Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2025.255619.1918
Vol. 16, No. 2, 2025, pp. 141-153
Research Paper

On Extremal General Multiplicative Zagreb Indices

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Keywords:
Maximum degree,
Diameter,
Tree,
Unicyclic graph

AMS Subject Classification (2020):

05C05; 05C07; 05C09

Article History:
Received: 20 October 2024
Accepted: 3 January 2025

Abstract

The first general multiplicative Zagreb index $P_1^a(G)$ is the product of the degree of each vertex v in G, raised to the power a and the second general multiplicative Zagreb index $P_2^a(G)$ is the product of the degree of each vertex v in G, raised to the power a times the degree of v, where a is a non-zero real number. In this study, we present bounds on the general multiplicative Zagreb indices for trees and unicyclic graphs. We also provide bounds for the first general multiplicative Zagreb index for trees. Additionally, we identify all the extremal graphs for each bound mentioned as best as possible.

1 Introduction

In this study, we examine connected simple graphs. $V(G)$ and $E(G)$ represent the vertex set and edge set of a graph G, respectively. The degree of v, $\deg_G(v)$, for a vertex v in G, is the number of edges incident to v. A vertex with degree one is called a pendant vertex. To indicate the highest degree of G, we utilize $\Delta = \Delta(G)$. The graph $G + uv$ represents the graph that is created by adding an edge uv to any two nonadjacent vertices u and v in G. The length of the shortest path between two vertices, u and v, is represented by $d_G(u, v)$. For each vertex $v \in V(G)$, the greatest distance between v and every other vertex in G is known as the eccentricity of vertex v in G, $\mathrm{ecc}_G(v)$. The diameter of G, represented by $d(G)$, is its maximum eccentricity, and the radius of G, represented by $r(G)$, is its minimum eccentricity. A diametrical path of G is the path $P_d = v_0v_1 \cdots v_d$.

A connected graph without any cycles is called a tree. A path and a star of order n are indicated by P_n and S_n respectively. For integers $l \geq 2$ and $n_1 \geq n_2 \geq 1$, $P_l(n_1, n_2)$ is a tree obtained from the path P_l by joining one end vertex of P_l to n_1 new vertices and the other end vertex of P_l to n_2 pendant vertices. Trees can be attached to any vertex in a cycle graph to create a unicyclic graph. A unicyclic graph with n vertices has n edges. A graph obtained by adding a new edge between the two pendant vertices of S_n is denoted by S_n^+.

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Academic Editor: Gholam Hossein Fath-Tabar,

Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$ with $\deg(v_1) \geq \deg(v_2) \geq \ldots \geq \deg(v_n)$. Let $\deg(v_i) = x_i$ for $i = 1, 2, \ldots, n$. The non-increasing sequence $D(G) = d_1, d_2, \ldots, d_n$ is called the degree sequence of G. Furthermore, $D(G) = [x_1^{a_1}, x_2^{a_2}, \ldots, x_t^{a_t}]$ means that the degree sequence of G consists of x_i (appearing a_i times), where $i = 1, 2, \ldots, t$. The superscript 1 of x_i is dropped if $a_i = 1$. If every other vertex in the set $\Gamma \subseteq V(G)$ is adjacent to at least one vertex in Γ, then the set is referred to as a dominant set. The number of vertices in the smallest dominating set is known as the domination number, represented by $\gamma(G)$. Additionally, for definitions of terminology not explicitly used in this article, consult [1].

In chemical and pharmaceutical research, topological indices are frequently employed for activities including combinatorial library design, drug design, chemical documentation, isomer discrimination, toxicity hazard evaluations, and QSPR/QSAR analysis. These indices make it possible to translate chemical structures into numerical values, which simplifies correlations with chemical and physical characteristics such as boiling temperatures and molar heats of formation. Topological indices quantify molecular structures and offer useful information for understanding chemical behavior, forecasting features, and improving molecular design.

The goal of recent drug design research has been to determine a chemical's qualities based solely on its molecular structure. Topological indices are used to quantify the biological, physicochemical, environmental, and toxicological characteristics of molecules. Preliminary research employing quantitative structure-activity relationships (QSAR) enables the selection of the most promising compounds, reducing the number of compounds synthesized because both trial-and-error synthesis and random screening for activity are time-consuming and unfeasible [2]. Many topological indices based on degree [3, 4] and distance [5–7] have been thoroughly investigated.

There are several uses for multiplicative Zagreb indices, which have been studied more in the last ten years. Because they are connected with many physical properties of molecules, they are important in the fields of chemistry, pharmaceutical sciences, materials science, and engineering. These chemical structures are described using graph theory, in which a compound's atoms are represented by the vertices of a graph and its chemical bonds by its edges.

In 1972, Gutman and Trinajstić presented the first and second Zagreb indices, which are degree-based molecular descriptors [8]. Zagreb indices are among the oldest topological indices, and because of their chemical significance, a lot of research has been done on them. Bounds on the first and second Zagreb indices for trees were examined by Lin [9] and Borovićanin [10]. The first and second multiplicative Zagreb indices of trees of a particular order were examined by Gutman [11] and Xu and Hua [12]. Bounds on these indices for trees with a specified number of maximum degree vertices and domination number [13–15], unicyclic and bicyclic graphs with given (total) domination [16], k-trees [17], molecular graphs [18], graphs of given order, size, and other parameters [19, 20], some derived graphs [21], graph operations [22, 23]; chemical trees [24] and bipartite graphs of given diameter [25] were examined.

In [3], $P_i^a, (i = 1, 2)$ indices were introduced.

$$P_1^a(G) = \prod_{v \in V(G)} \deg(v)^a \quad \text{and} \quad P_2^a(G) = \prod_{v \in V(G)} \deg(v)^{a \deg(v)},$$

where $a \neq 0$ is a real number. This is the definition of the first and second general multiplicative Zagreb indices. The traditional multiplicative Zagreb indices are generalized by these indices. The first multiplicative Zagreb index is P_1^2 for $a = 2$, and the Narumi-Katayama index is P_1^1 for $a = 1$. P_2^1 is the second multiplicative Zagreb index for $a = 1$. Note that we may restate the previous formula as $P_1^a(G) = P_1^a(X)$ and $P_2^a(G) = P_2^a(X)$ if the degree sequence of G is represented by $D(G) = X$.

Vetrik and Balachandran presented $P_i^a, (i = 1, 2)$ for trees with a given order, matching number and independence number [3, 26, 27]. Nanotubes [28], graphs with applications to

QSPR modeling [29], graphs with a number of bridges [30], graphs with a small number of cycles [31], graphs with a given clique number [4], unicyclic graphs [32], unicyclic graphs with a matching number [27], and polycyclic aromatic hydrocarbons and benzenoid systems [33] are all analyzed in great detail.

For trees with a known maximum degree and diameter, as well as for unicyclic graphs with a particular diameter for $a > 0$, we give an upper bound for the P_1^a index and a lower bound for the P_2^a index. Additionally, for trees with an identified domination number for $a > 0$, we give a lower bound for the P_1^a index. We also identify all the extremal graphs, suggesting that our bounds are optimal.

2 Preliminary results

Proposition 2.1. *For $a, b \in \mathbb{Z}_{\geq 2}$, $ab \geq a + b$.*

Proposition 2.2. *For an integer $n \geq 5$, $2^{\frac{n}{2}} > n$.*

Proposition 2.2 can be proved using the principle of mathematical induction.

Proposition 2.3. *For $a, b \in \mathbb{Z}_{\geq 2}$, $ab \geq 2(a + b - 2)$, and the equality holds when $a = b = 2$.*

Proof. $ab - 2(a + b - 2) = ab - 2a - 2b + 4 = a(b - 2) - 2(b - 2) = (b - 2)(a - 2) \geq 0$ because $a, b \geq 2$. Therefore, $ab \geq 2(a + b - 2)$. ∎

Proposition 2.4. *Let G be a graph different from P_n. Let $u, v \in V(G)$ such that $\deg_G(v) = 1$ and $\deg_G(u) \geq 2$. Let $u' \in V(G)$ such that $uu' \in E(G)$ and u' is at a larger distance from v in G than u. Let $G' = G - uu' + vu'$. Then for $a > 0$,*

$$P_1^a(G) \leq P_1^a(G') \quad \textit{and} \quad P_2^a(G) \geq P_2^a(G').$$

Proof. Since $G' = G - uu' + vu'$, we have $\deg_G(u) = p \geq 2$, $\deg_G(v) = 1$, $\deg_{G'}(u) = p - 1$, and $\deg_{G'}(v) = 2$. The degrees of all other vertices remain unchanged. Thus, for $a > 0$,

$$\frac{P_1^a(G)}{P_1^a(G')} = \frac{p^a}{2^a(p-1)^a} = \left(\frac{p}{2(p-1)}\right)^a \leq 1,$$

hence

$$P_1^a(G) \leq P_1^a(G').$$

Similarly,

$$\frac{P_2^a(G)}{P_2^a(G')} = \frac{p^{ap}}{2^{2a}(p-1)^{a(p-1)}} = \left(\frac{p^p}{2^2(p-1)^{(p-1)}}\right)^a \geq 1,$$

thus

$$P_2^a(G) \geq P_2^a(G') \quad \text{for} \quad p \geq 2.$$

∎

A tree that has exactly one vertex with a degree greater than two is said to be starlike. Consequently, it possesses a singular vertex of maximum degree $\Delta \geq 3$. Let T^* represent the set of Δ degree starlike trees.

Proposition 2.5. *For a tree $T \in T^*$,*

$$P_1^a(T) = \Delta^a \cdot 2^{a(n-\Delta-1)} \quad \textit{and} \quad P_2^a(T) = \Delta^{a\Delta} \cdot 2^{2a(n-\Delta-1)}.$$

Proof. Let n_i be the number of vertices of degree i. From the definition of a starlike tree and the Handshaking Lemma, we have

$$n_1 + n_2 + n_\Delta = n \Rightarrow n_1 + n_2 = n - 1, \tag{1}$$

$$n_1 + 2n_2 + \Delta n_\Delta = 2(n-1) \Rightarrow n_1 + 2n_2 + \Delta = 2n - 2. \tag{2}$$

By combining Equations (1) and (2), we have $n_2 = n - \Delta - 1$ and $n_1 = \Delta$. Therefore, $D(T) = [\Delta, 2^{(n-\Delta-1)}, 1^{\Delta}]$.

From the definition of P_1^a and P_2^a of a graph with respect to its degree sequence, we have

$$P_1^a(T) = \Delta^a \cdot 2^{a(n-\Delta-1)} \cdot 1^{a\Delta} = \Delta^a \cdot 2^{a(n-\Delta-1)},$$

and

$$P_2^a(T) = \Delta^{a\Delta} \cdot 2^{2a(n-\Delta-1)} \cdot 1^{a\Delta} = \Delta^{a\Delta} \cdot 2^{2a(n-\Delta-1)}.$$

■

3 Main results

3.1 Trees with a given diameter

Let the set of all trees of order n and diameter d be represented as $\mathscr{T}_{n,d}$, where $1 \leq d \leq n-1$. Only P_2 and S_n have $d = 1$ and $d = 2$, respectively, whereas P_n is the only tree with $d = n-1$. Consequently, we will only take into account trees whose diameter is $d \geq 3$.

Let $T_{n,d,i}$ represent the tree that is produced by attaching $n-d-1$ pendant vertices to v_i for $1 \leq i \leq d-1$ from $P_d : v_0v_1 \cdots v_d$. $T_{n,d,2}$, for example, is displayed in Figure 1. Consider the set $\mathcal{T}_{n,d} = \{T_{n,d,i} : 1 \leq i \leq d-1\}$.

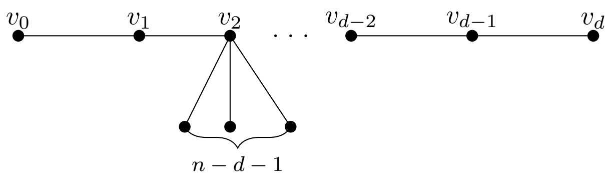

Figure 1: Tree $T_{n,d,2}$.

Lemma 3.1. *Let $T \in \mathscr{T}_{n,d}$, where $3 \leq d \leq n-2$. Then $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$ if and only if $T \in \mathcal{T}_{n,d}$.*

Proof. Let $T \in \mathcal{T}_{n,d}$. Clearly, $T \in \mathscr{T}_{n,d}$ and $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$. Conversely, let $T \in \mathscr{T}_{n,d}$ and $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$. We need to show that $T \in \mathcal{T}_{n,d}$.

Let $P_d : v_0v_1 \cdots v_d$ be the diametrical path of T. Clearly, v_0 and v_d are pendant vertices in T. Then $\deg_T(v_i) \geq 2$ for $i = 1, 2, \ldots, d-1$. Since $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$, there are just $d-1$ vertices of degree greater than 1 in T. If one of the vertices with maximum degree is not in $\{v_1, v_2, \ldots, v_{d-1}\}$, then there exists $i \in \{1, 2, \ldots, d-1\}$ such that $\deg_T(v_i) = 3$ and $\deg_T(v_j) = 2$ for all $j \in \{1, 2, \ldots, d-1\} \setminus \{i\}$. Clearly, $\deg_T(v_0) \neq n-d+1$ and $\deg_T(v_d) \neq n-d+1$ otherwise the diameter of T is greater than d. Thus, there are at least d vertices of degree greater than 1. This is a contradiction to $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$.

Therefore, there exists $k \in \{1, 2, \ldots, d-1\}$ such that $\deg_T(v_k) = n-d+1$. Since $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$, v_k is a unique vertex whose degree is $n-d+1$ in T and $1 \leq k \leq d-1$.

The number of vertices whose degree is 2 in $\{v_0, v_1, \ldots, v_d\}$ is equal to $d+1-2-1 = d-2$, which is the same as in $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$. Thus, there is no vertex $u \notin \{v_0, v_1, \ldots, v_d\}$ such that $\deg_T(u) \geq 3$. Hence, $T \in \mathcal{T}_{n,d}$. ■

Theorem 3.2. *Let $T \in \mathscr{T}_{n,d}$, where $3 \leq d \leq n-2$. For $a > 0$, we have*

$$P_1^a(T) \geq (n-d+1)^a 2^{a(d-2)} \quad \text{and} \quad P_2^a(T) \leq (n-d+1)^{a(n-d+1)} 2^{2a(d-2)}.$$

The equalities hold if and only if $T \in \mathcal{T}_{n,d}$.

Proof. Let T' be a tree with the smallest P_1^a (or the largest P_2^a) index among trees with n vertices and diameter d. We aim to show by contradiction that $T' \in \mathcal{T}_{n,d}$. Assume that $T' \in \mathscr{T}_{n,d}$ but $T' \notin \mathcal{T}_{n,d}$.

Since $T' \notin \mathcal{T}_{n,d}$, there are two vertices u and v on the path $P_d : v_0 v_1 \cdots v_d$ (the diametrical path of T') such that $\deg_{T'}(u) = r \geq 3$ and $\deg_{T'}(v) = q \geq 3$. Without loss of generality, consider $q \geq r \geq 3$. Let $u_1, u_2, \ldots, u_{r-2}$ be the vertices adjacent to u that are outside of P_d. That is, $u_i \notin \{v_0, v_1, \ldots, v_d\}$ for $i = 1, 2, \ldots, r-2$.

Let $T'' = T' - \{uu_1, uu_2, \ldots, uu_{r-2}\} + \{vu_1, vu_2, \ldots, vu_{r-2}\}$. Clearly, $T'' \in \mathscr{T}_{n,d}$. We have $\deg_{T'}(u) = r$, $\deg_{T'}(v) = q$, $\deg_{T''}(u) = 2$, and $\deg_{T''}(v) = q+r-2$, while $\deg_{T'}(x) = \deg_{T''}(x)$ for all $x \in V(T') \setminus \{u, v\}$. Thus,

$$\frac{P_1^a(T')}{P_1^a(T'')} = \frac{r^a q^a}{2^a (q+r-2)^a} = \left(\frac{rq}{2(q+r-2)}\right)^a.$$

By Proposition 2.3, we have $\frac{rq}{2(q+r-2)} > 1$, so $\frac{P_1^a(T')}{P_1^a(T'')} > 1$, implying $P_1^a(T') > P_1^a(T'')$, which is a contradiction. Similarly, we can show that $P_2^a(T') < P_2^a(T'')$, which is again a contradiction. Therefore, $T' \in \mathcal{T}_{n,d}$.

By Lemma 3.1, a tree $T \in \mathcal{T}_{n,d}$ has a degree sequence $D(T) = [n-d+1, 2^{d-2}, 1^{n-d+1}]$, and clearly,

$$P_1^a(T) = (n-d+1)^a 2^{a(d-2)} \quad \text{and} \quad P_2^a(T) = (n-d+1)^{a(n-d+1)} 2^{2a(d-2)}.$$

■

3.2 Trees with a given domination number

Any tree T with n vertices is a bipartite graph, where each partite set is a dominant set. As a result, there are at most $\frac{n}{2}$ vertices in one of the partite sets. We have $1 \leq \gamma \leq \frac{n}{2}$ for every tree T with n vertices and domination number γ. The inequalities are tight for all trees except for T being S_n or P_n (for even n), in which case equality holds on the corresponding sides.

The set of all trees of order n and domination number γ is represented by $\mathscr{T}_{n,\gamma}$. Let $T_{n,\gamma}$ represent a tree that is created by joining $\gamma - 1$ pendant vertices of $S_{n-\gamma+1}$ with a path of length 1. $D(T_{n,\gamma}) = [n-\gamma, 2^{\gamma-1}, 1^{n-\gamma}]$ as a result. For instance, $T_{4,1}$ is S_4, $T_{4,2}$ is P_4, $T_{5,2}$ is $P_2(2,1)$, and $T_{5,3}$ is P_5.

Theorem 3.3. *Let $T \in \mathscr{T}_{n,\gamma}$, and $a > 0$. Then*

$$P_1^a(T) \geq (n-\gamma)^a 2^{a(\gamma-1)}.$$

Equality holds if and only if T is $T_{n,\gamma}$.

Proof. If $\Delta(T) = 2$ and $n \geq 2$, then $T \cong P_n$. For $n = 2$, $T \cong T_{2,1} \cong P_2$, thus

$$P_1^a(T) = P_1^a(T_{2,1}) = P_1^a(P_2).$$

For $n = 3$, $T \cong T_{3,1} \cong P_3$, thus

$$P_1^a(T) = P_1^a(T_{3,1}) = P_1^a(P_3).$$

For $n = 4$, $T \cong T_{4,2} \cong P_4$, thus

$$P_1^a(T) = P_1^a(T_{4,2}) = P_1^a(P_4).$$

This shows that the equality holds for $n \leq 4$. If $n \geq 5$, then

$$P_1^a(P_n) = 2^{a(n-2)}.$$

Assume that $\gamma(P_n) = \frac{n}{2}$. So, for $a > 0$ and $n \geq 5$, using Proposition 2.2, we have

$$\frac{P_1^a(P_n)}{(n-\gamma)^a 2^{a(\gamma-1)}} = \frac{2^{a(n-2)}}{(n-\frac{n}{2})^a 2^{a(\frac{n}{2}-1)}} = \left(\frac{2^{\frac{n}{2}}}{n}\right)^a > 1.$$

Thus, $P_1^a(P_n) > (n-\gamma)^a 2^{a(\gamma-1)}$.

Therefore, when $\Delta(T) = 2$, the theorem is true. Trees with $\Delta(T) \geq 3$ are now under consideration. Let d be the diameter of T, and let $P_d : v_0 v_1 \cdots v_d$ be the diametrical path of T. Then $\deg_T(v_0) = \deg_T(v_d) = 1$. Since $D(T_{n,\gamma}) = [n-\gamma, 2^{\gamma-1}, 1^{n-\gamma}]$, we have $\Delta \leq n - \gamma$. Let $\Gamma(T)$, or simply Γ, be a dominant set of T such that $|\Gamma| = \gamma(T)$.

We will use the Principle of Mathematical Induction to prove the theorem for $\Delta(T) \geq 3$. The trees that satisfy the equality in the preceding theorem for $n \leq 5$ and $\Delta(T) \geq 3$ are $T_{4,1} \cong S_4$, $T_{5,2}$, and $T_{5,1} \cong S_5$. Assume that for $|T'| = n - 1$, the thesis holds true, that is,

$$P_1^a(T') \geq (n-1-\gamma)^a 2^{a(\gamma-1)}.$$

Let $T' = T - v_0$. Note that

$$\deg_{T'}(v) = \deg_T(v), \ \forall v \in V(T) \setminus \{v_0, v_1\}.$$

Also,

$$\deg_{T'}(v_1) = \deg_T(v_1) - 1.$$

We need to show that the theorem is true for $|T| = n$. Now consider two cases:

1. If $v_0 \notin \Gamma(T)$, then $v_0 \notin \Gamma(T')$, and thus $\gamma(T') = \gamma(T)$ and $\deg_T(v_1) \geq 2$. Since

$T' = T - v_0$, we have $\deg_T(v_0) = 1$ and $\deg_{T'}(v_1) = \deg_T(v_1) - 1 \geq 1$. Then

$$\begin{aligned}
P_1^a(T) &= \prod_{v \in V(T)} (\deg_T(v))^a \\
&= \left(\prod_{v \neq v_0, v_1} (\deg_T(v))^a \right) (\deg_T(v_0))^a (\deg_T(v_1))^a \\
&= \left(\prod_{v \neq v_1} (\deg_{T'}(v))^a \right) (\deg_T(v_1) - 1)^a \frac{(\deg_T(v_1))^a}{(\deg_T(v_1) - 1)^a} (\deg_T(v_0))^a \\
&= \left(\prod_{v \neq v_1} (\deg_{T'}(v))^a \right) (\deg_{T'}(v_1))^a \frac{(\deg_T(v_1))^a}{(\deg_T(v_1) - 1)^a} (\deg_T(v_0))^a \\
&= \left(\prod_{v \in V(T')} (\deg_{T'}(v))^a \right) \left(\frac{\deg_T(v_1)}{(\deg_T(v_1) - 1)} \deg_T(v_0) \right)^a \\
&= P_1^a(T') \left(\frac{\deg_T(v_1)}{(\deg_T(v_1) - 1)} \right)^a \quad \text{because} \quad \deg_T(v_0) = 1.
\end{aligned}$$

From the hypothesis,

$$\begin{aligned}
P_1^a(T) &\geq 2^{a(\gamma-1)} (n - 1 - \gamma)^a \left(\frac{\deg_T(v_1)}{(\deg_T(v_1) - 1)} \right)^a \\
&= 2^{a(\gamma-1)} (n - \gamma)^a \frac{(n - 1 - \gamma)^a}{(n - \gamma)^a} \left(\frac{\deg_T(v_1)}{(\deg_T(v_1) - 1)} \right)^a \\
&= 2^{a(\gamma-1)} (n - \gamma)^a \left(\frac{\frac{n-1-\gamma}{n-\gamma}}{\frac{\deg_T(v_1)-1}{\deg_T(v_1)}} \right)^a .
\end{aligned}$$

Since $\frac{n-1-\gamma}{n-\gamma} = 1 - \frac{1}{n-\gamma}$ and $\frac{\deg_T(v_1)-1}{\deg_T(v_1)} = 1 - \frac{1}{\deg_T(v_1)}$ and $\deg_T(v_1) \leq n - \gamma$, we have $\frac{1}{\deg_T(v_1)} \geq \frac{1}{n-\gamma}$, thus $\frac{\frac{n-1-\gamma}{n-\gamma}}{\frac{\deg_T(v_1)-1}{\deg_T(v_1)}} \geq 1$. This leads us to $P_1^a(T) \geq 2^{a(\gamma-1)}(n - \gamma)^a$.

2. If $v_0 \in \Gamma(T)$, then $v_0 \notin \Gamma(T')$. Thus, $v_0 \notin V(T')$, then we have $\gamma(T') = \gamma(T) - 1$.

We would obtain a path of length at least $d+1$ in T if v_1 were adjacent to a vertex $w \notin \{v_0, v_2\}$ in T that is not a pendant vertex. v_1 must be in every dominating set of size γ, (that means, $v_0 \notin \Gamma(T)$), if it were adjacent to a pendant vertex $w \notin \{v_0, v_2\}$. Therefore, the only neighbors of v_1 in T are v_0 and v_2. The following are true: $\deg_{T'}(v_1) = \deg_T(v_1) - 1 = 1$ and $\deg_T(v_0) = 1$.

Then,

$$\begin{aligned}
P_1^a(T) &= \prod_{v\in V(T)} (\deg_T(v))^a \\
&= \left(\prod_{v\neq v_0,v_1} (\deg_T(v))^a\right) (\deg_T(v_0))^a (\deg_T(v_1))^a \\
&= \left(\prod_{v\neq v_1} (\deg_{T'}(v))^a\right) (\deg_T(v_1)-1)^a \frac{(\deg_T(v_1))^a}{(\deg_T(v_1)-1)^a} (\deg_T(v_0))^a \\
&= \left(\prod_{v\neq v_1} (\deg_{T'}(v))^a\right) (\deg_{T'}(v_1))^a \frac{(\deg_T(v_1))^a}{(\deg_T(v_1)-1)^a} (\deg_T(v_0))^a \\
&= \left(\prod_{v\in V(T')} (\deg_{T'}(v))^a\right) \left(\frac{\deg_T(v_1)}{(\deg_T(v_1)-1)} \deg_T(v_0)\right)^a \\
&= P_1^a(T') \left(\frac{\deg_T(v_1)}{(\deg_T(v_1)-1)}\right)^a; \quad \text{because} \quad \deg_T(v_0)=1.
\end{aligned}$$

From the hypothesis,

$$\begin{aligned}
P_1^a(T) &\geq 2^{a(\gamma-1-1)}(n-1-(\gamma-1))^a \left(\frac{\deg_T(v_1)}{(\deg_T(v_1)-1)}\right)^a \\
&= 2^{a(\gamma-1-1)}(n-\gamma)^a \left(\frac{\deg_T(v_1)}{(\deg_T(v_1)-1)}\right)^a \\
&= 2^{a(\gamma-2)}(n-\gamma)^a \left(\frac{2}{2-1}\right)^a \\
&= 2^{a(\gamma-1)}(n-\gamma)^a.
\end{aligned}$$

This leads us to $P_1^a(T) \geq 2^{a(\gamma-1)}(n-\gamma)^a$. ■

3.3 Trees with a given maximum degree

The set of all trees of order n and maximum degree Δ is represented by $\mathscr{T}_{n,\Delta}$, where $1 \leq \Delta \leq n-1$. Only P_2 and P_n have $\Delta = 1$ and $\Delta = 2$, respectively, whereas S_n is the only tree with $\Delta = n-1$. Consequently, we will take into account trees with a maximum degree of $\Delta \geq 3$.

Theorem 3.4. *Let $T \in \mathscr{T}_{n,\Delta}$ and $3 \leq \Delta \leq n-1$. Then for $a > 0$,*

$$P_1^a(T) \leq \Delta^a \cdot 2^{a(n-\Delta-1)} \quad \textit{and} \quad P_2^a(T) \geq \Delta^{a\Delta} \cdot 2^{2a(n-\Delta-1)}.$$

The equality holds if and only if $T \in T^*$.

Proof. Let T' be a tree with the largest P_1^a (or the smallest P_2^a) index among trees with n vertices and maximum degree Δ. We need to show by contradiction that $T' \in T^*$. We claim the following:

Claim 1. T' has no vertex v such that $2 < \deg_{T'}(v) < \Delta$.

Assume that T' contains a vertex, say u, such that $3 \leq \deg_{T'}(u) = p \leq \Delta - 1$. Let u be the nearest vertex to a pendant vertex, say v, in T'. Let $u' \in V(T')$ such that $uu' \in E(T')$, but u' is further from v in T' than u is. Let $T'' = T' - uu' + vu'$. Clearly, $T'' \in \mathscr{T}_{n,\Delta}$. From Proposition 2.4,

$$P_1^a(T') < P_1^a(T'') \quad \text{and} \quad P_2^a(T') > P_2^a(T''),$$

for $a > 0$, which is a contradiction. Thus, Claim 1 is true.

Claim 2. T' has exactly one vertex with degree Δ.

Assume that T' contains two vertices, say u and v, such that $\deg_{T'}(u) = \deg_{T'}(v) = p = \Delta > 2$. Let $N_{T'}(u) = \{u_1, u_2, \ldots, u_p\}$, and let $w_1, w_2, \ldots, w_s$ be pendant vertices of T', where $s > p$. Let $T_1 = T' - uu_1 + w_1u_1$. Since $\deg_{T_1}(v) = \deg_{T'}(v) = \Delta > 2$, we have $T_1 \in \mathscr{T}_{n,\Delta}$. From Proposition 2.4,

$$P_1^a(T') < P_1^a(T_1) \quad \text{and} \quad P_2^a(T') > P_2^a(T_1), \qquad a > 0.$$

Let $T_2 = T_1 - uu_2 + w_2u_2$. Since $\deg_{T_2}(v) = \deg_{T_1}(v) = \deg_{T'}(v) = \Delta > 2$, we have $T_2 \in \mathscr{T}_{n,\Delta}$. From Proposition 2.4,

$$P_1^a(T_1) < P_1^a(T_2) \quad \text{and} \quad P_2^a(T_1) > P_2^a(T_2), \qquad a > 0.$$

Similarly, let $T_3 = T_2 - uu_3 + w_3u_3$. Since $\deg_{T_3}(v) = \deg_{T_2}(v) = \deg_{T_1}(v) = \deg_{T'}(v) = \Delta > 2$, we have $T_3 \in \mathscr{T}_{n,\Delta}$. By Proposition 2.4, we have

$$P_1^a(T_2) < P_1^a(T_3) \quad \text{and} \quad P_2^a(T_2) > P_2^a(T_3), \qquad a > 0.$$

Thus, using the same fashion as above, let $T_{k+1} = T_k - uu_k + w_ku_k$. Since $\deg_{T_k}(v) = \deg_{T'}(v) = \Delta > 2$, we have $T_k \in \mathscr{T}_{n,\Delta}$ for $1 \leq k \leq p-2$. Then for $1 \leq k \leq p-2$ and $a > 0$, by Proposition 2.4, we have

$$P_1^a(T_{k-1}) < P_1^a(T_k) \quad \text{and} \quad P_2^a(T_{k-1}) > P_2^a(T_k).$$

This approach gives us the following pattern in inequalities for $a > 0$:

$$P_1^a(T') < P_1^a(T_1) < P_1^a(T_2) < \cdots < P_1^a(T_{p-2}),$$

$$P_2^a(T') > P_2^a(T_1) > P_2^a(T_2) > \cdots > P_2^a(T_{p-2}).$$

This is a contradiction. Thus, Claim 2 is true.

Claim 3. T' has Δ pendant vertices.

Since T' is a tree, by Proposition 2.5, Claim 3 is true. ■

3.4 Unicyclic graphs with given maximum degree

The set of unicyclic graphs of order n with maximum degree Δ is represented by $\mathscr{C}_{n,\Delta}$, where $2 \leq \Delta \leq n-1$. The only unicyclic graphs with $\Delta = 2$ and $\Delta = n-1$ are C_n and S_n^+, respectively. Thus, unicyclic graphs with a maximum degree $\Delta \geq 3$ will be examined.

Assume that U^* is the set of unicyclic graphs that results from joining two pendant vertices of $T \in T^*$ with an edge. It is evident that the maximum degree Δ of these unicyclic graphs U^* and trees $T \in T^*$ is the same. Consequently, $U^* \subseteq \mathscr{C}_{n,\Delta}$, and $D(U^*) = [\Delta, 2^{n-\Delta+1}, 1^{\Delta-2}]$ is the degree sequence of U^*.

A unicyclic graph of order n is obtained when an edge is added between two vertices in a tree of order n. Let G be a unicyclic graph with maximum degree Δ, meaning that $G \in \mathscr{C}_{n,\Delta}$

and let $u, v \in V(G)$, so that $\deg_G(u) \neq \Delta$ and $\deg_G(v) \neq \Delta$. Let $T \in \mathscr{T}_{n,\Delta}$. Assume that u and v are vertices of the cycle in G, $\deg(u) \geq 2$ and $\deg(v) \geq 2$, respectively. Let $T = G - uv$. then $\deg_G(x) = \deg_T(x)$ for $x \in V(G)\backslash\{u, v\}$ but $\deg_G(u) = \deg_T(u)+1$ and $\deg_G(v) = \deg_T(v)+1$. Thus,

$$\begin{aligned} P_1^a(G) &= P_1^a(T)\left(\frac{\deg(u)\deg(v)}{(\deg(u)-1)(\deg(v)-1)}\right)^a \\ &\leq \Delta^a 2^{a(n-\Delta-1)} 2^{2a} = \Delta^a 2^{a(n-\Delta+1)} \\ &= P_1^a(U^*), \end{aligned}$$

since $\frac{t}{t-1} = 1 + \frac{1}{t-1} \leq 2$ for all integers $t \geq 2$. Also,

$$\begin{aligned} P_2^a(G) &= P_2^a(T)\left(\frac{(\deg(u))^{\deg(u)}(\deg(v))^{\deg(v)}}{(\deg(u)-1)^{(\deg(u)-1)}(\deg(v)-1)^{(\deg(v)-1)}}\right)^a \\ &\geq \Delta^{a\Delta} 2^{2a(n-\Delta-1)}\left(\frac{(\deg(u))^{\deg(u)}(\deg(v))^{\deg(v)}}{(\deg(u)-1)^{(\deg(u)-1)}(\deg(v)-1)^{(\deg(v)-1)}}\right)^a \\ &= \Delta^{a\Delta} 2^{2a(n-\Delta-1)}\left(\frac{(\deg(u))^{\deg(u)}}{(\deg(u)-1)^{(\deg(u)-1)}}\right)^a\left(\frac{(\deg(v))^{\deg(v)}}{(\deg(v)-1)^{(\deg(v)-1)}}\right)^a \\ &\geq \Delta^{a\Delta} 2^{2a(n-\Delta-1)} 2^{2a} 2^{2a} \\ &= \Delta^{a\Delta} 2^{2a(n-\Delta+1)} \\ &= P_2^a(U^*), \end{aligned}$$

since $t^t \geq 4(t-1)^{t-1}$ for all integers $t \geq 2$.

Thus, the extremal graph $G \in \mathscr{C}_{n,\Delta}$ with maximum P_1^a (minimum P_2^a) is U^*. Conversely, if G is obtained by connecting two vertices u and v of a starlike tree T with maximum degree Δ, i.e., let $G = T + uv$ where either $\deg_T(u) = 1$ and $\deg_T(v) = 2$, or $\deg_T(u) = \deg_T(v) = 2$. Let G_1 be obtained by connecting vertices u and v of a starlike tree T with maximum degree Δ such that $\deg_T(u) = 1$ and $\deg_T(v) = 2$. Then the degree sequence of G_1 is $D(G_1) = [\Delta, 3, 2^{n-\Delta-1}, 1^{\Delta-1}]$ and

$$P_1^a(G_1) = \Delta^a 3^a 2^{a(n-\Delta-1)} \quad \text{and} \quad P_2^a(G_1) = \Delta^{a\Delta} 3^{3a} 2^{2a(n-\Delta-1)}. \tag{3}$$

Let G_2 be obtained by connecting vertices u and v of a starlike tree T with maximum degree Δ such that $\deg_T(u) = \deg_T(v) = 2$. Then the degree sequence of G_2 is $D(G_2) = [\Delta, 3^2, 2^{n-\Delta-3}, 1^{\Delta}]$ and

$$P_1^a(G_2) = \Delta^a 3^{2a} 2^{a(n-\Delta-3)} \quad \text{and} \quad P_2^a(G_2) = \Delta^{a\Delta} 3^{6a} 2^{2a(n-\Delta-3)}. \tag{4}$$

Next, we establish the relation between the results obtained in Equations (3) and (4).

$$\frac{P_1^a(U^*)}{P_1^a(G_1)} = \frac{2^{a(n-\Delta+1)}}{3^a 2^{a(n-\Delta-1)}} = \frac{2^{2a}}{3^a} = \left(\frac{4}{3}\right)^a > 1,$$

$$\frac{P_1^a(G_1)}{P_1^a(G_2)} = \frac{3^a 2^{a(n-\Delta-1)}}{3^{2a} 2^{a(n-\Delta-3)}} = \frac{2^{2a}}{3^a} = \left(\frac{4}{3}\right)^a > 1.$$

Thus, we have

$$P_1^a(U^*) > P_1^a(G_1) > P_1^a(G_2).$$

and

$$\frac{P_2^a(U^*)}{P_2^a(G_1)} = \frac{2^{2a(n-\Delta+1)}}{3^{3a}2^{2a(n-\Delta-1)}} = \frac{2^{4a}}{3^{3a}} = \left(\frac{16}{27}\right)^a < 1,$$

$$\frac{P_2^a(G_1)}{P_2^a(G_2)} = \frac{3^{3a}2^{2a(n-\Delta-1)}}{3^{6a}2^{2a(n-\Delta-3)}} = \frac{2^{4a}}{3^{3a}} = \left(\frac{16}{27}\right)^a < 1.$$

Thus, we have

$$P_2^a(U^*) < P_2^a(G_1) < P_2^a(G_2).$$

That is, U^* has the maximum P_1^a (and minimum P_2^a). So, Theorem 3.5 follows.

Theorem 3.5. *Let $G \in \mathscr{C}_{n,\Delta}$ and $3 \leq \Delta \leq n-1$. For $a > 0$,*

$$P_1^a(G) \leq \Delta^a 2^{a(n-\Delta+1)} \quad \text{and} \quad P_2^a(G) \geq \Delta^{a\Delta} 2^{2a(n-\Delta+1)},$$

with equality if and only if $G \in U^*$.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

Acknowledgments. The authors thank the anonymous referees for their valuable feedback, which has significantly improved the quality of this work.

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