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Extremal Graphs with Respect to the Multiplicative Sum Zagreb Index

Batmend Horoldagva[a,*], **Chunlei Xu**[a,b],
Lkhagva Buyantogtokh[a], **Shiihar Dorjsembe**[a]

[a]*Department of Mathematics, Mongolian National University of Education, Baga toiruu-14, Ulaanbaatar 48, Mongolia*
[b]*School of Mathematics, Inner Mongolia University for Nationalities, Tongliao, People's Republic of China*
horoldagva@msue.edu.mn, xuchunlei1981@sina.cn,
buyantogtokh.l@msue.edu.mn, dorjsembe@msue.edu.mn

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Abstract

The multiplicative sum Zagreb index of a graph G, denoted by $\Pi_1^*(G)$, is the product of the sum of the degrees of adjacent vertices in G. This graphical invariant is the multiplicative version of the well known first Zagreb index and introduced by Eliasi, Iranmanesh and Gutman (*MATCH Commun. Math. Comput. Chem.* **68** (2012) 217–230). In this paper we determine the extremal graphs with respect to the multiplicative sum Zagreb index for several classes of graphs.

1 Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of the vertex u in G is denoted by $d_G(u)$. In chemical graph theory and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. The oldest and best known topological indices are the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G and they are defined as

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

*Corresponding author

These indices were first introduced about fifty years ago by Gutman and Trinajstić [12], and for details of the mathematical studies and chemical applications on the Zagreb indices, see [3, 13, 15, 21, 24] and the references cited therein. Moreover the classical Zagreb indices M_1 and M_2 were studied in the mathematical literature under other names [2, 6, 23, 28]. Also the relation and comparison between M_1 and M_2 were investigated in [5, 7, 10, 11, 16–18, 25].

Todeschini and Consonni [26] proposed the multiplicative versions of the classical Zagreb indices M_1 and M_2, which are defined as

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

Gutman [14] studied these two graph invariants and called the first and second multiplicative Zagreb indices, respectively. The recent results related to the multiplicative Zagreb indices and their other versions can be found in [1, 4, 8, 20, 22, 27, 29, 30, 32].

Eliasi, Iranmanesh and Gutman [9] introduced a new graphical invariant, which is the multiplicative version of the well known first Zagreb index M_1 and called the multiplicative sum Zagreb index by Xu and Das [31]. The multiplicative sum Zagreb index is defined as follows:

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

Although Π_1^* was introduced in 2012, it has been studied only to a limited extent for various class of graphs. Eliasi, Iranmanesh and Gutman [9] proved that among all connected graphs with a given order, the path has minimal Π_1^*-value. Also they determined the trees with the second minimal Π_1^*-value. Xu and Das [31] characterized the extremal trees, unicyclic and bicyclic graphs with a given order with respect to the multiplicative sum Zagreb index by introducing some graph transformations. Kazemi [19] studied the multiplicative Zagreb indices of molecular graphs with tree structure.

For vertices $u, v \in V(G)$, the distance between $d(u, v)$ is defined as the length of the shortest path between u and v. A cut edge in a graph G is an edge whose removal increases the number of connected components of G. For $uv \in E(G)$, denote by $G - uv$ the subgraph of G obtained from G by deleting the edge uv. For two nonadjacent vertices $u, v \in V(G)$, denote by $G + uv$ the graph obtained from G by adding the edge uv. The girth of a graph G is the length of a shortest cycle contained in G. Maximum degree of

G is denoted by Δ. Denote by $\mathcal{U}_{n,g}$ the class of all unicyclic graphs of order n with girth g. Denote by $\mathcal{G}_{n,k}$ the class of all connected graphs of order n with k cut edges.

The aim of this paper is to continue works started by Gutman [14], Eliasi et al. [9] and Xu et al. [31] on the multiplicative sum Zagreb index. We denote by $\mathcal{F}_{n,g}$ and $\mathcal{H}_{n,k}$ the class of graphs of order n with girth g and the class of graphs of order n with k pendant vertices, respectively. The paper is organized as follows. In section 2, we present the sharp upper bound on Π_1^* of graphs in $\mathcal{U}_{n,g}$ and characterize extremal graphs. Also, we determine the graphs that have minimal Π_1^*-value in $\mathcal{U}_{n,g}$ and $\mathcal{F}_{n,g}$. In section 3, we obtain the sharp upper bound on Π_1^* of graphs in $\mathcal{G}_{n,k}$ and characterize the corresponding extremal graphs. Moreover, we determine the graphs that have minimal and maximal Π_1^*-value in $\mathcal{G}_{n,k}$ and $\mathcal{H}_{n,k}$, respectively.

2 Extremal graphs in $\mathcal{U}_{n,g}$ and $\mathcal{F}_{n,g}$ with respect to Π_1^*

In this section, we obtain the extremal graphs with respect to multiplicative sum Zagreb index for the class of unicyclic graphs of order n with girth g. Also, we obtain the graphs that have minimal Π_1^*-value in the class of graphs of order n with girth g. Let $P = uu_1u_2\cdots u_k$ be a path in G such that $d_G(u) \geq 3$, $d_G(u_k) = 1$ and $d_G(u_i) = 2$ for $1 \leq i < k$. Then it is called a pendant path in G, u and k are called the origin and the length of P. The following results immediately follows from the definition of multiplicative sum Zagreb index.

Lemma 2.1. *Let G be a connected graph.*
(i) If $uv \notin E(G)$ then $\Pi_1^*(G) < \Pi_1^*(G + uv)$.
(ii) If $uv \in E(G)$ then $\Pi_1^*(G) > \Pi_1^*(G - uv)$.

Transformation A. Let P_1 and P_2 be two pendant paths with origin u and v in a connected graph G, respectively. Suppose that x is the neighbor of the vertex u on P_1 and y is the pendant vertex on P_2. Let G' be the graph obtained from G by deleting edge ux and adding new edge xy. (see Figure 1.)

Lemma 2.2. [31] Let G and G' be the graphs depicted in Figure 1. If $u \equiv v$ then $\Pi_1^*(G') < \Pi_1^*(G)$.

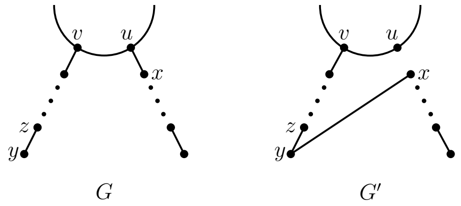

Figure 1. Transformation A

Lemma 2.3. *Let G and G' be the graphs depicted in Figure 1.*

(i) If $d_G(u) \geq 4$, then $\Pi_1^*(G') < \Pi_1^*(G)$.

(ii) If there exists $u_i \in N_G(u)$ such that $u_i \neq x$ and $d_G(u) + d_G(u_i) \leq 16$, then $\Pi_1^*(G') < \Pi_1^*(G)$.

Proof. Let z be the neighbor of the pendant vertex y. By the definition of Π_1^*, we have

$$\begin{aligned} \frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{(d_G(x)+2)(d_G(z)+2)}{(d_G(u)+d_G(x))(d_G(z)+1)} \prod_{u_i \in N_G(u)\setminus\{x\}} \frac{d_G(u)+d_{G_1}(u_i)-1}{d_G(u)+d_G(u_i)} \\ &= \frac{d_G(x)+2}{d_G(u)+d_G(x)} \cdot \left(1+\frac{1}{d_G(z)+1}\right) \prod_{u_i \in N_G(u)\setminus\{x\}} \left(1-\frac{1}{d_G(u)+d_G(u_i)}\right). \quad (1) \end{aligned}$$

(i) If the length of the pendant path P_2 is greater and equal to 2, then $d_G(z) = 2$. Clearly $d_G(x) \leq 2$. Then from (1), we get $\Pi_1^*(G') < \Pi_1^*(G)$ since $d_G(u) \geq 4$. If the length of the pendant path P_2 is equal to 1, then $z \equiv v$ and $d_G(z) \geq 3$. Hence, from (1) we have

$$\frac{\Pi_1^*(G')}{\Pi_1^*(G)} < \frac{5}{4} \cdot \frac{d_G(x)+2}{d_G(u)+d_G(x)}. \quad (2)$$

Since $d_G(u) \geq 4$ and $d_G(x) \leq 2$, it follows from (2) that $\Pi_1^*(G') < \Pi_1^*(G)$.

(ii) If $d_G(u) \geq 4$ then $\Pi_1^*(G') < \Pi_1^*(G)$ by (i). Let now $d_G(u) = 3$. Then, since there exists a neighbour u_i ($u_i \neq x$) of u such that $d_G(u) + d_G(u_i) \leq 16$, we have

$$\begin{aligned} \frac{\Pi_1^*(G')}{\Pi_1^*(G)} &< \frac{d_G(x)+2}{d_G(u)+d_G(x)} \cdot \left(1+\frac{1}{d_G(z)+1}\right)\left(1-\frac{1}{d_G(u)+d_G(u_i)}\right) \\ &\leq \frac{d_G(x)+2}{3+d_G(x)} \cdot \left(1+\frac{1}{d_G(z)+1}\right) \cdot \frac{15}{16} \quad (3) \end{aligned}$$

from (1). Clearly, we have $d_G(z) \geq 2$ and $d_G(x) \leq 2$. Therefore, it follows from (3) that $\Pi_1^*(G') < \Pi_1^*(G)$. ■

A unicyclic graph G is said to be a sun graph if $\Delta(G) = 3$ and the origin of all pendant paths lie on the unique cycle C. Denote by $\mathcal{S}(n, g)$ the class of all sun graphs of order n with girth g. Then we have $\mathcal{S}(n, g) \subset \mathcal{U}_{n,g}$.

Proposition 2.4. *Let $G \in \mathcal{U}_{n,g}$. If $\Pi_1^*(G)$ is minimum in $\mathcal{U}_{n,g}$ then $G \in \mathcal{S}(n, g)$.*

Proof. Suppose that $G \notin \mathcal{S}(n, g)$. Then there are two pendant paths P_1 and P_2 with common origin u. If we apply Transformation A for the paths P_1 and P_2, then $\Pi_1^*(G) > \Pi_1^*(G')$ by Lemma 2.2, which is a contradiction. ■

We denote by $C_{n,g}$ the sun graph of order n with girth g that has at most one pendant path. If $g = n$ then $C_{n,n}$ is the cycle of order n and it is denoted by C_n.

Theorem 2.5. *Let G be a unicyclic graph in $\mathcal{U}_{n,g}$ which is not isomorphic to $C_{n,g}$. Then $\Pi_1^*(G) > \Pi_1^*(C_{n,g})$.*

Proof. Suppose that $\Pi_1^*(G)$ is minimum in $\mathcal{U}_{n,g} \setminus C_{n,g}$. Then by Proposition 2.4, we have $G \in \mathcal{S}(n,\, g)$ and there exist at least two pendant paths P_1 and P_2 with origin u and v, respectively, such that $u, v \in V(C)$. Clearly $d_G(u) = 3$ and $d_G(u) + d_G(u_i) \leq 6$ for all $u_i \in N_G(u)$. We apply Transformation A for the paths P_1 and P_2, then $G' \in \mathcal{U}_{n,g}$ and $\Pi_1^*(G) > \Pi_1^*(G')$ by Lemma 2.3 (ii). If G' is not isomorphic to $C_{n,g}$, then we have a contradiction to the fact that $\Pi_1^*(G)$ is minimum in $\mathcal{U}_{n,g} \setminus C_{n,g}$. Otherwise, we get the required result. ■

Theorem 2.6. *Let G be a graph in $\mathcal{F}_{n,g}$. If $\Pi_1^*(G)$ is minimum in $\mathcal{F}_{n,g}$ then G is isomorphic to $C_{n,g}$.*

Proof. Let g be the girth of G and C be a cycle of length $g \geq 3$ in G. By deleting edges from a graph G, the multiplicative sum Zagreb index decreases by Lemma 2.1 (ii). Thus by deleting the edges of G, which does not lie on the cycle C, a sufficient number of times we arrive at a graph in $\mathcal{U}_{n,g}$. Then since $\Pi_1^*(G)$ is minimum in $\mathcal{F}_{n,g}$, it follows that G is isomorphic to $C_{n,g}$ by Theorem 2.5. This completes the proof. ■

Xu and Das [31] introduced the following transformation in order to characterize the trees, unicyclic and bicyclic graphs with maximal multiplicative sum Zagreb index.

Transformation B. Let uv be a cut edge of a graph G such that $d_G(u) \geq 2$ and $d_G(v) \geq 2$. Denote by $G' = G \cdot (uv) + uv$ the graph obtained by the contraction of uv onto the vertex u and adding a pendant vertex v to u. (see Figure 2.)

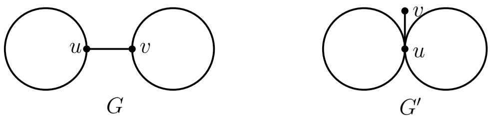

Figure 2. Transformation B

Lemma 2.7. [31] Let G and G' be the graphs depicted in Figure 2. Then $\Pi_1^*(G) < \Pi_1^*(G')$.

Proposition 2.8. *Let $G \in \mathcal{G}_{n,k}$. If $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,k}$, then all cut edges of G are pendant.*

Proof. Suppose, on the contrary, that G contains a non-pendant cut edge uv. Then $d_G(u) \geq 2$ and $d_G(v) \geq 2$. Let G' be the graph obtained from G by using Transformation B, i.e., $G' = G \cdot (uv) + uv$. Then $G' \in \mathcal{G}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G')$ by Lemma 2.7. Therefore, we have a contradiction to the assumption that $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,k}$. ■

Corollary 2.9. [31] Let T be a tree of order n which is different from S_n. Then $\Pi_1^*(T) < \Pi_1^*(S_n)$.

A unicyclic graph is called as cycle-caterpillar if deleting all its pendant vertices will reduce it to a cycle. Denote by $\mathcal{U}(n, g)$ the class of all cycle-caterpillars of order n with girth g. Then the following result immediately follows from Proposition 2.8.

Corollary 2.10. *Let $G \in \mathcal{U}_{n,g}$. If $\Pi_1^*(G)$ is maximum in $\mathcal{U}_{n,g}$ then $G \in \mathcal{U}(n, g)$.*

Denote by $U_{n,g}$ the unicyclic graph obtained by attaching $n-g$ pendant edges to a vertex of C_g.

Theorem 2.11. *Let $G \in \mathcal{U}_{n,g}$. Then*

$$\Pi_1^*(G) \leq 4^{g-2}(n-g+3)^{n-g}(n-g+4)^2 \tag{4}$$

with equality holding if and only if G is isomorphic to $U_{n,g}$.

Proof. If G is isomorphic to $U_{n,g}$, then $\Pi_1^*(G) = 4^{g-2}(n-g+3)^{n-g}(n-g+4)^2$, the equality holds. Suppose that G is not isomorphic to $U_{n,g}$ and $\Pi_1^*(G)$ is maximum in $\mathcal{U}_{n,g}$. Then by Corollary 2.10, we have $G \in \mathcal{U}(n, g)$. Let $v_1, v_2, \ldots, v_g$ be the vertices, which are numbered clockwise, of cycle $C(G)$ and n_i be the number of pendant vertices adjacent to vertex v_i, $i = 1, 2, \dots, g$. Without loss of generality we may assume that v_1 is maximum degree vertex of G. Then, since G is not isomorphic to $U_{n,g}$, there exists a vertex v_i such that $v_i \neq v_1$ and $n_i \geq 1$. Clearly, the vertices v_1 and v_i lie on the cycle $C(G)$. Let $x_1, x_2, \dots, x_{n_i}$ be the pendant neighbors of v_i. Consider the graph

$$G' = G - \{v_i x_1, v_i x_2, \dots, v_i x_{n_i}\} + \{v_1 x_1, v_1 x_2, \dots, v_1 x_{n_i}\}.$$

Then we have $d_{G'}(v_i) = 2$, $d_{G'}(v_1) = d_G(v_1) + n_i$ and $d_{G'}(v_j) = d_G(v_j)$ for $j \neq 1$ and $j \neq i$. Now, in order to prove that $\Pi_1^*(G') > \Pi_1^*(G)$ we distinguish the following three cases:

Case 1. $d(v_1, v_i) \geq 3$. By the definition of Π_1^*, we have

$$\begin{aligned}
\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{n_{i-1}+4}{n_i+n_{i-1}+4} \cdot \frac{n_{i+1}+4}{n_{i+1}+n_i+4} \cdot \frac{n_1+n_i+n_g+4}{n_1+n_g+4} \\
&\times \frac{n_1+n_i+n_2+4}{n_1+n_2+4} \cdot \frac{(n_1+n_i+3)^{n_1+n_i}}{(n_i+3)^{n_i}(n_1+3)^{n_1}} \\
&= \left(1 - \frac{n_i}{n_i+n_{i-1}+4}\right)\left(1 - \frac{n_i}{n_{i+1}+n_i+4}\right)\left(1 + \frac{n_i}{n_1+n_g+4}\right) \\
&\times \left(1 + \frac{n_i}{n_1+n_2+4}\right)\left(1 + \frac{n_1}{n_i+3}\right)^{n_i}\left(1 + \frac{n_i}{n_1+3}\right)^{n_1}. \qquad (5)
\end{aligned}$$

On the other hand we have $n_{i-1}, n_{i+1} \geq 0$ and $n_2, n_g \leq n_1$. Therefore from (5), by using these inequalities and well known Bernoulli's inequality, we get

$$\begin{aligned}
\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &\geq \left(1 - \frac{n_i}{n_i+4}\right)^2\left(1 + \frac{n_i}{2n_1+4}\right)^2\left(1 + \frac{n_1 n_i}{n_i+3}\right)\left(1 + \frac{n_1 n_i}{n_1+3}\right) \\
&\geq \left(1 - \frac{n_i}{n_i+4}\right)^2\left(1 + \frac{n_i}{2n_1+4}\right)^2\left(1 + \frac{n_1 n_i}{n_1+3}\right)^2 \\
&= \left(\frac{2(2n_1+n_i+4)(n_1+3+n_1 n_i)}{(n_i+4)(n_1+2)(n_1+3)}\right)^2 \\
&= \left(\frac{2(2n_1^2+10n_1+2n_1^2 n_i+3n_i+5n_1 n_i+n_1 n_i^2+12)}{n_1^2 n_i+4n_1^2+5n_1 n_i+20n_1+6n_i+24}\right)^2 \\
&= \left(1 + \frac{3n_1^2 n_i+5n_1 n_i+2n_1 n_i^2}{n_1^2 n_i+4n_1^2+5n_1 n_i+20n_1+6n_i+24}\right)^2 > 1.
\end{aligned}$$

Case 2. $d(v_1, v_i) = 2$. In this case we can assume that $i = 3$. Using similar argument as the above case, we get

$$\begin{aligned}
\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{n_1+n_3+n_2+4}{n_1+n_2+4} \cdot \frac{n_1+n_3+n_g+4}{n_1+n_g+4} \cdot \frac{n_2+4}{n_2+n_3+4} \\
&\times \frac{n_4+4}{n_3+n_4+4} \cdot \left(\frac{n_1+n_3+3}{n_1+3}\right)^{n_1} \cdot \left(\frac{n_1+n_3+3}{n_3+3}\right)^{n_3}
\end{aligned}$$

$$
\begin{aligned}
&= \left(1+\frac{n_3}{n_1+n_2+4}\right)\left(1+\frac{n_3}{n_1+n_g+4}\right)\left(1-\frac{n_3}{n_2+n_3+4}\right)\\
&\times \left(1-\frac{n_3}{n_3+n_4+4}\right)\left(1+\frac{n_3}{n_1+3}\right)^{n_1}\left(1+\frac{n_1}{n_3+3}\right)^{n_3}\\
&\geq \left(1+\frac{n_3}{2n_1+4}\right)^2\left(1-\frac{n_3}{n_3+4}\right)^2\left(1+\frac{n_1n_3}{n_1+3}\right)\left(1+\frac{n_1n_3}{n_3+3}\right)\\
&\geq \left(1+\frac{n_3}{2n_1+4}\right)^2\left(1-\frac{n_3}{n_3+4}\right)^2\left(1+\frac{n_1n_3}{n_1+3}\right)^2\\
&= \left(\frac{2(2n_1+4+n_3)(n_1+3+n_1n_3)}{(n_1+2)(n_3+4)(n_1+3)}\right)^2\\
&= \left(1+\frac{3n_1^2n_3+5n_1n_3+2n_1n_3^2}{n_1^2n_3+5n_1n_3+4n_1^2+20n_1+6n_3+24}\right)^2>1.
\end{aligned}
$$

Case 3. $d(v_1, v_i) = 1$. In this case we can assume that $i = 2$. Similarly as the above cases, we also get

$$
\begin{aligned}
\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{(n_1+n_2+4)(n_3+4)(n_1+n_2+n_g+4)(n_1+n_2+3)^{n_1+n_2}}{(n_1+n_2+4)(n_2+n_3+4)(n_1+n_g+4)(n_1+3)^{n_1}(n_2+3)^{n_2}}\\
&= \left(1-\frac{n_2}{n_2+n_3+4}\right)\left(1+\frac{n_2}{n_1+n_g+4}\right)\left(1+\frac{n_2}{n_1+3}\right)^{n_1}\left(1+\frac{n_1}{n_2+3}\right)^{n_2}\\
&\geq \left(1-\frac{n_2}{n_2+4}\right)\left(1+\frac{n_2}{2n_1+4}\right)\left(1+\frac{n_1n_2}{n_1+3}\right)\left(1+\frac{n_1n_2}{n_2+3}\right)\\
&\geq \left(1-\frac{n_2}{n_2+4}\right)\left(1+\frac{n_2}{2n_1+4}\right)\left(1+\frac{n_1n_2}{n_1+3}\right)^2\\
&\geq \left(1-\frac{n_2}{n_2+4}\right)\left(1+\frac{n_2}{2n_1+4}\right)\left(1+\frac{2n_1n_2}{n_1+3}\right)\\
&= \frac{2(2n_1+4+n_2)(n_1+3+2n_1n_2)}{(n_1+2)(n_2+4)(n_1+3)}\\
&= 1+\frac{7n_1^2n_2+13n_1n_2+4n_1n_2^2}{n_1^2n_2+4n_1^2+5n_1n_2+20n_1+6n_2+24}>1.
\end{aligned}
$$

In all of the above cases, we have $\Pi_1^*(G') > \Pi_1^*(G)$ and it contradicts to the assumption that $\Pi_1^*(G)$ is maximum in $\mathcal{U}_{n,g}$. ■

3 Extremal graphs in $\mathcal{G}_{n,k}$ and $\mathcal{H}_{n,k}$ with respect to Π_1^*

In this section, we obtain extremal graphs with respect to multiplicative sum Zagreb index for the class of connected graphs of order n with k cut edges. Also, we determine the graphs that have maximal Π_1^*-value in the class of graphs of order n with k pendant vertices. A connected graph of order n has at most $n-1$ cut edges and if $k = n-1$ then it is a tree. Eliasi, Iranmanesh and Gutman [9] proved that among all connected graphs with a given number of vertices, the path P_n has minimal Π_1^*-value. Also among all connected graphs with a given number of vertices, the star S_n has maximal Π_1^*-value by Corollary 2.9. Therefore, we further assume that $0 \le k < n-1$. Xu and Das [31] determined the graphs extremal with respect to multiplicative sum Zagreb index from the class of bicyclic graphs of order n.

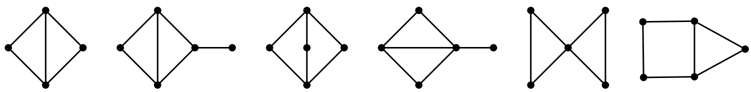

Figure 3. Bicyclic graphs of order 4 and 5.

Lemma 3.1. [31] Let G be a bicyclic graph of order $n \ge 6$. Then $\Pi_1^*(G) \ge 4^{n-4} \cdot 5^4 \cdot 6$.

Theorem 3.2. *Let G be a graph in $\mathcal{G}_{n,k}$ with $0 \le k < n-1$. If $\Pi_1^*(G)$ is minimum in $\mathcal{G}_{n,k}$ then G is isomorphic to $C_{n,n-k}$.*

Proof. Let G be a graph in $\mathcal{G}_{n,k}$ which is not isomorphic to $C_{n,n-k}$ such that $\Pi_1^*(G)$ is minimum. Then we show that $\Pi_1^*(G) > \Pi_1^*(C_{n,n-k})$. Since G is connected and $0 \le k < n-1$, we have $n \ge 3$. Let ν be the cyclomatic number of G. Since $k < n-1$, we have $\nu \ge 1$. If $\nu = 1$ then G is a unicyclic graph and the girth of G is $n-k$. Hence $G \in \mathcal{U}_{n,n-k}$. Since G is not isomorphic to $C_{n,n-k}$, we have $\Pi_1^*(G) > \Pi_1^*(C_{n,n-k})$ by Theorem 2.5.

Let now $\nu \ge 2$. Then $n \ge 4$. Let g be the girth of G and C be a cycle of length $g \ge 3$ in G. By deleting the non-cut edges of G, which does not lie on the cycle C, a sufficient number of times ($\nu - 1$-times) we arrive at a graph $G_{\nu-1}$ in $\mathcal{U}_{n,g}$. Thus by Lemma 2.1, we get the following sequence

$$\Pi_1^*(G) > \Pi_1^*(G_1) > \cdots > \Pi_1^*(G_{\nu-2}) > \Pi_1^*(G_{\nu-1}). \tag{6}$$

On the other hand one can easily calculate that

$$\Pi_1^*(C_{n,t}) = 3 \cdot 4^{n-4} \cdot 5^3 \tag{7}$$

for all $t < n-1$. Clearly $G_{\nu-2}$ is a bicyclic graph. Let $4 \le n \le 5$. Then all bicyclic graphs of order n are depicted in Figure 3 and $G_{\nu-2}$ is isomorphic to one of them. In this case one can easily check that $\Pi_1^*(G_{\nu-2}) > \Pi_1^*(C_{n,\,n-k})$. Let now $n \geq 6$. Then, by Lemma 3.1 and (7), we have

$$\begin{aligned} \Pi_1^*(G_{\nu-2}) &\geq 4^{n-4} \cdot 5^4 \cdot 6 > 4^{n-2} \cdot 5^2 = \Pi_1^*(C_{n,\,n-1}) \\ &> 3 \cdot 4^{n-4} \cdot 5^3 = \Pi_1^*(C_{n,\,n-k}) > 4^n = \Pi_1^*(C_n) \end{aligned} \tag{8}$$

for $k > 1$. From (6) and (8), we obtain that $\Pi_1^*(G) > \Pi_1^*(C_{n,\,n-k})$ for all $0 \leq k < n-1$. This completes the proof. ■

Denote by $\mathcal{G}(n,k)$ the class of graphs of order n with k pendant vertices in which the removal of all pendant vertices and their incident edges results in a complete graph of order $n-k$.

Lemma 3.3. *Let G be a graph in $\mathcal{G}_{n,\,k}$ with $0 \leq k < n-1$. If $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,\,k}$ then $G \in \mathcal{G}(n,k)$.*

Proof. Since $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,\,k}$, all cut edges of G are pendant by Proposition 2.8. If $G \notin \mathcal{G}(n,k)$, then there exist two non-adjacent vertices u and v in G whose degrees are greater than one. Now consider the graph $G' = G + uv$. Then $G' \in \mathcal{G}_{n,\,k}$ and $\Pi_1^*(G') > \Pi_1^*(G)$ by Lemma 2.2, so this is a contradiction. ■

Lemma 3.4. *Let a, b and c be non-negative real numbers. If $x \geq 0$ then*

$$\frac{x+a+b+c}{x+a+c} \cdot \frac{x+c}{x+b+c} \geq \frac{a+b+c}{a+c} \cdot \frac{c}{b+c}. \tag{9}$$

Proof. Let us consider a function

$$f(x) = \frac{x+a+b+c}{x+a+c} \cdot \frac{x+c}{x+b+c}.$$

Then, we have

$$\begin{aligned} f'(x) &= -\frac{b}{(x+a+c)^2} \cdot \frac{x+c}{x+b+c} + \frac{x+a+b+c}{x+a+c} \cdot \frac{b}{(x+b+c)^2} \\ &= \frac{b(x+a+b+c)(x+a+c) - b(x+b+c)(x+c)}{(x+a+c)^2(x+b+c)^2} \\ &\geq 0 \end{aligned}$$

and it follows that $f(x)$ is a non-decreasing function of x. Therefore $f(x) \geq f(0)$, which proves the inequality (9). ■

Denote by $G_{n,\,k}$ the graph obtained by attaching k pendant edges to a vertex of K_{n-k}.

Theorem 3.5. *Let G be a graph in $\mathcal{G}_{n,k}$. Then*

$$\Pi_1^*(G) \leq [2(n-k-1)]^{\frac{(n-k-1)(n-k-2)}{2}}(2n-k-2)^{n-k-1}n^k \tag{10}$$

with equality holding if and only if G is isomorphic to $G_{n,k}$.

Proof. If G is isomorphic to $G_{n,k}$ then one can easily see that the equality in (10) holds. Suppose that G is not isomorphic to $G_{n,k}$ and $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,k}$. Then by Lemma 3.3 we have $G \in \mathcal{G}(n,k)$. Let $v_1, v_2, \ldots, v_{n-k}$ be the vertices of the clique K_{n-k} and n_i be the number of pendant vertices adjacent to vertex v_i in G. Without loss of generality we can assume that v_1 is maximum degree vertex of G. Since G is not isomorphic to $G_{n,k}$, there exists a vertex v_t such that $v_t \neq v_1$ and $n_t \geq 1$. Let $x_1, x_2, \ldots, x_{n_t}$ be the pendant neighbors of v_t. Consider the graph

$$G' = G - \{v_t x_1, v_t x_2, \ldots, v_t x_{n_t}\} + \{v_1 x_1, v_1 x_2, \ldots, v_1 x_{n_t}\}.$$

Then we have $d_{G'}(v_t) = n-k-1$, $d_{G'}(v_1) = d_G(v_1) + n_t$ and $d_{G'}(v_j) = d_G(v_j)$ for $j \neq 1$ and $j \neq t$. Now we prove that $\Pi_1^*(G') > \Pi_1^*(G)$. If we set $x = n_i$, $a = n_1$, $b = n_t$, $c = 2(n-k-1)$ in inequality (9), then it follows that

$$\begin{aligned} &\frac{n_1+n_t+n_i+2(n-k-1)}{n_1+n_i+2(n-k-1)} \cdot \frac{n_i+2(n-k-1)}{n_t+n_i+2(n-k-1)} \\ &\geq \frac{n_1+n_t+2(n-k-1)}{n_1+2(n-k-1)} \cdot \frac{2(n-k-1)}{n_t+2(n-k-1)} \end{aligned} \tag{11}$$

by Lemma 3.4. Then by the definition of Π_1^* and (11), we have

$$\begin{aligned} &\Pi_1(G')/\Pi_1(G) \\ &= \frac{(n_1+n_t+n-k)^{n_1+n_t}}{(n_1+n-k)^{n_1}(n_t+n-k)^{n_t}} \prod_{i=2, i\neq t}^{n-k} \left[\frac{n_1+n_t+n_i+2(n-k-1)}{n_1+n_i+2(n-k-1)} \cdot \frac{n_i+2(n-k-1)}{n_t+n_i+2(n-k-1)}\right] \\ &\geq \frac{(n_1+n_t+n-k)^{n_1+n_t}}{(n_1+n-k)^{n_1}(n_t+n-k)^{n_t}} \prod_{i=2, i\neq t}^{n-k} \left[\frac{n_1+n_t+2(n-k-1)}{n_1+2(n-k-1)} \cdot \frac{2(n-k-1)}{n_t+2(n-k-1)}\right] \\ &= \frac{(n_1+n_t+n-k)^{n_1+n_t}}{(n_1+n-k)^{n_1}(n_t+n-k)^{n_t}} \frac{[2(n-k-1)+n_1+n_t]^{n-k-2}}{[2(n-k-1)+n_1]^{n-k-2}} \frac{[2(n-k-1)]^{n-k-2}}{[2(n-k-1)+n_t]^{n-k-2}} . \end{aligned}$$

Let us consider the following functions

$$f(x) = [2(n-k-1)+x]^{n-k-2}(x+n-k)^x, \quad x \geq 0 \tag{12}$$

and

$$h(x) = lnf(x) + lnf(0) - lnf(x-n_t) - lnf(n_t). \tag{13}$$

Then, the above inequality is rewritten as

$$\frac{\Pi_1^*(G')}{\Pi_1^*(G)} \geq \frac{f(n_1+n_t)f(0)}{f(n_1)f(n_t)} \tag{14}$$

and from (12) it follows that

$$lnf(x) = (n-k-2)ln[2(n-k-1)+x] + xln(x+n-k).$$

Therefore,

$$(lnf(x))' = \frac{n-k-2}{2(n-k-1)+x} + ln(x+n-k) + \frac{x}{x+n-k}$$

and

$$\begin{aligned}(lnf(x))'' &= \frac{-(n-k-2)}{[2(n-k-1)+x]^2} + \frac{1}{x+n-k} + \frac{n-k}{(x+n-k)^2} \\ &= \frac{x+2(n-k)}{(x+n-k)^2} - \frac{n-k-2}{[2(n-k-1)+x]^2}\ .\end{aligned} \tag{15}$$

On the other hand, one can easily seen that

$$x+2(n-k) > n-k-2, \quad (x+n-k)^2 < [2(n-k-1)+x]^2 \tag{16}$$

since $n-k \geq 3$. Combining (15) and (16) we obtain that $(lnf(x))'' > 0$. Hence $(lnf(x))'$ is an increasing function when $x \geq 0$ and it follows that $(lnf(x))' > (lnf(x-n_t))'$. From this, $h'(x) = (lnf(x) + lnf(0) - lnf(x-n_t) - lnf(n_t))' > 0$ for $0 < n_t \leq x$. Thus $h(x)$ is an increasing function when $0 < n_t \leq x$ from (13) and it follows that $h(x) > h(n_t) = 0$. So $lnf(x) + lnf(0) > lnf(x-n_t) + lnf(n_t)$. If set $x = n_1 + n_t$, then we get $ln(f(n_1+n_t)f(0)) > ln(f(n_1)f(n_t))$, that is

$$f(n_1+n_t)f(0) > f(n_1)f(n_t). \tag{17}$$

Combining (14) and (17) we obtain $\Pi_1^*(G') > \Pi_1^*(G)$ and it contradicts to the assumption that $\Pi_1^*(G)$ is maximum in $\mathcal{G}_{n,g}$. ■

Theorem 3.6. *Let G be a graph in $\mathcal{H}_{n,k}$. If $\Pi_1^*(G)$ is maximum in $\mathcal{H}_{n,k}$ then G is isomorphic to $G_{n,k}$.*

Proof. Suppose that $G \notin \mathcal{G}(n,k)$. Then there exist two non-adjacent vertices u and v in G whose degrees are greater than one. Let us consider the graph $G' = G + uv$. Then $G' \in \mathcal{H}_{n,k}$ and $\Pi_1^*(G') > \Pi_1^*(G)$ by Lemma 2.1 (i). This contradicts to the fact that $\Pi_1^*(G)$ is maximum in $\mathcal{H}_{n,k}$. The rest of the proof is similar to the proof of Theorem 3.5. Hence, we get the required result. ■

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