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Extremal Values of Total Multiplicative Sum Zagreb Index and First Multiplicative Sum Zagreb Coindex on Unicyclic and Bicyclic Graphs

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Abstract

The total multiplicative sum Zagreb index of a simple graph G is defined as $\prod^{T}(G) := \prod_{u,v \in V(G)} (d_G(u) + d_G(v))$, while $\overline{\Pi}_1(G) := \prod_{uv \notin E(G)} (d_G(u) + d_G(v))$ represents the first multiplicative sum Zagreb coindex. Both graphical invariants were introduced by Xu, Das and Tang in [10]. We obtained extremal values of those indices on the class of unicyclic and bicyclic graphs.

1 Introduction

In this paper we consider only finite simple graphs. Let $G = (V, E)$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. For each vertex $v \in V$, let $d_G(v)$ denote the degree of a vertex v in G and $\Delta(G)$ the maximum vertex degree of the graph G. We will omit the subscript G whenever the graph is clear from the context.

A *graphical invariant* is a some number related to a graph whose value remains fixed under graph automorphisms. In chemical graph theory, these invariants are also called the *topological indices*. In this paper, we consider few topological indices: *multiplicative* *sum Zagreb index*

$$\Pi_1^*(G) := \prod_{uv\in E(G)} (d_G(u) + d_G(v)),$$

first multiplicative Zagreb coindex

$$\overline{\Pi}_1(G) := \prod_{uv\notin E(G)} (d_G(u) + d_G(v)),$$

and *total multiplicative sum Zagreb index*

$$\overset{T}{\prod}(G) := \prod_{u,v\in V(G)} (d_G(u) + d_G(v)).$$

While the first one was introduced and studied in [1], the other two were introduced in [10]. Considering definitions of those topological indices, we cannot avoid an impression that the names of the multiplicative sum Zagreb index and first multiplicative Zagreb coindex do not reflect the substantial mathematical relation between them. Nevertheless, that connection is nicely highlighted in Lemma 2.5 of [10]

$$\overline{\prod}_1(G) \cdot \prod{}_1^*(G) = \overset{T}{\prod}(G). \qquad (\star)$$

It is this connection that allowed us to come to a result given in the title of the paper.

The paper is organized as follows. In Section 2 we listed some graph transformations and show how they affect total multiplicative sum Zagreb index. We used those graph transformations in Section 3, and presented extremal values of total multiplicative sum Zagreb index on the class of unicyclic graphs. Following the same approach in Section 4 and Section 5, we obtained the extremal values of total multiplicative sum Zagreb index on the class of and bicyclic graphs graphs. Relying on the identity $(\star)$ and results in the sections 3, 4 and 5, we easily got extremal values of first multiplicative Zagreb coindex on the the class of unicyclic and bicyclic graphs.

2 Transformations and the degree sequence theorem

The *degree sequence* of an undirected graph is the non-increasing sequence of its vertex degrees.

Remark 1: If G and $\widetilde{G}$ are two graphs with the same degree sequences, then $\overset{T}{\prod}(G) = \overset{T}{\prod}(\widetilde{G})$.

For the sake of brevity, from now on we write *total index* instead of *total multiplicative sum Zagreb index*.

In this section, we give an overview of some known and some new graph transformations that will be used in the course of searching for extremal values of the total index and consequently multiplicative coindex for unicyclic and bicyclic graphs. We should emphasize that some of transformations, presented in this section, have already been introduced, as in [9], under different names like: *transformation A, transformation B*, ... However, we consider that the names we propose have a stronger *visual impression* and therefore make the proofs more comprehensive.

For each transformation we will show how that transformation affects the total index; that is, we will compare the total index of the initial and resulting graph. In order to obtain these comparisons we will need the following theorem:

Theorem 2.1 **(Degree sequence theorem).** *Let G, $\widetilde{G}$ be nontrivial graphs, with common vertex set V and $u, v \in V$ such that $d_G(u) = a$, $d_G(v) = b$, $d_{\widetilde{G}}(u) = a + k$, $d_{\widetilde{G}}(v) = b - k$, for some $k \geq 0$, and $d_{\widetilde{G}}(x) = d_G(x)$ for each $x \in V \backslash \{u, v\}$. Then, it holds:*

1. $\prod^T(G) = \prod^T(\widetilde{G})$ *if and only if* $k = 0$ *or* $k = b - a$.
2. $\prod^T(G) < \prod^T(\widetilde{G})$ *if and only if* $k < b - a$.
3. $\prod^T(G) > \prod^T(\widetilde{G})$ *if and only if* $k > b - a$.

Proof. Denote by N set $V \backslash \{u, v\}$. Since the degrees of vertices from N are the same in G and $\widetilde{G}$, we will use d_y instead of $d_G(y)$ and $d_{\widetilde{G}}(y)$ for each $y \in N$.

By the definition of total index, we have

$$\frac{\prod^T(G)}{\prod^T(\widetilde{G})} = \frac{\prod\limits_{y \in N}(d_y + a)(d_y + b)}{\prod\limits_{y \in N}(d_y + a + k)(d_y + b - k)}.$$

It is easy to see that

$$(d_y + a)(d_y + b) = (d_y + a + k)(d_y + b - k) \iff k = 0 \text{ or } k = b - a,$$

and, for $k > 0$ and for each $y \in N$

$$k < b - a \implies (d_y + a)(d_y + b) < (d_y + a + k)(d_y + b - k),$$

$$b - a < k \implies (d_y + a)(d_y + b) > (d_y + a + k)(d_y + b - k).$$

These implies the final conclusion. ■

Now, we are ready to introduce some useful graph transformations.

Pendant-paths (PP) transformation. Let G be a nontrivial graph and $u, v \in G$ vertices, not necessarily different, such that $d_G(v) \geqslant 3$ and $P : uu_1 \dots u_\ell$ and $Q : vv_1v_2 \dots v_s$ be two paths in G that hang on these two vertices. Denote by $\widetilde{G}$ the graph created from G in a way that these two paths are being "concatenated", so the tail $v_1v_2 \dots v_s$ of path Q is attached to u_ℓ. Thus, we get the path: $uu_1 \dots u_\ell v_1 v_2 \dots v_s$ in the new graph $\widetilde{G}$.

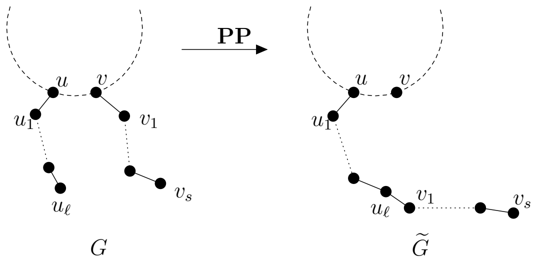

Figure 1

Since $d_G(v) \geqslant 3$ and $d_G(u_\ell) = 1$ and since the PP transformation increases by $k = 1$ the degree of vertex u_ℓ and decreases by $k = 1$ the degree of vertex v, it follows, by Theorem 2.1, that the PP transformation increases the total index.

Contraction to path (CP) transformation. Let G be a nonempty graph whose vertex u has degree $d_G(u) \geqslant 3$ and u is the starting vertex of the path $P : uu_1u_2 \dots u_\ell$ of length $\ell \geqslant 1$. Let v be the neighbor of u so that v is out of P, u and v have no common neighbor and $d_G(v) \geqslant 2$. Let us denote by $G \cdot uv$ graph obtained from G by the contraction of edge uv onto vertex u, and denote by $\widetilde{G}$ graph obtained from $G \cdot uv$ by inserting vertex v on the edge $u_{\ell-1}u_\ell$ (i.e. by subdivision of edge $u_{\ell-1}u_\ell$ with vertex v).

If $d_G(u) = a$ and $d_G(v) = b$, then

$$d_{\widetilde{G}}(u) = a + b - 2, \qquad d_{\widetilde{G}}(v) = 2.$$

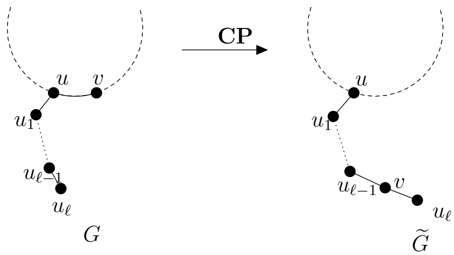

Figure 2

Hence, CP transformation increases the degree of vertex u by $k = b-2$, and decreases the degree of the vertex v by $k = b - 2$. The degrees of all other vertices remain unchanged.

By using Theorem 2.1 we conclude the following:

(i) if $d_G(v) > 2$, then the CP transformation increases total index;

(ii) if $d_G(v) = 2$, then the CP transformation doesn't change total index.

The *comet* $H_{n,i}$ is a unicyclic graph with the cycle C_i on which is attached a path of length $n - i$, $i = 3, \ldots, n - 1$.

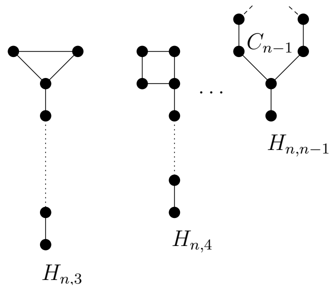

Figure 3

Conclusion. The comets $H_{n,3}, \ldots, H_{n,n-1}$ have the same total index. The same conclusion follows immediately from Remark 1.

Contraction to star (CS) transformation. Let u and v be adjacent vertices of the graph G that have no common neighbor in G and $d_G(u) = a$, $d_G(v) = b$, where $a \geqslant b \geqslant 2$. If $e := uv$, let us denote by $\widetilde{G} = (G \cdot e) + uv$ the graph obtained by the contraction of the edge e onto the vertex u and then adding a pendent vertex v to u.

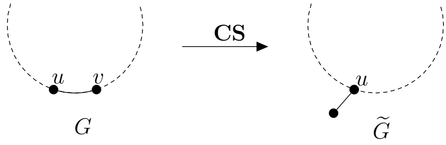

Figure 4

Now we have:

$$d_{\widetilde{G}}(u) = a + b - 1 \qquad \text{and} \qquad d_{\widetilde{G}}(v) = 1.$$

Hence, the CS transformation increases the degree of vertex u by $k = b - 1 > 0$, degree of the vertex v decreases by $k = b - 1$, while degrees of all the other vertices remain unchanged.

If $a = b$ then $k > b - a$, so by using Theorem 2.1 (inequality 3.), then the CS transformation decreases the total index i.e.

$$\prod^{T}(G) > \prod^{T}(\widetilde{G}).$$

Remark 2: The total index of cycle C_n is greater than the total index of comet $H_{n,i}$ for each $i = 3, \ldots, n-1$.

If $a > b$ then $k > b - a$. Thus, by Theorem 2.1 (inequality 3.) the CS transformation decreases the total index.

Star translation (ST) transformation. Let $v \in V(G)$ and let $v_1, v_2, \ldots, v_k$ be pendent vertices and neighbours of v. Let $u \in V(G) \backslash \{v_1, \ldots, v_k\}$.

Let us denote by $\widetilde{G}$ graph

$$(G - \{vv_1, \ldots, vv_k\}) + \{uv_1, \ldots, uv_k\}$$

obtained by "moving" the star $H = G[v, v_1, v_2, \ldots, v_k]$ from vertex v to vertex u.

Let $d_G(v) = b$ and $d_G(u) = a$.

By using Theorem 2.1 we have

(1) if $b - k = a$ then the ST transformation doesn't change the total index;

(2) if $b - k > a$ then the ST transformation increases the total index;

(3) if $b - k < a$ then the ST transformation decreases the total index.

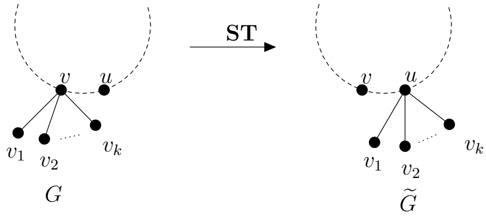

Figure 5

Edge to path (EP) transformation. Let G be a nontrivial graph and $u, v \in G$ two adjacent vertices, such that $d_G(u) \geq 3$. Let $W : uu_1 \dots u_\ell$ be a path in G. Denote by $\widetilde{G}$ the graph created from G in a way that the edge uv is removed and the new edge $u_\ell v$ is added.

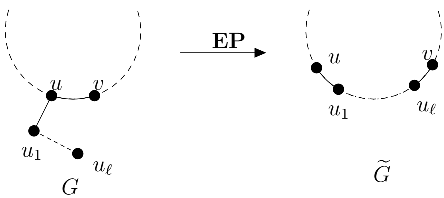

Figure 6

By using the EP transformation, the degree of vertex u decreases by 1, the degree of the vertex u_ℓ increases by 1, while the degrees of all other vertices remain unchanged.

Consider two vertices, u and u_ℓ, in the sense of Theorem 2.1. Clearly $d_G(u_\ell) = 1$, $d_G(u) \geq 3$, while after the transformation we have $d_{\widetilde{G}}(u_\ell) = d_G(u_\ell) + 1$, $d_G(u) = d_{\widetilde{G}}(u) - 1$. Thus, $k = 1$, and since $k < d_{\widetilde{G}}(u) - d_{\widetilde{G}}(u_\ell)$, it follows that $\prod^{T}(G) < \prod^{T}(\widetilde{G})$.

3 Unicyclic graphs extremal with respect to total index

By iterative use of the PP transformation, any tree of a unicyclic graph G can be transformed into a path, and all paths will make, by the PP transformation, a unique path. We have already concluded that the PP transformation increases the total index, so in the family of unicyclic graphs with n vertices and whose cycle contains k vertices, maximum of the total index is attained on the comet $H_{n,k}$. Now, by Remark 2, it follows that in the family of unicyclic graphs with n vertices, maximum of the total index is attained on the cycle C_n.

Similarly, by iterative use of the CS transformation on a unicyclic graph G, one can obtain the unicyclic graph with stars attached on its cycle. Then, by further applying the ST transformation we get a graph H with only one star attached on the cycle. Hence,

$$\prod^{T}(H) \leqslant \prod^{T}(G).$$

It follows that in the family of unicyclic graphs with n vertices and cycle C_k, minimum of the total index is attained on the graph C_n^k, whose cycle C_k contains a vertex adjacent to $n-k$ pendent vertices.

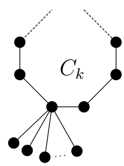

Figure 7. The graph C_n^k.

By further repeating of the CS transformation, we obtain a unicyclic graph with the cycle C_3 containing one vertex adjacent to $n-3$ pendent vertices. Therefore, we conclude that among unicyclic graphs with n vertices, the minimum of the total index is attained on the graph presented by the Figure 8.

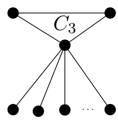

Figure 8. The graph C_n^3.

4 Maximum of total index on bicyclic graphs

Denote by $\mathcal{B}(n)$ the set of connected bicyclic graphs of order n. As in [8] and [9], the structure of two independent 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 u;

(II) The two cycles C_p and C_q in G are linked by a path of length $r > 0$;

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

The graphs $C_{p,q}$, $C_{p,r,q}$ and $\Theta_{k,i,j}$ (where $1 \leq k \leq \min\{i, j\}$) corresponding to the cases above shown in the Figure 9 are called **main subgraphs** of $G \in \mathcal{B}(n)$ of type (I), (II) and (III), respectively.

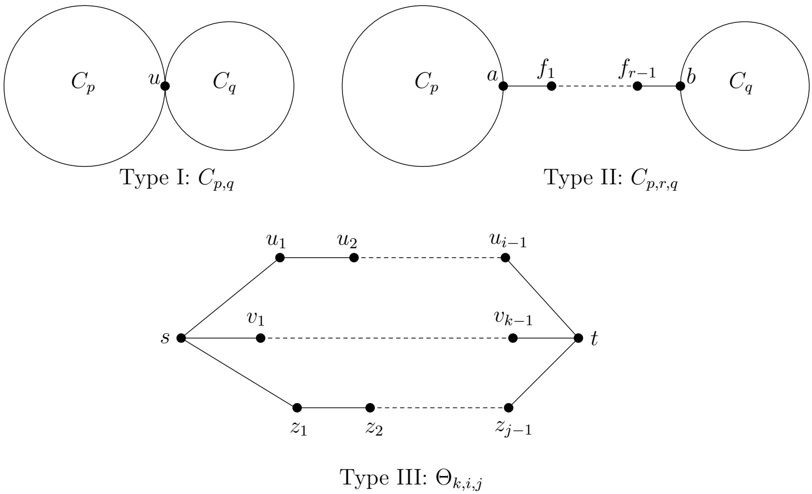

Figure 9. Main subgraphs of bicyclic graphs.

By iterative use of the PP transformation, one can transform every tree in a graph G into a path, and later, employing the same transformation, we get an unique path concatenating all other paths. As we already stated, the PP transformation increases the total index of a graph. Therefore, we end up with a graph whose main subgraph is one of the three types given above and that has one pendant path $W : w_1\, w_2\, \ldots\, w_\ell$ attached at some vertex. Depending on which vertex the path W is attached to, we consider some situations.

1. **The main subgraph of a graph is of type I.**

   If the path W is attached to the vertex u, then we can move it and attach to any vertex x in those two cycles, C_p or C_q. Now, we can apply the EP transformation on the vertex x and some of its adjacent vertices y of degree 2. As we already determined, it also increases the total index of a graph. Finally, we get a graph of type I, where one of the circles is expanded by the size of the path W.

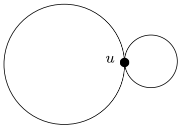

Figure 10. Bicyclic graph G_1 of type I.

2. **The main subgraph of a graph is of type II.**

   If the path W were attached to any of the vertices: $a, b, f_1, \ldots, f_{r-1}$, we can move it and attach to any vertex x inside one of the cycles, other than a or b. Now, we can apply the EP transformation on the vertex x and some of its adjacent vertices y of degree 2, which again increases the total index of a graph. Note, it is still a graph of type II with one of the circles expanded by the size of path W. Further, we can insert vertices $\{f_1, \ldots, f_{r-1}\}$ into one of the circles, which does not change the degrees of the graph and therefore does not change the total index. Finally, we get the graph with two cycles, connected by the edge ab as in the figure below

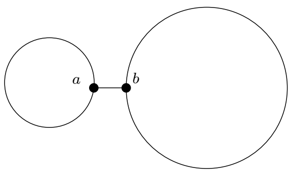

Figure 11. Bicyclic graph G_2 of type II.

   As we can see, it is still a graph of type II, where the path between two cycles is reduced to the length 1.

3. **The main subgraph of a graph is of type III.**

   In this case, we can basically copy the approach from the previous case. So, let us suppose that the path W were attached to any of the vertices: $s, t, v_1, \ldots, v_{k-1}$. As before, we move it and attach to some vertex inside one of the cycles, other than s or t, which, by Theorem 2.1, increases the total index of a graph. Again, we apply the EP transformation on the vertex x and some of its adjacent vertices y of degree 2, which also increases the total index of a graph. Further, we can insert vertices $\{v_1, \ldots, v_{k-1}\}$ into one of the circles; that does not change the degrees of the graph and therefore does not change the total index. Finally, we get a graph of type III, with two cycles sharing the st edge, as in the figure below

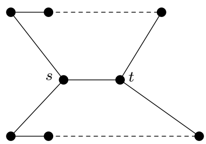

Figure 12. Bicyclic graph G_3 of type III.

As we can see, it is still a graph of type III, where two cycles share just one edge.

It has been shown that every bicyclic graph from $\mathcal{B}(n)$ could be transformed into one of the basic three types of bicyclic graphs: G_1 (Figure 10), G_2 (Figure 11) or G_3 (Figure 12), which have greater total index compared to the original graph we considered. Therefore, we need to determine which one of the three graphs G_1, G_2 or G_3 has the greatest total index. Certainly, all three graphs are of order n and it is clear that the degree sequences of G_2 and G_3 are the same. Hence, we should just compare G_1 and G_2.

There are $n-1$ vertices of degree 2 and one vertex of degree 4 in G_1. Hence

$$\prod^{T}(G_1) = (2+2)^{\binom{n-1}{2}}(2+4)^{n-1} = 4^{\binom{n-1}{2}}6^{n-1}.$$

There are $n-2$ vertices of degree 2 and two vertices of degree 3 in G_2, so

$$\prod^{T}(G_2) = (2+2)^{\binom{n-2}{2}}(2+3)^{n-2}(2+3)^{n-2}(3+3) = 4^{\binom{n-2}{2}}5^{2n-4}\cdot 6.$$

Therefore,

$$\frac{\prod^{T}(G_2)}{\prod^{T}(G_1)} = \left(\frac{25}{24}\right)^{n-2},$$

which means that $\prod^{T}(G_2) > \prod^{T}(G_1)$. This fact leads to the conclusion that the maximum of the total index for the class of bicyclic graphs $\mathcal{B}(n)$ is achieved on graphs G_2 or G_3.

5 Minimum of total index on bicyclic graphs

In order to find the bicyclic graph with the minimal total index we use a technique similar to the one of unicyclic graphs: consecutive repetition of the CS transformation leads to the bicyclic graph with two triangles and hanging stars, whose total index is less than the index of the starting graph. In the next step we repeat the ST transformation until we carry over the incoming graph of type I or III to the graph R_1 (Figure 13), or in the case of incoming graph of type II to the graph R_2 (Figure 13).

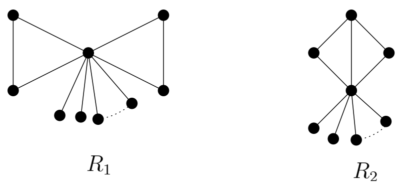

Figure 13

Now, it remains to compare the total index of the graphs R_1 and R_2 with $n \geqslant 5$ vertices. We obtain

$$\frac{\overset{T}{\prod}(R_1)}{\overset{T}{\prod}(R_2)} = \frac{2^{\binom{n-5}{2}} \cdot n^{n-5} \cdot 3^{4(n-5)} \cdot (n+1)^4 \cdot 4^{\binom{4}{2}}}{2^{\binom{n-4}{2}} \cdot n^{n-4} \cdot 3^{2(n-4)} \cdot 4^{n-3} \cdot (n+1)^2 \cdot (n+2) \cdot 5^2}$$
$$= \frac{3^{2n-12}\,(n+1)^2}{2^{3n-23}\,25n(n+2)} = \frac{8388608 \cdot 9^n}{13286025 \cdot 8^n} \cdot \frac{(n+1)^2}{n^2+2n}$$

which is greater than 1 for each $n \geqslant 5$.

6 Unicyclic and bicyclic graphs extremal with respect to multiplicative sum Zagreb coindex

Firstly, we quote Lemma 2.5 of [10]:

Lemma 6.1. *For a connected graph G, we have $\overline{\prod}_1(G) \cdot \prod_1^*(G) = \overset{T}{\prod}(G)$.*

By using this Lemma, Theorem 3.8 of [9], and Section 3, it follows

Theorem 6.2. *In the family of unicyclic graphs with n vertices, the maximum of the multiplicative sum Zagreb coindex is attained on the cycle C_n, and the minimum of the multiplicative sum Zagreb coindex is attained on the graph C_n^3 (Figure 8).*

In the same manner, by using Lemma 6.1, Theorem 3.11 of [9], and Section 5, we have the next assertion

Theorem 6.3. *In the family of bicyclic graphs the minimum of the multiplicative sum Zagreb coindex is achieved on graph R_1 (Figure 13).*

Finally, by using Lemma 6.1, Theorem 3.11 of [9], and Section 4, we obtain

Theorem 6.4. *In the family of bicyclic graphs the maximum of the multiplicative sum Zagreb coindex is achieved on graphs G_2 and G_3 (Figure 11, 12).*

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