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Extremal graphs of multiplicative sum Zagreb index

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Abstract: The multiplicative sum Zagreb index, regarded as the multiplicative version of the first Zagreb index, is defined as the product of the degree sum over all pairs of adjacent vertices. In this paper, we determine the extremal values of the multiplicative sum Zagreb index for three class of trees. Some bounds on the multiplicative sum Zagreb index are obtained, and the corresponding extremal graphs with these bounds are characterized.

Keywords: Extremal value, Extremal graph, Tree, Bound.
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1 Introduction

In mathematical chemistry and chemical graph theory, topological indices can be seen as descriptors of a molecule graph. Since the Wiener index was introduced in 1972, a series of topological indices have been defined over the past fifty years. The most famous and well-known ones are the first Zagreb index and the second Zagreb index, and they were defined as

$$M_1(G) = \sum_{v_iv_j \in E(G)} (d_G(v_i) + d_G(v_j)) \quad \text{and} \quad M_2(G) = \sum_{v_iv_j \in E(G)} (d_G(v_i)d_G(v_j)),$$

where G is a graph with vertex set $V(G)$ and edge set $E(G)$, $d_G(v_i)$ is the degree of vertex $v_i \in V(G)$. In the literature of the mathematical properties and chemical applications of M_1 and M_2, see details in [1, 3, 5, 7, 10, 12, 17, 18]. The main results with respect to the properties of M_1 and M_2 were summarized in [8, 11, 15, 16].

In 2012, Eliasi, Iranmanesh and Gutman [9] introduced a topological index which is called "*multiplicative sum Zagreb index*", its definition is

$$\Pi_1^* = \Pi_1^*(G) = \prod_{v_iv_j \in E(G)} (d_G(v_i) + d_G(v_j)).$$

For the latest results with respect to the multiplicative sum Zagreb index, see details in [9, 13, 14, 19, 20].

To avoid repetition, the basic definitions and notations used in this paper refer to Bondy and Murty's book [2]. Other terminology and notations will be listed when necessary.

This paper is organized in the following way. In Section 2, we give a simple method to determine the minimal second Π_1^*-value for trees, and then determine the second maximal Π_1^*-value for trees. Moreover, the extremal Π_1^*-values for Banana trees, Kragujevac trees are also obtained in this section. In Section 3, some bounds are established, and the graphs with these bounds are entirely characterized.

2 Extremal Π_1^*-values on trees

In this section, we determine the second minimal Π_1^*-value by using a different method from the one given in [9] by Eliasi, Iranmanesh and Gutman. Then the second maximal Π_1^*-values for trees are obtained. At the end of this section, we determine the extremal values of the multiplicative sum Zagreb index for Banana trees and Kragujevac trees.

Lemma 2.1. [19] *For any graph G,*

(i) *If $uv \in E(G)$, then $\Pi_1^*(G - uv) < \Pi_1^*(G)$.*

(ii) *If $xy \notin E(G)$, then $\Pi_1^*(G + xy) > \Pi_1^*(G)$.*

Denote by $\mathcal{T}_n$ the class of all trees of order n. In 2012, Eliasi, Iranmanesh and Gutman [9] determined the second minimal Π_1^*-value in $\mathcal{T}_n$. We now present an alternative approach that is slightly simpler to achieve the same result. To begin with, we employ three sets defined in [6] as follows

$$A = \{uv \in E(T) : d_T(u) + d_T(v) = 3\},$$
$$B = \{uv \in E(T) : d_T(u) + d_T(v) = 4\},$$
$$C = \{uv \in E(T) : d_T(u) + d_T(v) \geq 5\}.$$

Following the definition and notation in [9], denote by $\mathcal{T}_n^*$ the class of trees of order n which can be obtained from a path $P_{n-k} = v_1 v_2 \cdots v_{n-k}$ by attaching a pendent path P_k onto v_i, where $3 \leq i \leq n-k-2$ and $2 \leq k \leq n-2$. Denote by $Q_{n,i}$ the tree constructed from a path $P_{n-1} = x_1 \cdots x_i \cdots x_{n-1}$ by attaching a pendent edge $x_i x_n$ onto x_i, where $2 \leq i \leq n-3$. Denote by R_n the tree of order n which can be constructed from path $P_{n-2} = y_2 y_3 \cdots y_{n-1}$ by attaching two pendent edges $y_3 y_1$ and $y_{n-2} y_n$ onto y_3 and y_{n-2}, respectively. Denote by W_n the tree of order n which can be constructed from path $P_{n-2} = z_2 z_3 z_4 \cdots z_{n-1}$ by attaching two pendent edges $z_3 z_1$ and $z_4 z_n$ onto z_3 and z_4, respectively.

Lemma 2.2. [6] *For any tree $T \in \mathcal{T}_n$ with $T \ncong P_n$, $|C| \geq |A|$.*

Theorem 2.3. [9] *If $P_n \ncong T \in \mathcal{T}_n$ and $n \geq 7$, then $\Pi_1^*(T) \geq 3^3 4^{n-7} 5^3$, where the equality holds if and only if $T \in \mathcal{T}_n^*$.*

Proof. For the sake of simplicity, denote by p, q, r the cardinalities of sets A, B, C, respectively. Then $p + q + r = n - 1$. Obviously, $r \geq p$ since Lemma 2.2. Now we distinguish the following three cases:

Case 1. If $r = 1$, then $\Delta = 3$, and there exists only one edge uv in T such that $d_T(u) + d_T(v) = 5$ or $d_T(u) + d_T(v) = 6$. Therefore, $d_T(u) + d_T(v) = 5$ for $n \geq 7$, which means $T \cong Q_{n,2}$. By the definition of the multiplicative sum Zagreb index,

$$\Pi_1^*(Q_{n,2}) = 3 \cdot 4^{n-3} 5 > 3^3 4^{n-7} 5^3.$$

Case 2. If $r = 2$, then $\Delta = 3$, and there are exactly two different edges uv and xy such that $(d_T(u) + d_T(v), d_T(x) + d_T(y))$ is $(5, 5)$ or $(5, 6)$ or $(6, 6)$.

If $(d_T(u) + d_T(v), d_T(x) + d_T(y)) = (5, 5)$, then $T \cong R_n$ or $T \cong Q_{n,i}$, $i \geq 3$. Hence, by the definition of the multiplicative sum Zagreb index,

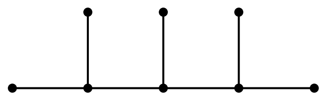
$$\Pi_1^*(R_n) = 4^{n-3} 5^2 > 3^3 4^{n-7} 5^3 \quad \text{and} \quad \Pi_1^*(Q_{n,i}) = 3^2 4^{n-5} 5^2 > 3^3 4^{n-7} 5^3.$$

If $(d_T(u) + d_T(v), d_T(x) + d_T(y)) = (5, 6)$, then $T \cong W_n$. Hence, by the definition of the multiplicative sum Zagreb index,

$$\Pi_1^*(W_n) = 3 \cdot 4^{n-4} 5 \cdot 6 > 3^3 4^{n-7} 5^3.$$

If $(d_T(u) + d_T(v), d_T(x) + d_T(y)) = (6, 6)$, then $T \cong T_1$ (see Figure 1). Hence, by the definition of the multiplicative sum Zagreb index,

$$\Pi_1^*(T_1) = 4^5 6^2 > 3^3 \cdot 4 \cdot 5^3 = 3^3 4^{n-7} 5^3 \Big|_{n=8}.$$



T_1

Figure 1. Trees T_1

<u>Case 3.</u> If $r \geq 3$, then by the definition of the multiplicative sum Zagreb index,

$$\begin{aligned}\Pi_1^*(T) &= \prod_{uv \in A}(d_T(u)+d_T(v)) \cdot \prod_{wx \in B}(d_T(w)+d_T(x)) \cdot \prod_{yz \in C}(d_T(y)+d_T(z)) \\ &\geq 3^p 4^{n-1-p-r} 5^r \;=\; 3^p 4^{n-1-p}\left(\frac{5}{4}\right)^r \qquad (1)\\ &\geq 3^p 4^{n-1-p}\left(\frac{5}{4}\right)^p \;=\; 3^p 4^{n-1-2p} 5^p. \qquad (2)\end{aligned}$$

If $p \geq 3$, then inequality (2) can be rewritten as $\Pi_1^*(T) \geq 3^3 4^{n-7} 5^3$, which means that the equality holds if and only if $p = 3$ and there are $n-7$ edges $e_i = u_i v_i$ such that $d_T(u_i) + d_T(v_i) = 4$ for $i = 1, 2, \ldots, n-7$.

If $p = 1$ or $p = 2$, then inequality (1) can be rewritten as

$$\Pi_1^*(T) \;\geq\; 3^p 4^{n-1-p-r} 5^r \;>\; 3^p 4^{n-4-p} 5^3 \;>\; 3^3 4^{n-7} 5^3.$$

By combining the three cases above, we finish the proof of this theorem. □

In Theorem 2.3, we only considered the case $n \geq 7$. For $n = 5$ and $n = 6$, we refer to [9], where Eliasi, Iranmanesh and Gutman have already determined the second minimal Π_1^*-values, so we omit these cases here.

Lemma 2.4. [13] Let H_1 and H_2 be two subgraphs of G such that there is exactly one cut edge $uv \in E(G)$ connecting H_1 and H_2, where $u \in V(H_1)$ and $v \in V(H_2)$. Denote by $G' = (G \cdot uv) + uv$ the graph obtained by deleting edge uv, merging u and v into the new vertex u, adding a new edge also named uv. Then $\Pi_1^*(G') > \Pi_1^*(G)$.

Now we look for the second maximum Π_1^*-value in $\mathcal{T}_n$. Recall that the *diameter* of graph G is the greatest length of a path in G. Suppose that $K_{1,p}$ and $K_{1,q}$ are two stars of order $p+1$ and $q+1$, respectively, where $p \geq q$. Then the *double star*, denoted by $DS(p,q)$, is a tree obtained from $K_{1,p}$ and $K_{1,q}$ by jointing a new edge between the two central vertices of $K_{1,p}$ and $K_{1,q}$. Note that $V(DS(p,q)) = p+q+2$.

Theorem 2.5. *If $T \in \mathcal{T}_n$ and $T \ncong S_n \cong K_{1,n-1}$, then $\Pi_1(T) \leq 3\,n(n-1)^{n-3}$, where the equality holds if and only if $T \cong DS(n-3,1)$.*

Proof. According to the evaluation of the diameter d of T, we consider following two cases:

<u>Case 1.</u> If $d = 3$, then $T \cong DS(p,q)$. Without loss of generality, we assume that $p \geq q \geq 1$ and $(p+1)+(q+1) = n$. By the definition of the multiplicative sum Zagreb index,

$$\Pi_1^*(DS(p,q)) = n\,(p+2)^p(q+2)^q.$$

Now we consider a function $f(x) = (x+2)^x(n-x)^{n-x-2}$, $\lceil \frac{n-2}{2} \rceil \leq x \leq n-3$. Since $x+2 \geq n-x$,

$$f'(x) = f(x)\left(\ln(x+2) + \frac{x}{x+2} - \ln(n-x) - \frac{n-x-2}{n-x}\right) > 0.$$

Hence, $f(x)$ is increasing for $\lceil \frac{n-2}{2} \rceil \leq x \leq n-3$. It gives that $f(x)_{\max} = f(n-3) = 3\,(n-1)^{n-3}$. Therefore, for any $T \in \mathcal{T}_n$ and $T \ncong S_n \cong K_{1,n-1}$,

$$\Pi_1^*(T) \leq \Pi_1^*(DS(p,q)) \leq \Pi_1^*(DS(n-3,1)) = 3\,n(n-1)^{n-3}.$$

Case 2. If $d \geq 4$, then by repeatedly using Lemma 2.4 on $T \in \mathcal{T}_n$, there exists $T' \in \mathcal{T}_n$ such that $\Pi_1^*(T') > \Pi_1^*(T)$ and $d(T') = 3$. By the same discussion as in Case 1, we obtain $\Pi_1^*(T) \leq 3\,n(n-1)^{n-3}$. □

Denote by $B(n_1, n_2, \ldots, n_p)$ the *Banana tree* [4] which can be constructed from p stars $K_{1,n_1}, K_{1,n_2}, \ldots, K_{1,n_p}$ by jointing p new edges onto one end vertex of each star, where $n_1 \geq n_2 \geq \cdots \geq n_p > 1$, $p \geq 2$. Write $B^* = B(t, 1, 1, \ldots, 1)$, $B_* = B(t_1, t_2, \ldots, t_p)$, where $t = \sum_{i=1}^{p} n_i - 2\,p + 1$ and $|t_i - t_j| \leq 1$, for $1 \leq i < j \leq p$. See the Banana trees B_* and B^* in Figure 2.

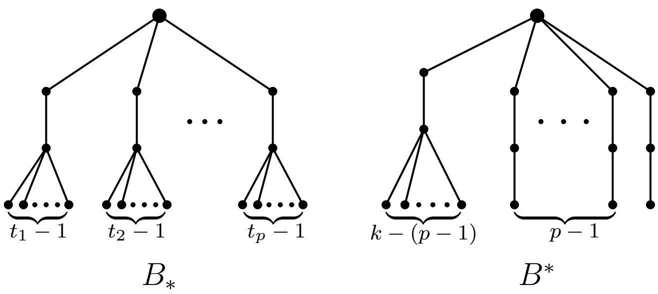


Figure 2. Banana trees B_* and B^*

Lemma 2.6. *Suppose that* $B(n_1, \ldots, n_i, \ldots, n_j, \ldots, n_p)$ *and* $B(n_1, \ldots, n_i+1, \ldots, n_j-1, \ldots, n_p)$ *are two Banana trees, where* $n_i \geq n_j$*, then*

$$\Pi_1^*(B(n_1, \ldots, n_i, \ldots, n_j, \ldots, n_p)) < \Pi_1^*(B(n_1, \ldots, n_i+1, \ldots, n_j-1, \ldots, n_p)).$$

Proof. Without loss of generality, we assume that $i = 1, j = 2$, and $n_1 \geq n_2$. For the sake of simplicity, write $B_1 = B(n_1, n_2, \ldots, n_p)$ and $B_2 = B(n_1+1, n_2-1, \ldots, n_p)$. By the definition of the multiplicative sum Zagreb index,

$$\frac{\Pi_1^*(B_2)}{\Pi_1^*(B_1)} = \frac{(n_1+2)^{n_1} n_2^{n_2-2}(n_1+3)(n_2+1)}{(n_1+1)^{n_1-1}(n_2+1)^{n_2-1}(n_1+2)(n_2+2)}. \tag{3}$$

Now we consider two functions

$$f(x) = (x+1)^{x-1}(x+2), \quad x \geq 1,$$
$$g(x) = \ln f(x) = (x-1)\ln(x+1) + \ln(x+2), \quad x \geq 1.$$

Then (3) can be rewritten as

$$\frac{\Pi_1^*(B_2)}{\Pi_1^*(B_1)} = \frac{f(n_1+1)f(n_2-1)}{f(n_1)f(n_2)}. \tag{4}$$

By derivation,

$$g''(x) = [\ln f(x)]' = \frac{x+3}{(x+1)^2} - \frac{1}{(x+2)^2} > 0,$$

which means that $[\ln f(x)]'$ is increasing in $[1, +\infty)$. It is deduced that $[\ln f(x) - \ln f(x-1)]' > 0$. So, $\ln f(n_1+1) - \ln f(n_1) > \ln f(n_2) - \ln f(n_2-1)$, that is

$$\ln[f(n_1)f(n_2)] < \ln[f(n_1+1)f(n_2-1)].$$

Therefore, from (4) we get $\Pi_1^*(B_2)/\Pi_1^*(B_1) > 1$. □

Theorem 2.7. *For the Banana tree $B(n_1, n_2, \dots, n_p)$,*

$$(p+2)^p \left(\left\lfloor \frac{k}{p} \right\rfloor + 2\right)^{(p-r)} \left(\left\lceil \frac{k}{p} \right\rceil + 2\right)^r \left(1 + \left\lfloor \frac{k}{p} \right\rfloor\right)^{\lfloor \frac{k}{p} \rfloor - 1)(p-r)} \left(1 + \left\lceil \frac{k}{p} \right\rceil\right)^{(\lceil \frac{k}{p} \rceil - 1)r}$$
$$\leq \Pi_1^*(B) \leq 12^{p-1}(p+2)^p(t+2)^t(t+3), \tag{5}$$

where the left equality holds if and only if $B \cong B_*$ and the right equality holds if and only if $B \cong B^*$, where $k = n_1 + n_2 + \cdots + n_p - p$, and $k = ps + r,\ 0 \leq r < p$.

Proof. To begin with, we claim that if $B(n_1, n_2, \dots, n_p)$ has its minimum Π_1^*-value in the set $\{B(l_1, l_2, \dots, l_p) : k = l_1 + l_2 + \cdots + l_p - p\}$, then for any pair (i, j) with $1 \leq i < j \leq p$, the inequality $|n_i - n_j| \leq 1$ holds. Otherwise, there exists a pair (i, j) such that $|n_i - n_j| \geq 2$. By Lemma 2.6, we can construct a Banana tree B' satisfying $\Pi_1^*(B') < \Pi_1^*(B)$, which contradicts the assumption that B achieves the minimum Π_1^*-value. For the left-hand equality in (5), the desired result follows directly via straightforward computation.

Now for the maximum Π_1^*-value in $\{B(l_1, l_2, \dots, l_p) : k = l_1 + l_2 + \cdots + l_p - p\}$, by using Lemma 2.6 enough times on B until $B(t, 1, 1, \dots, 1)$ is obtained, where $t = \sum_{i=1}^{p} n_i - (p-1)$. By directly calculating, $\Pi_1^*(B) \leq \Pi_1^*(B^*) = 12^{p-1}(p+2)^p(t+2)^t(t+3)$. □

Denote by A_k the rooted tree with $2k+1$ vertices constructed by attaching k two-vertex branches onto the root, see A_0, A_1, A_2, A_3, A_k in Figure 3.

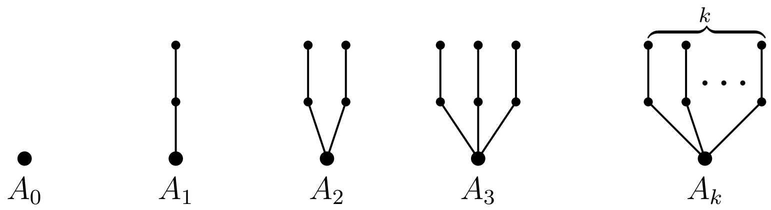


Figure 3. Tress A_0, A_1, A_2, A_3, A_k

The *Kragujevac tree*, denoted by $Kg(k_1, k_2, \ldots, k_t)$, is a tree obtained from t rooted trees $A_1, A_2, \ldots, A_t$ by connecting their roots to a new vertex, where $k_1 \geq k_2 \geq \cdots \geq k_t \geq 0$. Set $K = \sum_{i=1}^{t} k_i = rt + s$, where $0 \leq s < t$. See an example in Figure 4.

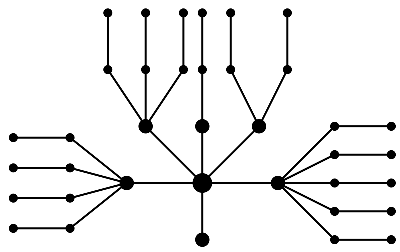


Figure 4. Kragujevac tree $Kg(5, 4, 3, 2, 1, 0)$

Theorem 2.8. *For any Kragujevac tree* $Kg(k_1, k_2, \ldots, k_t)$,

$$3^K \left(t+1+\left\lfloor \frac{K}{t} \right\rfloor\right)^{t-s} \left(t+1+\left\lceil \frac{K}{t} \right\rceil\right)^{s} \left(2+\left\lfloor \frac{K}{t} \right\rfloor\right)^{(t-s)\lfloor \frac{K}{t} \rfloor} \left(2+\left\lceil \frac{K}{t} \right\rceil\right)^{s\lceil \frac{K}{t} \rceil}$$
$$\leq \Pi_1^*(Kg(k_1, k_2, \cdots, k_t) \ \leq \ 3^K (K+3)^K (t+1)^{t-1} (t+K+1), \tag{6}$$

where the left-hand equality holds if and only if $G \cong Kg(\underbrace{r+1, \ldots, r+1}_{s}, \underbrace{r, \ldots, r}_{t-s})$ *and the right-hand equality holds if and only if* $G \cong Kg(K, 0, 0, \ldots, 0)$.

Proof. Without loss of generality, let $i < j$. By the definition of the Kragujevac tree, $k_i \geq k_j$. It is sufficient to prove

$$\Pi_1^*(Kg(k_1, \ldots, k_i + 1, \ldots, k_j - 1, \ldots, k_t)) > \Pi_1^*(Kg(k_1, \ldots, k_i, \ldots, k_j, \ldots, k_t)). \tag{7}$$

Now we consider the functions

$$f(x) = (x+3)^x (x+1+t), \quad x \geq 1, t \geq 2.$$
$$g(x) = \ln f(x) = x \ln(x+3) + \ln(x+1+t), \quad x \geq 1, t \geq 2.$$

By derivation,

$$g''(x) = [\ln f(x)]'' = \frac{x+6}{(x+3)^2} - \frac{1}{(x+1+t)^2} \ > \ 0,$$

which means $g'(x) = [\ln f(x)]'$ is increasing in the interval $[1, +\infty)$.

Hence, $[\ln f(x+1) - \ln f(x)]' > 0$. It gives $\ln f(k_1+1) - \ln f(k_1) > \ln f(k_2) - \ln f(k_2-1)$, that is $f(k_1+1)f(k_2-1) > f(k_1)f(k_2)$. By the definition of the multiplicative sum Zagreb index,

$$\frac{\Pi_1^*(Kg(k_1+1, k_2-1, k_3, \ldots, k_t))}{\Pi_1^*(Kg(k_1, k_2, k_3, \ldots, k_t))} = \frac{(k_1+4)^{k_1+1}(k_1+2+t)(k_2+2)^{k_2-1}(k_2+t)}{(k_1+3)^{k_1}(k_1+1+t)(k_2+3)^{k_2}(k_2+1+t)}$$
$$= \frac{f(k_1+1)f(k_2-1)}{f(k_1)f(k_2)}$$
$$> 1.$$

After proving (7), the construction above can be seen as a transformation. By using this transformation enough times, we get

$$\Pi_1^*(k_1,k_2,\ldots,k_t) \le \Pi_1^*(Kg(K,0,0,\ldots,0)) = 3^K(K+2)^K(t+1)^{t-1}(t+K+1),$$

so it follows that the right-hand equality holds in (6) if and only if $G \cong Kg(K,0,0,\ldots,0)$. If there exists a pair k_i, k_j admitting $|k_i - k_j| \ge 2$, then we use the transformation once. Therefore, we can use this transformation enough times (if necessary) until $Kg(\underbrace{r+1,\ldots,r+1}_{s},\underbrace{r,\ldots,r}_{t-s})$ is obtained. Meanwhile, by direct calculation,

$$\begin{aligned}&\Pi_1^*(Kg(k_1,k_2,\ldots,k_t)\\ =\;& 3^K\left(t+1+\left\lfloor\frac{K}{t}\right\rfloor\right)^{t-s}\left(t+1+\left\lceil\frac{K}{t}\right\rceil\right)^{s}\left(2+\left\lfloor\frac{K}{t}\right\rfloor\right)^{(t-s)\lfloor\frac{K}{t}\rfloor}\left(2+\left\lceil\frac{K}{t}\right\rceil\right)^{s\lceil\frac{K}{t}\rceil}.\end{aligned}$$

Furthermore, if the transformation is used once more, then the Π_1^*-value will be increased. Thus, we obtain the minimum Π_1^*-value for the Kragujevac tree $Kg(k_1,k_2,\ldots,k_t)$, that is the left-hand equality holds in (6). □

3 Bounds of multiplicative sum Zagreb index

Denote by $\mathcal{G}_n, \mathcal{G}(m), \mathcal{G}_n(m)$ the class of graphs of order n, the class of graphs with m edges, and the class of graphs of order n with m edges, respectively. In this section, we obtain some bounds for the multiplicative sum Zagreb index and characterize the graphs with these bounds.

Theorem 3.1. *If $G \in \mathcal{G}(m)$, then $(2\,\delta)^m \le \Pi_1^*(G) \le (2\,\Delta)^m$, where the equality holds if and only if G is isomorphic to a δ- (or Δ-) regular graph.*

Proof. Clearly, $2\,\delta \le d_G(u) + d_G(v) \le 2\,\Delta$. Therefore, by the definition of the multiplicative sum Zagreb index,

$$(2\,\delta)^m \le \Pi_1^*(G) = \prod_{v_iv_j\in E(G)} (d_G(v_i)+d_G(v_j)) \le (2\,\Delta)^m.$$

For the equality, one can get the required results by direct calculation. □

Theorem 3.2. *If $G \in \mathcal{G}_n$, then $(2\,\delta)^{\frac{n\delta}{2}} \le \Pi_1^*(G) \le (2\,\Delta)^{\frac{n\Delta}{2}}$, where the equality holds if and only if G is isomorphic to a regular graph.*

Proof. By the famous Handshaking Lemma,

$$n\delta \le \sum_{v_i\in V(G)} d_G(v_i) = 2\,|E(G)| \le n\Delta.$$

Hence we get $\frac{n\delta}{2} \le |E(G)| \le \frac{n\Delta}{2}$. Therefore,

$$(2\,\delta)^{\frac{n\delta}{2}} \le \Pi_1^*(G) = \prod_{v_iv_j\in E(G)} (d_G(v_i)+d_G(v_j)) \le (2\,\Delta)^{\frac{n\Delta}{2}}. \tag{8}$$

Clearly, the equality holds in (8) if and only if G is isomorphic to a regular graph. □

Theorem 3.3. *If $G \in \mathcal{G}_n$, then*

$$\Pi_1^*(G)\Pi_1^*(\overline{G}) \le (2\,n-2)^{\frac{n(n-1)}{2}},$$

where the equality holds if and only if $G \cong K_n$ or $G \cong \overline{K}_n$.

Proof. Obviously, if $G \in \mathcal{G}_n$, then for any edge $u_iu_j \in E(G)$, $d_G(u_i) + d_G(u_j) \le 2\,(n-1)$. Hence, by the definition of the multiplicative sum Zagreb index,

$$\begin{aligned}\Pi_1^*(G)\Pi_1^*(\overline{G}) &= \prod_{u_iu_j \in E(G)} (d_G(u_i) + d_G(u_j)) \cdot \prod_{v_iv_j \in E(\overline{G})} (d_{\overline{G}}(v_i) + d_{\overline{G}}(v_j)) \\ &\le (2\,n-2)^{\binom{n}{2}} \;=\; (2\,n-2)^{\frac{n(n-1)}{2}} \end{aligned} \tag{9}$$

since $\left|E(G)\right| + \left|E(\overline{G})\right| = \binom{n}{2} = \frac{n(n-1)}{2}$. For the equality in (9), one can get the required result by direct calculation. □

Theorem 3.4. *If G is a triangle-free graph in $\mathcal{G}_n(m)$, then $\Pi_1^*(G) \le n^m$, where the equality holds if and only if G is isomorphic to a semi-regular graph with degrees p and q, where $p + q = n$.*

Proof. Since $G \in \mathcal{G}_n$ is triangle-free, for any $v_iv_j \in E(G)$, $d_G(v_i) + d_G(v_j) \le n$. Hence, by the definition of the multiplicative sum Zagreb index,

$$\Pi_1^*(G) = \prod_{v_iv_j \in E(G)} (d_G(v_i) + d_G(v_j)) \le n^m. \tag{10}$$

For the equality in (10), it is easy to see that for any edge $xy \in E(G)$, $d_G(x) + d_G(y) = n$, that is G is isomorphic to a semi-regular graph with degree p and q, and $p + q = n$. □

Theorem 3.5. [9] *If $T \in \mathcal{T}_n$, then $9 \cdot 4^{n-3} \le \Pi_1^*(T) \le n^{n-1}$, where the left equality holds if and only if $T \cong P_n$ and the right equality holds if and only if $T \cong S_n$.*

Set $p + q = n$, denote by $\mathcal{B}_{p,q}$ the class of all bipartite graphs with two parties of sizes p and q, respectively. Denote by $\mathcal{K}_{p,q}$ the class of all complete bipartite graphs with two parties of sizes p and q, respectively. The following theorem wholly determines the extremal Π_1^*-values in $\mathcal{B}_{p,q}$.

Theorem 3.6. *For any graph $G \in \mathcal{B}_{p,q}$,*

$$9 \cdot 4^{n-3} \le \Pi_1^*(G) \le \begin{cases} n^{\frac{n^2-1}{4}}, & \text{if } n \text{ is odd}, \\ n^{\frac{n^2}{4}}, & \text{if } n \text{ is even}, \end{cases} \tag{11}$$

where the right equality holds if and only if $G \cong K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Proof. Obviously, P_n is a bipartite graph. Hence, by Theorem 3.5, for any $G \in \mathcal{B}_{p,q}$, $\Pi_1^*(G) \ge \Pi_1^*(P_n) = 9 \cdot 4^{n-3}$.

For any $G \in \mathcal{B}_{p,q}$, $\Pi_1^*(G) \le \Pi_1^*(K_{p,q})$ due to Lemma 2.1. Now we consider function $f(x) = n^{x(n-x)},\ x \ge 1$. By derivation, $f'(x) = (n - 2\,x)\, n^{x(n-x)} \ln n$. Hence, $f(x)$ is increasing when $x \le \frac{n}{2}$ and is decreasing when $x \ge \frac{n}{2}$, which means when $x = \frac{n}{2}$, $f(x)$ attains the maximum value. It gives for any $G \in \mathcal{B}_{p,q}$,

$$\Pi_1^*(G) \le \Pi_1^*(K_{p,q}) \le \Pi_1^*(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}) = n^{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}.$$

For the equality in (11), one can get the required result by direct calculation. □

Denote by $CS(n,\alpha)$ the *complete split graph*, which is the graph obtained from a complete graph $K_{n-\alpha}$ and a stable set consisted of α separated vertices such that for any vertex u in stable set, u is linked to every vertex in $K_{n-\alpha}$.

Theorem 3.7. *If $G \in \mathcal{G}_n$ and the independent number of G is α, then*

$$\Pi_1^*(G) \le (2\,n-2)^{\binom{n-\alpha}{2}}(2\,n-1-\alpha)^{\alpha(n-\alpha)},$$

where the equality holds if and only if $G \cong CS(n,\alpha)$.

Proof. By direct calculation, one can easily obtain that

$$\Pi_1^*(CS(n,\alpha)) \le (2\,n-2)^{\binom{n-\alpha}{2}}\,(2\,n-1-\alpha)^{\alpha(n-\alpha)}\,.$$

Now we assume that $G \not\cong CS(n,\alpha)$, then by Lemma 2.1 (ii) and the independent number of G is α,

$$\Pi_1^*(G) < \Pi_1^*(CS(n,\alpha)) \le (2\,n-2)^{\binom{n-\alpha}{2}}[2\,n-1-\alpha)^{\alpha(n-\alpha)}.$$

We complete the proof of this theorem. □

If a path $P_k = v_1 v_2 \cdots v_k$ is a subgraph of G such that $d_G(v_1) \ge 3$, $d_G(v_k) = 1$, $d_G(v_i) = 2$ for $2 \le i \le k-1$, then P_k is called a *pendent path* of G and v_1 is the *origin* of P_k.

Lemma 3.8. [13] *Suppose that P and Q are two pendent paths at origin u and v in G, $ux \in E(P)$ and y is a pendent vertex in Q, respectively. If $G' = G - ux + yx$, then*

(i) *If $d_G(u) \ge 4$, then $\Pi_1^*(G') < \Pi_1^*(G)$.*
(ii) *If there exists a vertex $u_i \in N_G(u)$ such that $u_i \ne x$ and $d_G(u) + d_G(u_i) \le 16$, then $\Pi_1^*(G') < \Pi_1^*(G)$.*

Denote by $\mathcal{W}(n,\omega)$ the class of graphs of order n with clique number ω. Denote by $\mathcal{W}_{n,\omega}$ the class of graphs of order n constructed from the complete graph K_ω by attaching pendent path(s) onto the vertex (or vertices) of K_ω such that the order of all pendent path(s) is $n-\omega$. The *long kite graph*, denoted by $Ki_{n,\omega}$, is a graph obtained from a complete graph K_ω by attaching a path $P_{n-\omega}$ of length $n-\omega$ onto one vertex in K_ω. Specially, if $\omega = n$, then $Ki_{n,\omega} \cong K_n$. Therefore, by assuming that $\omega \le n-2$, we get

$$\Pi_1^*(Ki_{n,\omega}) = 3 \cdot 4^{(n-\omega-2)}(\omega+2)(2\,\omega-1)^{\omega-1}(2\,\omega-2)^{\binom{\omega-1}{2}}.$$

Theorem 3.9. *If $G \in \mathcal{W}(n,\omega)$, then*

$$\Pi_1^*(G) \ge 3 \cdot 4^{(n-\omega-2)}(\omega+2)(2\,\omega-1)^{\omega-1}(2\,\omega-2)^{\binom{\omega-1}{2}},$$

where the equality holds if and only if $G \cong Ki_{n,\omega}$.

Proof. By Lemma 2.1 (i) and Lemma 2.4, if G has the minimum Π_1^*-value in $\mathcal{W}(n,\omega)$, then $G \in \mathcal{W}_{n,\omega}$. In other words, there are some pendent paths on several vertices in K_ω. If $\omega \ge 4$, then we can choose a vertex which is attaching a pendent path in K_ω, and this vertex is of degree ≥ 4. By using Lemma 3.8 (i), we can get a graph G' such that $\Pi_1^*(G') < \Pi_1^*(G)$. If $\omega \leq 3$, then there must exist an vertices u and v in K_ω such that $d_G(u) + d_G(v) < 16$. Thus, by using Lemma 3.8 (ii), we can get a graph G'' admitting that $\Pi_1^*(G'') < \Pi_1^*(G)$. Therefore, by using Lemma 3.8, we obtain that if G has the minimum Π_1^*-value and $G \in \mathcal{W}_{n,\omega}$, then $G \cong Ki_{n,\omega}$. □

Corollary 3.10. [9] *If G is a connected graph of order n, then $\Pi_1^*(G) \geq 9 \cdot 4^{n-3}$, where the equality holds if and only if $G \cong P_n$.*

Proof. Assume that the clique number of G is ω. It is easy to see that $\omega \geq 2$. Then we obtain a Π_1^*-value sequence as follows

$$\Pi_1^*(G) \geq \Pi_1^*(Ki_{n,\omega-1}) \geq \Pi_1^*(Ki_{n,\omega-2}) \geq \cdots \geq \Pi_1^*(P_n) = 9 \cdot 4^{n-3}$$

by Lemma 2.1. Therefore, we get the required result. □

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