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Cactus Graphs with Maximal Multiplicative Sum Zagreb Index

Chunlei Xu [1,2,*], Batmend Horoldagva [1,*] and Lkhagva Buyantogtokh [1]

[1] Department of Mathematics, Mongolian National University of Education, Baga toiruu-14, Ulaanbaatar 210648, Mongolia; buyantogtokh.l@msue.edu.mn
[2] College of Mathematics and Physics, Inner Mongolia University for Nationalities, Tongliao 028000, China
* Correspondence: xuchunlei1981@sina.cn (C.X.); horoldagva@msue.edu.mn (B.H.)

Abstract: A connected graph G is said to be a cactus if any two cycles have at most one vertex in common. The multiplicative sum Zagreb index of a graph G is the product of the sum of the degrees of adjacent vertices in G. In this paper, we introduce several graph transformations that are useful tools for the study of the extremal properties of the multiplicative sum Zagreb index. Using these transformations and symmetric structural representations of some cactus graphs, we determine the graphs having maximal multiplicative sum Zagreb index for cactus graphs with the prescribed number of pendant vertices (cut edges). Furthermore, the graphs with maximal multiplicative sum Zagreb index are characterized among all cactus graphs of the given order.

Keywords: multiplicative sum Zagreb index; cactus graph; pendant vertex; cut edge

MSC: 05C35; 05C09; 92E10; 05C07

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1. Introduction

In chemical graph theory and mathematical chemistry, a degree-based topological index, also known as a connectivity index, is a type of molecular descriptor calculated based on the molecular graph of a chemical compound. Symmetry has played an important role in chemical graph theory; in recent years, this role has increased in the study of topological indices. Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The *degree* of the vertex v in G is denoted by $d_G(v)$. The oldest and most well-known graph invariants are the first Zagreb index M_1 and the second Zagreb index M_2 of a graph G, and they are defined as

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

These indices were first introduced about fifty years ago by Gutman and Trinajstić [1]; for details of the mathematical studies and chemical applications on the Zagreb indices, see [2–6]. Moreover, the relation and comparison between them were studied in [7–13].

Todeschini and Consonni [14] 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 [15] studied these two graphical invariants and called them first and second multiplicative Zagreb indices, respectively. Recent results related to the multiplicative Zagreb indices and their other versions can be found in [16,17].

Eliasi, Iranmanesh, and Gutman [18] 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 [19]. 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 classes of graphs. Elias, Iranmanesh, and Gutman [18] proved that among all connected graphs with a given order, the path has minimal Π_1^*-value. They also determined the trees with the second minimal Π_1^*-value. Xu and Das [19] characterized the extremal trees, unicyclic and bicyclic graphs with a given order with respect to the multiplicative sum Zagreb index. Azari and Iranmanesh [17] gave some lower bounds for the multiplicative sum Zagreb index of graph operations. Kazemi [20] studied the multiplicative Zagreb indices of molecular graphs with a tree structure. The extremal graphs with respect to the multiplicative sum Zagreb index for several classes of graphs were determined in [21].

A connected graph G is said to be a cactus if any two cycles have at most one vertex in common. For the class of cactus graphs, the graphs were characterized that have the extremal Zagreb indices [22], the difference between Zagreb indices [23], and multiplicative Zagreb indices [24]. Recently, Liu, Yao, and Das [25] characterized the extremal cactus graphs with respect to several well-known vertex degree-based graph invariants. A vertex of degree one is called pendent, and an edge incident with a pendent vertex is called pendent. For $v \in V(G)$, $N_G(v)$ denotes the set of neighbors of v. A cut edge in a graph G is an edge whose removal increases the number of connected components of G. For $X \subset E(G)$, denote by $G - X$ the subgraph of G obtained from G by deleting all edges in X. For $Y \subset E(\bar{G})$, denote by $G + Y$ the supergraph of G obtained from G by adding all edges in Y, where $\bar{G}$ is a complement of G.

Denote by $\mathcal{C}_{n,k}$ the class of cactus graphs of order n with k pendent vertices, and denote by $\mathcal{C}_n^k$ the class of cactus graphs of order n with k cut edges. This paper is organized as follows. In Section 2, we present several graph transformations that increase the Π_1^*-value. In Section 3, by using these transformations, we determine the graphs that have maximal Π_1^*-value in $\mathcal{C}_{n,k}$ and $\mathcal{C}_n^k$. Moreover, the graphs with maximal Π_1^*-value are characterized among all cactus graphs of the given order.

2. Transformations

In this Section, we introduce several transformations that will be used in the proof of the main results of this paper. We begin by recalling the following two lemmas due to Xu and Das [19].

Lemma 1 ([19]). *Let G be a graph with $uv \notin E(G)$. Then $\Pi_1^*(G + uv) > \Pi_1^*(G)$.*

An edge contraction is an operation which removes an edge from a graph while simultaneously merging the two vertices that it previously joined.

Lemma 2 ([19]). Let uv be a non-pendent cut edge of graph G. Denote by $G' = G \cdot (uv) + uv$ the graph obtained by the contraction of uv onto the vertex u and adding a new pendent vertex v to u. Then $\Pi_1^*(G) < \Pi_1^*(G')$.

Transformation A. Let $x_0x_1x_2 \cdots x_lx_0$ ($l \geq 4$) be a cycle of a connected graph G. If $x_0x_2, x_0x_3 \notin E(G)$ then $G' = G - x_2x_3 + \{x_0x_2, x_0x_3\}$ (see Figure 1).

Lemma 3. *Let G and G' be the graphs depicted in Figure 1. Then $\Pi_1^*(G) < \Pi_1^*(G')$.*

Proof. From the definition of G', we have $d_G(v) = d_{G'}(v)$ for all $v \in V(G) \setminus \{x_0\}$. Then by the definition of Π_1^*, we have

$$\frac{\Pi_1^*(G')}{\Pi_1^*(G)} = \frac{(d_G(x_0)+2+d_G(x_2))(d_G(x_0)+2+d_G(x_3))}{d_G(x_2)+d_G(x_3)} \cdot \prod_{v \in N_G(x_0)} \frac{d_G(x_0)+2+d_G(v)}{d_G(x_0)+d_G(v)} > \frac{2(d_G(x_2)+d_G(x_3))}{d_G(x_2)+d_G(x_3)} > 1$$

and it follows that $\Pi_1^*(G) < \Pi_1^*(G')$. □

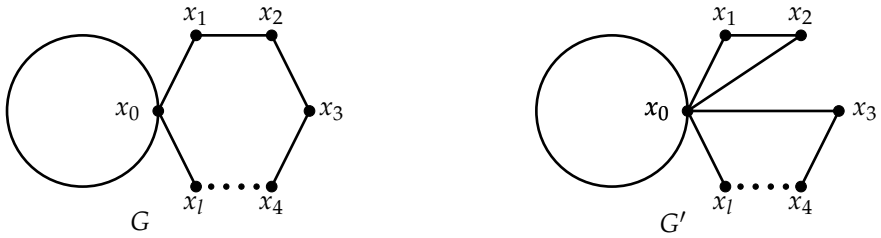

Figure 1. Transformation A.

Transformations B and C. Let $x_0x_1x_2x_3x_0$ and $y_0y_1y_2y_3y_0$ be cycles in connected graphs H_1 and H_2, respectively ($x_0x_2 \notin E(H_1)$, $y_0y_2 \notin E(H_2)$). Let G be the graph obtained from H_1 and H_2 by identifying x_0 with y_0 and denote this vertex x_0 (see Figure 2). Without loss of generality, we can assume that $d_G(x_1) \geq d_G(x_3)$, $d_G(y_1) \geq d_G(y_3)$, and $d_G(x_1) \geq d_G(y_1)$. Let $G' = G - \{x_2x_3, y_2y_3\} + \{x_0x_2, x_0y_2, x_3y_3\}$ and $G'' = G - \{x_2x_3, y_2y_3, x_0y_1\} + \{x_0x_2, x_1y_1, x_1y_2, x_3y_3\}$ (see Figure 2).

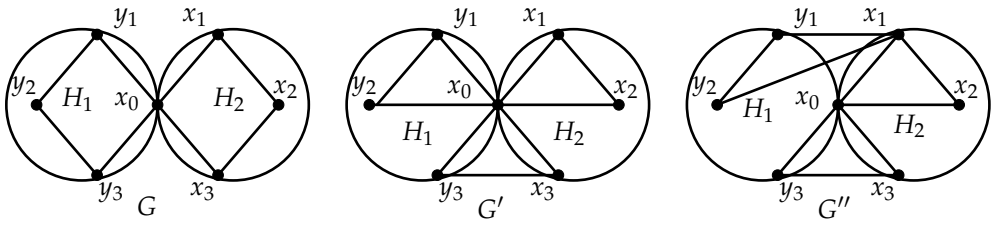

Figure 2. Transformations B and C.

Lemma 4. *Let G, G', and G'' be the graphs depicted in Figure 2.*

(i) *If $d_G(x_2) \geq d_G(x_3)$ then $\Pi_1^*(G) < \Pi_1^*(G')$.*
(ii) *If $d_G(x_2) < d_G(x_3)$ then $\Pi_1^*(G) < \Pi_1^*(G'')$.*

Proof. Set $d_G(x_0) = a \geq 4$, $d_G(x_i) = a_i$, and $d_G(y_i) = b_i$, $i = 1, 2, 3$.

(i) Then $d_{G'}(x_0) = a + 2$ and $d_G(v) = d_{G'}(v)$ for all $v \in V(G) \setminus \{x_0\}$. Therefore, we have

$$\frac{\Pi_1^*(G')}{\Pi_1^*(G)} = \frac{(a+2+a_2)(a+2+b_2)(a_3+b_3)}{(a_2+a_3)(b_2+b_3)} \cdot \prod_{v \in N_G(x_0)} \frac{a+2+d_G(v)}{a+d_G(v)} > \frac{(a_2+b_2+a_2b_2)(a_3+b_3)}{a_2b_2+a_2b_3+a_3b_2+a_3b_3} > 1$$

since $a_2 \geq a_3 > 1$ and $b_2 > 1$.

(ii) Then $d_{G''}(x_1) = a_1 + 2$ and $d_G(v) = d_{G''}(v)$ for all $v \in V(G) \setminus \{x_1\}$. From the assumption, we have $a_1 \geq b_1 \geq b_3$ and hence we get $a_1 + 2 + b_2 > b_2 + b_3$. Therefore, we have

$$\begin{aligned}\frac{\Pi_1^*(G'')}{\Pi_1^*(G)} &= \frac{(a_1+2+b_1)(a_1+2+b_2)(a+a_2)(a_3+b_3)}{(a+b_1)(a_2+a_3)(b_2+b_3)} \cdot \prod_{v \in N_G(x_1)} \frac{a_1+2+d_G(v)}{a_1+d_G(v)} \\ &> \frac{(a_1+b_1)(a+a_2)(a_3+b_3)}{aa_2+aa_3+a_2b_1+a_3b_1} > \frac{aa_1+aa_3+a_2b_1+a_3b_1}{aa_2+aa_3+a_2b_1+a_3b_1} > 1\end{aligned}$$

since $a_2 < a_3 \leq a_1$ and $a_1 \geq b_1 > 1$. □

Transformation D. Let $u_1u_2u_3u_4u_1$ and $v_1v_2v_3v_4v_1$ be two disjoint cycles of length 4 in a connected graph G. Suppose that $u_1u_3, v_1v_3, u_1v_2, u_2v_2 \notin E(G)$ and

$$d_G(u_1) = \max\{d_G(u_1), \ldots, d_G(u_4), d_G(v_1), \ldots, d_G(v_4)\}.$$

Let $G' = G - \{u_2u_3, v_1v_2, v_2v_3\} + \{u_1u_3, v_1v_3, u_1v_2, u_2v_2\}$ (see Figure 3).

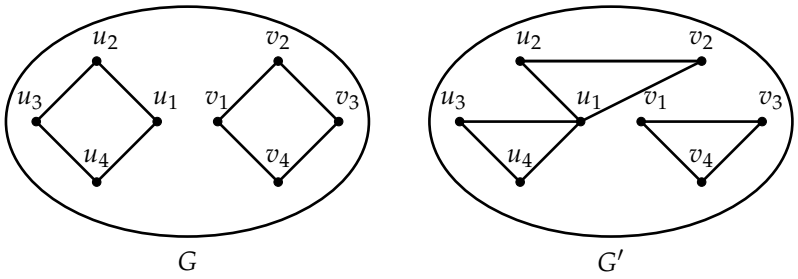

Figure 3. Transformation D.

Lemma 5. *Let G and G' be the graphs depicted in Figure 3. Then $\Pi_1^*(G) < \Pi_1^*(G')$.*

Proof. Set $d_G(u_i) = a_i$, $d_G(v_i) = b_i$, $i = 1, 2, 3$. Then $d_{G'}(u_1) = a_1 + 2$ and $d_{G'}(w) = d_G(w)$ for all $w \in V(G) \setminus \{u_1\}$. Therefore, we have

$$\begin{aligned}\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{(a_1+2+a_3)(a_1+2+b_2)(b_1+b_3)(a_2+b_2)}{(a_2+a_3)(b_1+b_2)(b_2+b_3)} \cdot \prod_{x \in N_G(u_1)} \frac{a_1+2+d_G(x)}{a_1+d_G(x)} \\ &> \frac{(a_1+2+a_3)(a_1+2+b_2)(b_1+b_3)(a_2+b_2)}{(a_2+a_3)(b_1+b_2)(b_2+b_3)} > \frac{(b_1+b_3)(a_2+b_2)}{b_2+b_3} > 1\end{aligned}$$

since $a_1 \geq a_2$, $a_1 \geq b_1$ and $a_2, b_1, b_2, b_3 \geq 2$. □

Transformation E. Let uv be an edge in a connected graph G such that $d_G(u) \geq 3$, $d_G(v) \geq 3$ and $N_G(u) \cap N_G(v) = \emptyset$. Assume that $y_1 \in N_G(v)$ is the maximum degree vertex in $N_G(u) \cup N_G(v) \setminus \{u, v\}$. Let $G' = (G - vy_1) \cdot (uv) + uv + vy_1$ be the graph obtained by the contraction of uv onto the vertex u and adding a new vertex v of degree two to u and y_1 (see Figure 4).

Lemma 6. *Let G and G' be the graphs depicted in Figure 4. Then $\Pi_1^*(G) < \Pi_1^*(G')$.*

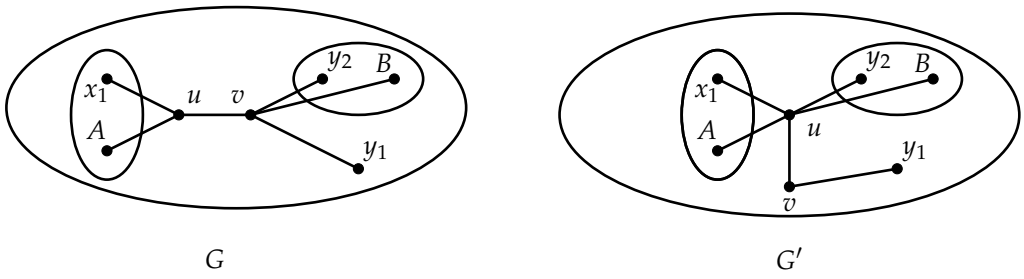

Figure 4. Transformation E.

Proof. Set $A = N_G(u) \setminus \{v\}$, $B = N_G(v) \setminus \{u, y_1\}$ and $|A| = a$, $|B| = b$. Then $d_G(u) = a + 1$, $d_G(v) = b + 2$, $d_{G'}(u) = a + b + 1$, $d_{G'}(v) = 2$, and $d_{G'}(w) = d_G(w)$ for all $w \in V(G) \setminus \{u, v\}$. Let x_1 and y_2 be maximum degree vertices in A and B, respectively. By the definition of Π_1^* and Bernoulli's inequality, we have

$$\begin{aligned}\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \prod_{x\in A}\frac{a+b+1+d_G(x)}{a+1+d_G(x)}\cdot\prod_{y\in B}\frac{a+b+1+d_G(y)}{b+2+d_G(y)}\cdot\frac{2+d_G(y_1)}{b+2+d_G(y_1)}\\ &\geq \left(1+\frac{b}{a+1+d_G(x_1)}\right)^a\cdot\left(1+\frac{a-1}{b+2+d_G(y_2)}\right)^b\cdot\frac{2+d_G(y_1)}{b+2+d_G(y_1)}\\ &\geq \left(1+\frac{ab}{a+1+d_G(x_1)}\right)\cdot\left(1+\frac{ab-b}{b+2+d_G(y_2)}\right)\cdot\frac{2+d_G(y_1)}{b+2+d_G(y_1)} \qquad (1)\end{aligned}$$

since $d_G(x_1)$, $d_G(y_2)$ are maximum in A and B, respectively. Denote $d_G(x_1) + 1 = s$, $d_G(y_2) + 2 = r$ and $d_G(y_1) + 2 = t$. Then we have $t > s$ and $t \geq r$ since $d_G(y_1)$ is maximum in $N_G(u) \cup N_G(v) \setminus \{u, v\}$. From (1), we have

$$\begin{aligned}\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &\geq \frac{(ab+a+s)(ab+r)t}{(a+s)(b+r)(b+t)}\\ &= \frac{a^2b^2t+a^2bt+abst+abrt+art+srt}{ab^2+abt+abr+art+sb^2+bst+srb+srt} > 1\end{aligned}$$

since $a^2b^2t \geq 2ab^2t > ab^2 + b^2t > ab^2 + b^2s$, $abst \geq 2bst \geq bst + bsr$ and $abrt > ab(r + t)$. Hence, we get $\Pi_1^*(G) < \Pi_1^*(G')$. □

Transformation F. Let uv be an edge in a connected graph G such that $d_G(u) \geq 3$, $d_G(v) \geq 3$ and $N_G(u) \cap N_G(v) = \{w\}$. Let $G' = (G - vw) \cdot uv + \{uv, vw\}$ be the graph obtained by the contraction of uv in $G - vw$ onto the vertex u and adding a new vertex v of degree two to u and w (see Figure 5).

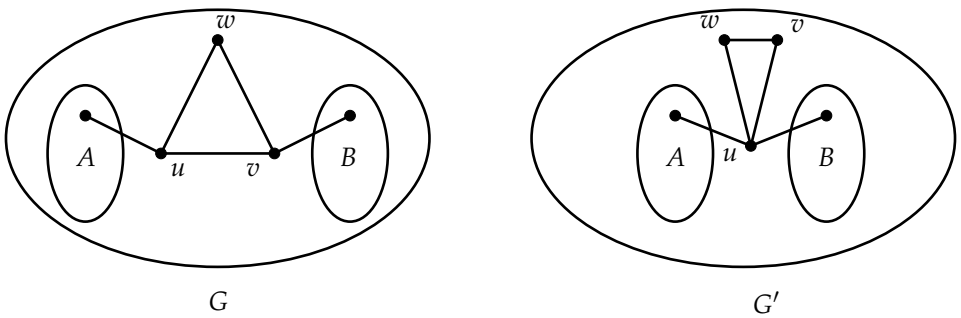

Figure 5. Transformation F.

Lemma 7. *Let G and G' be the graphs in Figure 5. If $d_G(u)$ is the maximum degree in $N_G(v) \setminus \{w\}$, then $\Pi_1^*(G) < \Pi_1^*(G')$.*

Proof. Clearly, $d_{G'}(z) = d_G(z)$ for all $z \in V(G) \setminus \{u, v\}$. Set $A = N_G(u) \setminus \{v, w\}$, $B = N_G(v) \setminus \{u, w\}$ and $|A| = a$, $|B| = b$, $d_G(w) = c - 2$. Then $d_G(u) = a + 2$, $d_G(v) = b + 2$ and $d_{G'}(u) = a + b + 2$, $d_{G'}(v) = 2$. Let $d_G(x_1)$ and $d_G(y_1)$ be the maximum degrees in A and B, respectively. By the definition of Π_1^* and Bernoulli's inequality, we have

$$\begin{aligned}\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &= \frac{c(a+b+c)}{(b+c)(a+c)} \cdot \prod_{x \in A} \frac{a+b+2+d_G(x)}{a+2+d_G(x)} \cdot \prod_{y \in B} \frac{a+b+2+d_G(y)}{b+2+d_G(y)} \\ &\geq \frac{c(a+b+c)}{(b+c)(a+c)} \cdot \left(1 + \frac{b}{a+2+d_G(x_1)}\right)^a \cdot \left(1 + \frac{a}{b+2+d_G(y_1)}\right)^b \\ &\geq \frac{c(a+b+c)}{(b+c)(a+c)} \cdot \left(1 + \frac{ab}{a+2+d_G(x_1)}\right) \cdot \left(1 + \frac{ab}{b+2+d_G(y_1)}\right). \qquad (2)\end{aligned}$$

Denote $d_G(x_1) + 2 = p$ and $d_G(y_1) + 2 = q$. Then from (2), we get

$$\begin{aligned}\frac{\Pi_1^*(G')}{\Pi_1^*(G)} &\geq \frac{(ab+a+p)(ab+b+q)(ac+bc+c^2)}{(a+p)(b+q)(ab+ac+bc+c^2)} \\ &= \frac{abc(ab+a+b+p+q)(a+b+c) + (a+p)(b+q)(ac+bc+c^2)}{(ab+aq+bp+pq)ab + (a+p)(b+q)(ac+bc+c^2)} \\ &> \frac{ab(ab+aq+bp+(a+c)p) + (a+p)(b+q)(ac+bc+c^2)}{(ab+aq+bp+pq)ab + (a+p)(b+q)(ac+bc+c^2)} \geq 1\end{aligned}$$

since $a + c \geq a + 4 = d_G(u) + 2 \geq d_G(y_1) + 2 = q$, and the proof is complete. □

3. Cactus Graphs with Maximal Π_1^*-Value

In this Section, we determine the graphs with maximal Π_1^*-value. A tree containing exactly two non-pendent vertices is called a double star.

Lemma 8. *Let G be a cactus graph different from a double star. If $\Pi_1^*(G)$ is maximum in $\mathcal{C}_{n,k}$ then there is no non-pendent cut edge. Moreover, the length of all k pendent paths in G is one.*

Proof. Suppose there exists a non-pendent cut edge uv in G. Then $d_G(u) \geq 2$ and $d_G(v) \geq 2$, and it follows that there exist vertices w_1 ($w_1 \neq v$) and w_2 ($w_2 \neq u$) such that $uw_1, vw_2 \in E(G)$. If we cannot choose w_1 and w_2 such that $d_G(w_1) \geq 2$ or $d_G(w_2) \geq 2$ then G is isomorphic to a double star and it is a contradiction. Therefore we can assume that $d_G(w_1) \geq 2$. First suppose that $d_G(u) = 2$. Clearly, $vw_1 \notin E(G)$, since uv is a cut edge of G. Then, since the path w_1uv has no common edge with any cycle in G, we have $G + w_1v \in \mathcal{C}_{n,k}$ and it follows that

$$\Pi_1^*(G) < \Pi_1^*(G + vw_1)$$

by Lemma 1. This contradicts the fact that $\Pi_1^*(G)$ is maximum in $\mathcal{C}_{n,k}$.

Now suppose that $d_G(u) \geq 3$ and $d_G(v) = 2$. If $d_G(w_2) \geq 2$ then $G + w_2u \in \mathcal{C}_{n,k}$ and again it follows that $\Pi_1^*(G) < \Pi_1^*(G + vw_1)$ by Lemma 1. Let now $d_G(w_2) = 1$. Consider $G_1 = G - \{uw_1, vw_2\} + \{uw_2, w_1w_2\}$. Then, $G_1 \in \mathcal{C}_{n,k}$. By the definition of Π_1^*, we have

$$\begin{aligned}\frac{\Pi_1^*(G_1)}{\Pi_1^*(G)} &= \frac{(d_G(u)+1)(d_G(u)+2)(d_G(w_1)+2)}{3(d_G(u)+2)(d_G(u)+d_G(w_1))} \\ &= \frac{(d_G(u)-2)(d_G(w_1)-1) + 3(d_G(u)+d_G(w_1))}{3(d_G(u)+d_G(w_1))} > 1\end{aligned}$$

since $d_G(u) > 2$ and $d_G(w_1) > 1$. It follows that $\Pi_1^*(G) < \Pi_1^*(G_1)$, and we get a contradiction. Hence we have $d_G(u) \geq 3$ and $d_G(v) \geq 3$. Denote by y_1 the maximum degree vertex in $N_G(u) \cup N_G(v) \setminus \{u, v\}$. Without loss of generality we can assume that $y_1 \in N_G(v) \setminus \{u\}$. If $G' = (G - vy_1) \cdot (uv) + uv + vy_1$ is the graph obtained from G by Transformation E

(see Figure 4), then we have $G' \in \mathcal{C}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G')$ by Lemma 6. This is also a contradiction. Clearly, the length of any pendent path is one, since there is no non-pendent cut edge. Hence, the proof is complete. □

Lemma 9. *Let G be a cactus graph with maximum multiplicative sum Zagreb index in $\mathcal{C}_{n,k}$. Then, the length of any cycle in G is at most four. Moreover, the number of cycles of length four in G is at most one.*

Proof. Suppose there exists a cycle $x_0x_1x_2\cdots x_lx_0$ in G of length at least five ($l \geq 4$). Since G is a cactus graph, we have $x_0x_2, x_0x_3 \notin E(G)$. If $G_1 = G - x_2x_3 + \{x_0x_2, x_0x_3\}$ is the graph obtained from G by Transformation A, then $G_1 \in \mathcal{C}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G_1)$ by Lemma 3. This is a contradiction. Hence, we conclude that the length of any cycle in G is at most four.

Now suppose that there are two cycles of length four in G. If they have a common vertex x_0, then we call them $x_0x_1x_2x_3x_0$ and $x_0y_1y_2y_3x_0$. Without loss of generality, we can assume that $d_G(x_1) \geq d_G(x_3)$, $d_G(y_1) \geq d_G(y_3)$, and $d_G(x_1) \geq d_G(y_1)$. Let $G' = G - \{x_2x_3, y_2y_3\} + \{x_0x_2, x_0y_2, x_3y_3\}$ and $G'' = G - \{x_2x_3, y_2y_3, x_0y_1\} + \{x_0x_2, x_1y_1, x_1y_2, x_3y_3\}$ be the graphs obtained from G by Transformations B and C (see Figure 2). Then $G', G'' \in \mathcal{C}_{n,k}$, and $\Pi_1^*(G) < \max\{\Pi_1^*(G'), \Pi_1^*(G'')\}$ by Lemma 4. This contradicts the fact that $\Pi_1^*(G)$ is maximal in $\mathcal{C}_{n,k}$. If the two cycles of length four are disjoint then we call them $u_1u_2u_3u_4u_1$ and $v_1v_2v_3v_4v_1$, where $d_G(u_1) = \max\{d_G(u_1), \ldots, d_G(u_4), d_G(v_1), \ldots, d_G(v_4)\}$. Let v_2 be the farthest vertex from u_1. Since G is a cactus graph and v_2 is the farthest vertex from u_1, one can easily see that $u_1u_3, v_1v_3, u_1v_2, u_2v_2 \notin E(G)$. Let $G_2 = G - \{u_2u_3, v_1v_2, v_2v_3\} + \{u_1u_3, u_1v_2, u_2v_2, v_1v_3\}$ be the graph obtained from G by Transformation D (see Figure 3). Obviously, the cycles $u_1u_3u_4u_1$ and $v_1v_3v_4v_1$ have no common edge with any cycle in G_2. Since G is a cactus graph and v_2 is the farthest vertex, each path from u_1 and u_2 to v_2 contains the vertex v_4. Hence, the cycle $u_1u_2v_2u_1$ has no common edge with any cycle in G_2. Therefore, $G_2 \in \mathcal{C}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G_2)$ by Lemma 5. This contradicts the fact that $\Pi_1^*(G)$ is maximal. This completes the proof. □

Let n and k be integers such that $n \geq 1$ and $k \geq 0$. If $n-k$ is odd then denote by $C_{n,k}^1$ the graph obtained from the star $K_{1,n-1}$ by adding $(n-k-1)/2$ independent edges. If $n-k$ is even then denote by $C_{n,k}^2$ the graph obtained from $C_{n-1,k}^1$ by inserting a new vertex of degree two on a non-pendent edge of it. Then, clearly the graphs $C_{n,k}^1$ and $C_{n,k}^2$ belong to $\mathcal{C}_{n,k}$ (see Figure 6).

Figure 6. The graphs $C_{7,2}^1$ and $C_{8,2}^2$.

Theorem 1. *Let G be a graph in $\mathcal{C}_{n,k}$.*

(i) *If $n-k$ is odd then $\Pi_1^*(G) \leq 2^{n-k-1}n^k(n+1)^{n-k-1}$ and equality holds if and only if G is isomorphic to $C_{n,k}^1$*

(ii) *If $n-k$ is even and $k \neq n-2$, then $\Pi_1^*(G) \leq 2^{n-k}(n-1)^k n^{n-k-2}$ and equality holds if and only if G is isomorphic to $C_{n,k}^2$.*

(iii) *If $k = n-2$ then $\Pi_1^*(G) \leq 3n(n-1)^{n-3}$ and equality holds if and only if G is isomorphic to a double star of order n with maximum degree $n-2$.*

Proof. Suppose that $\Pi_1^*(G)$ is maximum in $\mathcal{C}_{n,k}$. By Lemma 9, we have the length of all cycles, except one cycle of length four (if it exists) in G is three. Now we distinguish the following three cases.

(i) Let $n-k$ be odd. Then G is different from a double star. Hence, G has no non-pendent cut edge by Lemma 8. If G has a cycle of length four then $|E(G)| = k+3(t-1)+4 = k+3t+1$, where t is the number of cycles in G since there is no non-pendent cut edge and the length of each cycle except one cycle of length four is three. If we delete an edge from each cycle of G, then the resulting graph is a spanning tree of G. Hence we have $n-1 = k+3t+1-t = k+2t+1$, and this contradicts our assumption that $n-k$ is odd. Therefore, the length of all cycles of G is three.
Now, let $u \in V(G)$ be a vertex of maximum degree. If all neighbors of u are pendent, then $k = n-1$ and $G \cong K_{1,n-1} \cong C^1_{n,n-1}$ since G is connected. If $k < n-1$ then at least one cycle contains u. Let $uvwu$ be any cycle in G, where $d_G(v) \geq d_G(w)$. If $d_G(v) \geq 3$ then $d_G(u) \geq 3$ and $d_G(u)$ is the maximum in $N_G(v) \setminus \{w\}$ since $d_G(u)$ is maximum. If G' is the graph obtained from G by Transformation F (see Figure 5) then $G' \in \mathcal{C}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G')$ by Lemma 7. Hence we get $d_G(v) = d_G(w) = 2$ for any cycle $uvwu$ in G. Therefore, all cycles have length three and contain vertex u, and all pendent vertices are adjacent to u. This means that $G \cong C^1_{n,k}$.

(ii) Let $n-k$ be even and $k \neq n-2$. Then G is different from a double star since $k \neq n-2$. Hence G has no non-pendent cut edge by Lemma 8. If all cycles of G have length three, then $|E(G)| = k+3t$, where t is the number of cycles in G since all cut edges are pendent. Similarly, as in the above case, we have $n-1 = k+3t-t = k+2t$ and a contradiction. Therefore, G has a unique cycle of length four, as $C = ux_1vx_2u$.
Without loss of generality, we assume that u is a vertex of maximum degree among all vertices in $V(C)$. If $d_G(u) = 2$, then $n = 4$, $k = 0$, and we are done. Therefore, we have $d_G(u) \geq 3$. Now, suppose that $d_G(x_i) \geq 3$ ($i = 1$ or 2). One can easily see that $N_G(u) \cap N_G(x_i) = \emptyset$. Consider the graph G' obtained from G by Transformation F (see Figure 5). Then $G' \in \mathcal{C}_{n,k}$ and $\Pi_1^*(G) < \Pi_1^*(G')$ by Lemma 7. This is a contradiction with the fact that $\Pi_1^*(G)$ is maximum in $\mathcal{C}_{n,k}$. Hence, we get $d_G(x_1) = d_G(x_2) = 2$.
Let H be the connected component of $G - \{x_1u, x_2u\}$ which contains v. Let v_1 be a maximum degree vertex in H. Suppose that v_1 is different from v. Then there is a cycle v_1yzv_1 that contains v_1 such that $d_G(y) \geq 3$ since G has no non-pendent cut edge. Clearly, $d_G(v_1) \geq 3$. Let $G_1 = (G-yz)\cdot(v_1y) + \{v_1y, yz\}$ be the graph obtained from G by Transformation F. Then since $d_G(v_1)$ is maximum in $N_G(y) \cup N_G(z)$, we have $\Pi_1^*(G) < \Pi_1^*(G_1)$ by Lemma 7 and a contradiction. Therefore, v is a maximum degree vertex in H. If any neighbor of v has degree at least three in H then we also get a contradiction by Lemma 7. It follows that all cycles in H contain v and all pendent vertices in H are adjacent to v. Similarly, we can show that all cycles in H_1 contain u and all pendent vertices in H_1 are adjacent to u, where H_1 is the connected component of $G - \{x_1v, x_2v\}$ which contains u. Hence, G is isomorphic to the graph $G(a,b,k_1,k_2)$ in Figure 7, where $a+b = (n-k-4)/2$ and $k_1+k_2 = k$.
Without loss of generality, we can assume that $\min\{k_1+2a, k_2+2b\} = k_2+2b$. Then, it is easy to calculate that

$$\begin{aligned}\Pi_1^*(G(a,b,k_1,k_2)) &= (k_1+2a+2+1)^{k_1}\cdot(k_2+2b+2+1)^{k_2}\cdot 4^a\cdot 4^b \\ &\quad\cdot(k_1+2a+2+2)^{2a+2}\cdot(k_2+2b+2+2)^{2b+2}. \qquad (3)\end{aligned}$$

Now we show that

$$\Pi_1^*(G(a,b,k_1,k_2)) \leq \Pi_1^*(G(a+b,0,k_1+k_2,0)) = \Pi_1^*(C^2_{n,k})$$

and equality holds if and only if $b = k_2 = 0$.

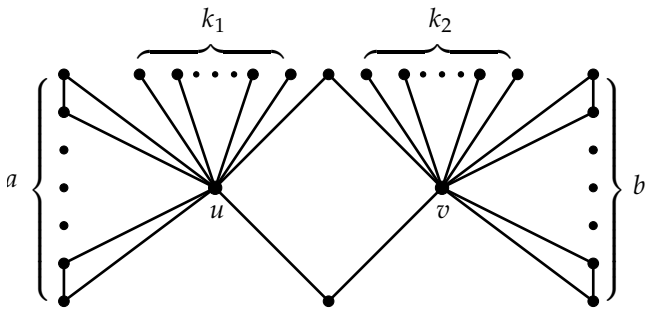

Figure 7. The graph $G(a, b, k_1, k_2)$.

If $k_2 + 2b = 0$ then $k_2 = 0$ and $b = 0$. Hence, we are done since $a + b = (n - k - 4)/2$ and $k_1 + k_2 = k$. Let now $k_2 + 2b \geq 1$. From (3) and Bernoulli's inequality, we obtain

$$\begin{aligned}
\frac{\Pi_1^*(G(a+b,0,k_1+k_2,0))}{\Pi_1^*(G(a,b,k_1,k_2))} &= \frac{4}{k_1+2a+4}\left(1+\frac{k_2+2b}{k_1+2a+3}\right)^{k_1}\left(1+\frac{k_2+2b}{k_1+2a+4}\right)^{2a+1} \\
&\quad \cdot\frac{4}{k_2+2b+4}\left(1+\frac{k_1+2a}{k_2+2b+3}\right)^{k_2}\left(1+\frac{k_1+2a}{k_2+2b+4}\right)^{2b+1} \\
&\geq \frac{4}{k_1+2a+4}\left(1+\frac{k_1(k_2+2b)}{k_1+2a+3}\right)\left(1+\frac{(2a+1)(k_2+2b)}{k_1+2a+4}\right) \\
&\quad \cdot\frac{4}{k_2+2b+4}\left(1+\frac{k_2(k_1+2a)}{k_2+2b+3}\right)\left(1+\frac{(2b+1)(k_1+2a)}{k_2+2b+4}\right) \\
&> \frac{4}{k_1+2a+4}\left(1+\frac{k_1(k_2+2b)}{k_1+2a+3}+\frac{(2a+1)(k_2+2b)}{k_1+2a+4}\right) \\
&\quad \cdot\frac{4}{k_2+2b+4}\left(1+\frac{k_2(k_1+2a)}{k_2+2b+3}+\frac{(2b+1)(k_1+2a)}{k_2+2b+4}\right) \\
&> \frac{4}{k_1+2a+4}\left(1+\frac{(k_1+2a+1)(k_2+2b)}{k_1+2a+4}\right) \\
&\quad \cdot\frac{4}{k_2+2b+4}\left(1+\frac{(k_2+2b+1)(k_1+2a)}{k_2+2b+4}\right) \\
&\geq \frac{4}{k_1+2a+4}\left(1+\frac{2}{5}(k_2+2b)\right) \\
&\quad \cdot\frac{4}{k_2+2b+4}\left(1+\frac{2}{5}(k_1+2a)\right) > 1
\end{aligned}$$

since $\frac{k_1+2a+1}{k_1+2a+4} \geq \frac{2}{5}$ and $\frac{k_2+2b+1}{k_2+2b+4} \geq \frac{2}{5}$. Hence we get $G \cong C_{n,k}^2$.

(iii) Let $k = n - 2$. Then G is isomorphic to a double star. Let u and v be the non-pendent vertices in G and $d_G(u) = p + 1$, $d_G(v) = q + 1$, where $p + q + 2 = n$. By Bernoulli's inequality, we have

$$3 \cdot \left(\frac{p+q+1}{p+2}\right)^p \geq 3 \cdot \left(1+\frac{p(q-1)}{p+2}\right) \geq 3 \cdot (1 + 1/3(q-1)) = q+2$$

since $\frac{p}{p+2} \geq \frac{1}{3}$. Hence we obtain $3 \cdot (p+q+1)^p \geq (p+2)^p(q+2)$. Therefore, we have

$$\begin{aligned}
\Pi_1^*(G) &= n(p+2)^p(q+2)^q \leq 3n(p+q+1)^p(q+2)^{q-1} \\
&\leq 3n(p+q+1)^{p+q-1} = 3n(n-1)^{n-3}
\end{aligned}$$

and equality holds if and only if G is isomorphic to a double star of order n with maximum degree $n-2$. The proof is complete. □

Now we characterize the graphs with maximum Π_1^*-value among all cactus graphs of the given order.

Theorem 2. *Let G be a cactus graph of order n.*

(i) *If n is odd then $\Pi_1^*(G) \leq 2^{n-1}(n+1)^{n-1}$ and equality holds if and only if G is isomorphic to $C_{n,0}^1$.*

(ii) *If n is even then $\Pi_1^*(G) \leq 2^{n-2}n(n+1)^{n-2}$ and equality holds if and only if G is isomorphic to $C_{n,1}^1$.*

Proof. Let k be the number of pendent vertices in G.

(i) Let n be odd. Then by Theorem 1, we get

$$\Pi_1^*(G) \leq \begin{cases} 2^{n-k-1}n^k(n+1)^{n-k-1} & \text{if } k \text{ is even,} \\ 2^{n-k}(n-1)^k n^{n-k-2} & \text{if } k \text{ is odd} \end{cases} \leq \begin{cases} 2^{n-1}(n+1)^{n-1} \\ 2^{n-1}(n-1)n^{n-3} \end{cases} \leq 2^{n-1}(n+1)^{n-1}$$

and equality holds if and only if G is isomorphic to $C_{n,0}^1$.

(ii) Let n be even. Then by Theorem 1, we get

$$\Pi_1^*(G) \leq \begin{cases} 2^{n-k-1}n^k(n+1)^{n-k-1} & \text{if } k \text{ is odd,} \\ 2^{n-k}(n-1)^k n^{n-k-2} & \text{if } k \text{ is even} \end{cases} \leq \begin{cases} 2^{n-2}n(n+1)^{n-2} \\ 2^n n^{n-2} \end{cases} \leq 2^{n-2}n(n+1)^{n-2}$$

and equality holds if and only if G is isomorphic to $C_{n,1}^1$. □

From Lemma 2, the following lemma holds immediately.

Lemma 10. *Let G be a cactus graph with maximum multiplicative sum Zagreb index in $\mathcal{C}_n^k$. Then all cut edges of G are pendent.*

The same argument as in the proof of Theorem 1 yields the following result.

Theorem 3. *Let G be a graph in $\mathcal{C}_n^k$.*

(i) *If $n-k$ is odd then $\Pi_1^*(G) \leq 2^{n-k-1}n^k(n+1)^{n-k-1}$ and equality holds if and only if G is isomorphic to $C_{n,k}^1$.*

(ii) *If $n-k$ is even then $\Pi_1^*(G) \leq 2^{n-k}(n-1)^k n^{n-k-2}$ and equality holds if and only if G is isomorphic to $C_{n,k}^2$.*

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