3}(n_1, n_2)$ with $n_1+n_2 = n-5$ or of the form $\theta_{2,1,2}(n_1, n_2)$ with $n_1+n_2 = n-4$.

By definition, we have

$$\begin{aligned}\prod_1^*(C_{3,3}(n_1, n_2)) &= 4(n_1 + n_2 + 6)(n_1 + 4)(n_1 + 3)^{n_1}(n_2 + 6)^3(n_2 + 5)^{n_2}\\ &= 4(n + 1)(n_1 + 4)(n_1 + 3)^{n_1}(n_2 + 6)^3(n_2 + 5)^{n_2},\\ \prod_1^*(\theta_{2,1,2}(n_1, n_2)) &= 4(n_1 + n_2 + 5)(n_1 + 5)(n_1 + 3)^{n_1}(n_2 + 5)(n_2 + 6)(n_2 + 4)^{n_2}\\ &= 4(n + 1)(n_1 + 5)(n_1 + 3)^{n_1}(n_2 + 5)(n_2 + 6)(n_2 + 4)^{n_2}.\end{aligned}$$

Claim 2. $\prod_1^*(C_{3,3}(n_1, n_2))$ reaches its its maximum value when $n_1 = 0, n_2 = n - 5$.

Proof of Claim 2. In order to prove this claim, we have to find the maximum value of $(n_2+6)^3(n_2+5)^{n_2}(n_1+4)(n_1+3)^{n_1}$, where $n_1+n_2 = n-5$. From the factors, one can see easily that the maximum value occurs only when $n_2 \geq n_1$, that is, $n_1 \leq (n-5)/2$. Thus we have to find the maximum value of $(n-n_1+1)^3(n-n_1)^{n-n_1-5}(n_1+4)(n_1+3)^{n_1}$,

$n_1 \le (n-5)/2$. For this let us consider a function

$$f(x) = (x+4)(x+3)^x(n-x+1)^3(n-x)^{n-x-5}, \quad 0 \le x \le (n-5)/2 \ .$$

Then

$$f'(x) = f(x)\Big[-\frac{1}{(x+3)(x+4)} - \frac{2(n-2x-2)}{(n-x+1)(x+3)} + \frac{5}{(n-x)(n-x+1)} + \ln\Big(\frac{x+3}{n-x}\Big)\Big] \ .$$

Since $0 \le x \le (n-5)/2$, we have $x+3 < n-x$ and $n-2x-2 \ge 3$. Using these results, we have

$$-\frac{2(n-2x-2)}{(n-x+1)(x+3)} + \frac{5}{(n-x)(n-x+1)} < 0 \ .$$

Moreover,

$$0 \le \frac{x+3}{n-x} \le 1 \ \text{ and hence } \ln\Big(\frac{x+3}{n-x}\Big) \le 0 \ .$$

Hence

$$f'(x) < 0 \ .$$

Thus $f(x)$ is a decreasing function on $x \le (n-5)/2$ and hence $f(x) \le 4(n+1)^3 n^{n-5}$ with maximum value occurs only when $x = 0$, that is, $n_1 = 0$, $n_2 = n-5$. This completes the proof of this claim.

Similarly we can prove that the maximum value of $\prod_1^*(\theta_{2,1,2}(n_1, n_2))$ is attained at $n_1 = 0, n_2 = n-4$. By the above arguments, we claim that G_0 is one of two graphs $C_{3,3}(0, n-5)$ and $\theta_{2,1,2}(n_1, n_2) \cong B'_n$. Moreover,

$\prod_1^*(C_{3,3}(0, n-5)) = 16(n+1)^4 n^{n-5}$,

$\prod_1^*(\theta_{2,1,2}(0, n-4)) = 20(n+1)^2(n+2)n^{n-4}$, thus,

$$\begin{aligned}\textstyle\prod_1^*(\theta_{2,1,2}(0, n-4)) - \prod_1^*(C_{3,3}(0, n-5)) &= 4(n+1)^2 n^{n-5}[5(n+2)n - 4(n+1)^2] \\ &= 4(n+1)^2 n^{n-5}(n^2+2n-4) > 0.\end{aligned}$$

Therefore we complete the proof of this theorem. □

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

$\mathcal{B}_1(n) = \{C_{p,q} : p+q-1 = n\}$;

$\mathcal{B}_2(n) = \{C_{p,l,q} : p+q+l-1 = n\}$;

$\mathcal{B}_3(n) = \{\theta_{k,l,m} : k+l+m-1 = n\}$.

Let G_i be any graph from $\mathcal{B}_i(n)$ for $i = 1, 2, 3$. Then,

$\prod_1^*(G_1) = 6^4 4^{n-3}$;

$\prod_1^*(G_2) = 5^4 \times 6 \times 4^{n-4}$ if $l = 1$, $\prod_1^*(G_2) = 5^6 \times 4^{n-5}$ if $l > 1$;

$\prod_1^*(G_3) = 5^4 \times 6 \times 4^{n-4}$ when $l = 1$, $\prod_1^*(G_3) = 5^6 \times 4^{n-5}$ when $l > 1$.

Theorem 3.10. *Let G be a graph in $\mathcal{B}(n) \setminus \mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ with $n \geq 6$ and H be a graph in $\mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ with $l = 1$. Then we have $\prod_1^*(H) < \prod_1^*(G)$.*

Proof. Using Lemmas 2.1 and 2.4, and noting Remark 2.1, we conclude that the graph from $\mathcal{B}(n)$ with minimal multiplicative sum Zagreb index $\prod_2$ must be a 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

$\prod_1^*(G_1) - \prod_1^*(G_2) > 0$ and $\prod_1^*(G_1) - \prod_1^*(G_3) > 0$.

Considering the difference of $\prod_1^*(G_i)$ for $i = 2, 3$ when l is different, the result follows immediately. $\square$

Now we present the following theorem in which the graphs extremal with respect to multiplicative sum Zagreb index from $\mathcal{B}(n)$ are completely determined.

Theorem 3.11. *Assume that H is any graph from $\mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ with $l = 1$. Let G be a graph in $\mathcal{B}(n) \setminus \mathcal{B}_2(n) \bigcup \mathcal{B}_3(n)$ different from B_n'. Then $\prod_1^*(H) < \prod_1^*(G) < \prod_1^*(B_n')$.*

Considering the graphs from $\mathcal{T}(n), \mathcal{U}(n)$ and $\mathcal{B}(n)$ extremal with respect to the second multiplicative Zagreb index (see [24]), it seems that there is some interesting relationship between the second multiplicative Zagreb index ($\prod_2$) and the multiplicative sum Zagreb index ($\prod_1^*$). This may be a research topic in the coming future.

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