Sharp Bounds for the Modified Multiplicative Zagreb Indices of Graphs with Vertex Connectivity at Most $k$

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Abstract. Zagreb indices and their modified versions of a molecular graph originate from many practical problems such as two dimensional quantitative structure-activity (2D QSAR) and molecular chirality. Nowadays, they have become important invariants which can be used to characterize the properties of graphs from different aspects.

Let $V_k^c$ (or $E_k^c$ respectively) be a set of graphs of $n$ vertices with vertex connectivity (or edge connectivity respectively) at most $k$. In this paper, we explore some properties of the modified first and second multiplicative Zagreb indices of graphs in $V_k^c$ and $E_k^c$. By using analytic and combinatorial tools, we obtain some sharp lower and upper bounds for these indices of graphs in $V_k^c$ and $E_k^c$. In addition, the corresponding extremal graphs which attain the lower or upper bounds are characterized. Our results enrich outcomes on studying Zagreb indices and the methods developed in this paper may provide some new tools for investigating the values on modified multiplicative Zagreb indices of other classes of graphs.

1. Introduction

In many fields like Physics, Chemistry and Electric Network, the boiling point, the melting point, the chemical bonds and the bond energy are all important quantifiable parameters in their fields.

To understand physic-chemical properties of chemical compounds or network structures and practical problems, mathematical modelings, such as graphs, have been built.

A molecular structured graph is a simple finite connected graph which represents the carbon-atom skeleton of an organic molecule of a hydrocarbon. The vertices of a molecular graph represent the carbon atoms while their undirected edges represent the carbon bounds. Studying graphs is a constant focus in chemical graph theory and its applications in the effort to better understand molecular structures.

Secondly, many abstract concepts were defined based on degree or distance, and collectively named topological descriptors or topological indices after mathematical modelings. Different indices represent their corresponding chemical structures in graph-theoretical terms via arbitrary molecular graphs. Large number
of articles about related all topological indices are proposed and based on edges or vertices in a molecular graph ([11-28]).

In the last decades, as a powerful approach, these two dimensional topological indices have been used to design or discover many new drugs such as Anticonvulsants, Anineoplastics, Antimalarials or Antiallergics and Silico generation ([4, 11-13, 26]). These topological indices play a key role in the process of drug discovery and other research areas ([5-8, 21]).

Among degree-based topological indices, Zagreb indices are the oldest ones and the most studied. Large numbers of articles about Zagreb indices and related indices have been published in the last decades (see for example [1, 3, 9, 10, 18, 19]). Recently, Gutman, Eliasi and Iranmanesh, respectively ([3, 9]) introduced the modified first multiplicative Zagreb index and defined as follows:

\[ \prod_1(G) = \prod_{u \in \mathcal{E}(G)} [d(u) + d(v)]. \]

In 2016, Basavanagoud et al.([1]) studied several derived graphs and introduced another multiplicative version called the modified second multiplicative Zagreb index and defined as

\[ \prod_2(G) = \prod_{u \in \mathcal{E}(G)} [d(u) + d(v)]^{d(u) + d(v)}. \]

With respect to Zagreb indices and modified versions, researchers are interested in finding upper and lower bounds for these indices of graphs and characterizing the graphs in which the maximal (respectively minimal) index values are attained (see [10, 15, 20, 27, 28]). And mathematical and computational properties on Zagreb indices have also been considered. Furthermore, other directions include studies of relation between multiplicative Zagreb indices and the corresponding invariants of elements of the graph G (vertices, pendent vertices, diameter, maximum degree, girth, cut edge, cut vertex, perfect matching, connectivity). For example, Li and Zhou [16] found the maximum and minimum Zagreb indices of graphs with vertex connectivity at most k. Wang [25] extended the results and obtained the maximum and minimum multiplicative Zagreb indices of graphs under the same condition.

Since the modified multiplicative Zagreb indices are relatively new concepts and involve the sum of degrees of both vertices of every edge, their values are usually more difficult to determine. Thus, we need to search for new tools to deal with these kind of indices. For this purpose, in this paper we study properties of modified multiplicative Zagreb indices of graphs with vertex connectivity or edge connectivity at most k. We manage to use some basic analytic functions to find the upper and lower bounds for the modified first and second multiplicative Zagreb indices and characterize their extremal graphs:

**Theorem 1.1.** Given \( n, k \in \mathbb{N} \), \( n \geq 3 \) and \( k \geq 1 \), let \( G \) be a graph with \( n \) vertices and vertex connectivity at most \( k \) and \( K_n^k \) be a graph obtained by adding a vertex to a clique \( K_{n-1}^k \) and joining the vertex to exactly \( k \) vertices of \( K_{n-1}^k \). Then

\[ \prod_1(G) \leq \prod_1(K_n^k) \]

and

\[ \prod_2(G) \leq \prod_2(K_n^k) \]

where the equalities hold if and only if \( G \cong K_n^k \), where

\[ \prod_1(K_n^k) = 2^{\frac{k(k-1)}{2}} \cdot (n-1) \cdot (n-2) \cdot (2n-3)^{k-1} \cdot (n+k-1) \cdot (n+k-1)^k, \]

\[ \prod_2(K_n^k) = 2^{(n-1)(k-1) + (n-2)(n-k-1)(k-2)} \cdot (n-1)^{(k-1)} \cdot (n-2)^{(n-k-1)} \cdot (n-k-2) \cdot (n-k-1)(n-k-2) \cdot (2n-3)^{k-1} \cdot (n+k-1)^k. \]

On the lower bounds for the modified first and second multiplicative Zagreb indices, we obtain the following:
Theorem 1.2. Let $G$ be a graph with $n$ vertices and vertex connectivity at most $k$, where $n \geq 3$ and $k \geq 1$. Then $\Pi_1(G) \geq 9 \cdot 4^{n-3}$ and $\Pi_2(G) \geq 729 \cdot 256^{n-3}$, and the equalities hold if and only if $G \cong P_n$, where $P_n$ is a path on $n$ vertices.

The methods we develop in this paper are expected to be used to study the properties of other indices of graphs. We first give some notations and graph operation properties of the modified first and second multiplicative Zagreb indices in Section 2 and then we prove our main results in Section 3.

2. Preliminaries and properties

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. If a vertex $v \in V(G)$, then the neighborhood of $v$ denotes the set $N(v) = N_G(v) = \{w \in V(G) : vw \in E(G)\}$, and the degree of $v$ is $d_G(v) = |N(v)|$, also denoted by $d(v)$. Let $n_i$ denote the number of vertices of degree $i \geq 0$.

Given $V_1, V_2 \subseteq V(G)$, denote $E[V_1, V_2] = \{vw \in E(G) : u \in V_1, v \in V_2\}$. Given $S \subseteq V(G)$ and $F \subseteq E(G)$, we denote by $G[S]$ the subgraph of $G$ induced by $S$, $G[F]$ the subgraph induced by $F$, $G - S$ the subgraph induced by $V(G) - S$ and $G - F$ for the subgraph of $G$ obtained by deleting $F$. If $G - S$ contains at least 2 components, then $S$ is said to be a vertex cut set of $G$. Similarly, if $G - F$ contains at least 2 components, then $E$ is called an edge cut set. In our exposition we will use the terminology and notations of (chemical) graph theory (see [2, 22]).

A graph $G$ is said to be $k$-connected with $k \geq 1$, if either $G$ is complete graph $K_{k+1}$, or it has at least $k + 2$ vertices and contains no $(k - 1)$-vertex cut. The vertex connectivity of $G$, denoted by $\kappa(G)$, is defined as the maximal value of $k$ for which a connected graph $G$ is $k$-connected. Similarly, for $k \geq 1$, a graph $G$ is called $k$-edge-connected if it has at least two vertices and does not contain a $(k - 1)$-edge cut. The maximal value of $k$ for which a connected graph $G$ is $k$-edge-connected is said to be the edge connectivity of $G$, denoted by $\kappa'(G)$. By the definitions, the following proposition is obtained.

**Proposition 2.1.** Let $G$ be a graph with $n$ vertices. Then

(i) $\kappa(G) \leq \kappa'(G) \leq n - 1$,

(ii) $\kappa(G) = n - 1$, $\kappa'(G) = n - 1$ and $G \cong K_n$ are equivalent.

Let $\mathcal{V}_n^k$ be a set of connected graphs with $n$ vertices and vertex connectivity at most $k$, $\kappa(G) \leq k \leq n - 1$. Denote by $\mathcal{E}_n^k$ a set of connected graphs with $n$ vertices and edge connectivity at most $k$, $\kappa'(G) \leq k \leq n - 1$. Let $P_n$ and $S_n$ be, respectively, a path and a star of $n$ vertices. Let $K_n$ denote a complete graph. The graph $K_n^k$ is obtained by joining $k$ vertices of $K_{n-1}$ to an isolated vertex (see Figure 1). Then $K_n^k \in \mathcal{E}_n^k \subset \mathcal{V}_n^k$.

![Figure 1.](image)

According to the definitions of $\Pi_1(G)$ and $\Pi_2(G)$, the following proposition is routinely obtained.

**Proposition 2.2.** Let $e$ be an edge of a graph $G \in \mathcal{V}_n^k$ ($\mathcal{E}_n^k$ respectively). Then

(i) $G - e \in \mathcal{V}_n^k$ ($\mathcal{E}_n^k$ respectively),

(ii) $\Pi_i(G - e) < \Pi_i(G)$, $i = 1, 2$. 
Lemma 2.5. Let \( u \) and \( v \) be a graph with vertex set \( V(G_1) \cup V(G_2) \) and edge set \( E(G_1) \cup E(G_2) \cup \{uv, u \in V(G_1), v \in V(G_2)\} \).

Proof. It is easy to verify that this proposition holds for \( M = 2, 3 \). Below we may assume that \( M \geq 4 \). By the fact \( \frac{2}{M} < 1 \) for any \( i = 4, \cdots, M \), we have

\[
C_M^i(M + 3)^{M-i} \cdot 2^i = \sum_{i=4}^{M} C_M^i(M + 3)^{M-i} \cdot 2^i < (M + 3)^M.
\]

By Binomial Theorem, we obtain

\[
(M + 5)^M = [(M + 3) + 2]^M = (M + 3)^M + 2M \cdot (M + 3)^{M-1} + 2M(M - 1) \cdot (M + 3)^{M-2} + \frac{1}{2}M(M + 1)(M - 2) \cdot (M + 3)^{M-3} + \sum_{i=4}^{M} C_M^i(M + 3)^{M-i} \cdot 2^i.
\]

Thus,

\[
(M + 5)^M < (M + 3)^{M+2}.
\]

We first provide some lemmas, which will play very important roles in the proofs of our main results. According to the definitions of \( \Pi_1^f(G) \) and \( \Pi_2^f(G) \), we have the following lemmas.

**Lemma 2.5.** Let \( u, v \in V(G) \) and \( uv \notin E(G) \). Then

\[
\Pi_1^f(G) < \Pi_1^f(G + uv), \quad \Pi_2^f(G) < \Pi_2^f(G + uv).
\]

Given two graphs \( G_1 \) and \( G_2 \), if \( V(G_1) \cap V(G_2) = \emptyset \), then the join graph \( G_1 \oplus G_2 \) is a graph with vertex set \( V(G_1) \cup V(G_2) \) and edge set \( E(G_1) \cup E(G_2) \cup \{uv, u \in V(G_1), v \in V(G_2)\} \).

Let \( G(j, H, n-k-j) = K_j \oplus H_k \oplus K_{n-k-j} \) be a graph with \( n \geq 3 \) vertices, in which \( K_j \) and \( K_{n-k-j} \) are cliques, and \( H_k \) is a graph with \( k \) vertices (see Figure 2). Specially, \( G(j, K_2, n-k-j) \) plays a key bridge role in this paper.
**Lemma 2.6.** For any $G(j, H_k, n - k - j) = K_j \oplus H_k \oplus K_{n-k-j}$ with $n \geq 3$, $k \geq 1$ and $1 \leq j \leq \frac{n-k}{2}$, we have

$$d_G(v) = \begin{cases} 
  k + j - 1, & \text{if } v \in V(K_j), \\
  d_H(v) + n - k, & \text{if } v \in V(H_k), \\
  n - j - 1, & \text{if } v \in V(K_{n-k-j}). 
\end{cases}$$

The next lemma is a key lemma in the proofs for upper bounds of our main results.

**Lemma 2.7.** Let $G(j, K_k, n - k - j) = K_j \oplus K_k \oplus K_{n-k-j}$ be a graph with $n$ vertices, in which $K_j$, $K_k$ and $K_{n-k-j}$ are cliques. If $n \geq 3$, $k \geq 1$ and $2 \leq j \leq \frac{n-k}{2}$, then

$$\prod_1'(G(j, K_k, n - k - j)) < \prod_1'(G(1, K_k, n - k - 1))$$

and

$$\prod_2'(G(j, K_k, n - k - j)) < \prod_2'(G(1, K_k, n - k - 1)).$$

**Proof.** Let the graph $G = G(j, K_k, n - k - j)$ for any $n \geq 3$, $k \geq 1$ and $2 \leq j \leq \frac{n-k}{2}$. By Lemma 2.6, we know that

$$d_G(v) = \begin{cases} 
  k + j - 1, & \text{if } v \in V(K_j), \\
  n - 1, & \text{if } v \in V(K_k), \\
  n - j - 1, & \text{if } v \in V(K_{n-k-j}). 
\end{cases}$$

Let $E_1 = E[V(K_j)] \cap E(G)$, $E_2 = E[V(K_k)] \cap E(G)$, $E_3 = E[V(K_{n-k-j})] \cap E(G)$, $B_1 = E[V(K_j)] \cap E(G)$, $B_2 = E[V(K_k)] \cap E(G)$, and $B_3 = E[V(K_{n-k-j})] \cap E(G)$. Then

$$|E_1| = \frac{j(j - 1)}{2},$$

$$|E_2| = \frac{k(k - 1)}{2},$$

$$|E_3| = \frac{(n - k - j)(n - k - j - 1)}{2},$$

$$|B_1| = jk,$$
Let \( f(x, y) \) be the unified function of \( \prod_1' \) and \( \prod_2' \). By the concepts of \( \prod_1' \), \( \prod_2' \) and the structure of the class of the graph \( G = G(j, K_k, n - k - j) \), we have

\[
\prod_1'(G) = \prod_{u \in E(G)} f(d(u), d(v))
\]

\[
= \prod_{v \in E_1} f(d(u), d(v)) \cdot \prod_{v \in E_2} f(d(u), d(v)) \cdot \prod_{v \in E_3} f(d(u), d(v)) \cdot \prod_{v \in E_4} f(d(u), d(v))
\]

\[
= [f(k + j - 1, k + j - 1)]^{E_1} \cdot [f(n - 1, n - 1)]^{E_2} \cdot [f(n - j - 1, n - j - 1)]^{E_3} \cdot [f(k + j - 1, n - 1)]^{E_4} \cdot [f(n - 1, n - j - 1)]^{E_5},
\]

where \( i = 1, 2 \).

With respect to \( \prod_1'(G) \), its corresponding function is \( f(x, y) = x + y \). After calculations, we have

\[
\prod_1'(G) = \prod_{v \in E(G)} [d_c(u) + d_c(v)]
\]

\[
= [2(k + j - 1)]^{E_1} \cdot [2(n - 1)]^{E_2} \cdot [2(n - j - 1)]^{E_3} \cdot [2(n + k - 2)]^{E_4} \cdot [2(n - j - 2)]^{E_5}.
\]

\[
(\star 1)
\]

**Claim 1.** Let \( G = G(j, K_k, n - k - j) \) with given \( n \geq 3 \) and \( k \geq 1 \). Then \( \prod_1'(G) \) is a strictly decreasing discrete function with respect to the variable \( j \), where \( 1 \leq j < \frac{n - k}{2} \).

Furthermore, if \( \frac{n - k}{2} \geq 2 \) is an integer, then

\[
\prod_1'(G(\frac{n - k}{2}, K_k, \frac{n - k}{2})) < \prod_1'(G(1, K_k, n - k - 1)).
\]

**Proof of Claim 1.**

Since \( \prod_1'(G) > 0 \) for \( 1 \leq j \leq \frac{n - k}{2} \), \( \ln[\prod_1'(G)] \) has the same monotonicity as \( \prod_1'(G) \).

Define the corresponding real function

\[
\prod_1'(x) = \frac{[2(k + x - 1)]^{(x+1)}}{x - 2)^k \cdot [2(n - 1)]^{(n-k-1)} \cdot [2(n - x - 1)]^{(n-k-1)} \cdot [n + k + x - 2]}^{k(n-k-2)}
\]

with respect to one variable \( x \) in the interval \([1, \frac{n - k}{2}]\).

By Derivative Theory of a function with one variable, we first need to prove that

\[
\frac{d[\ln(\prod_1'(x))]}{dx} < 0.
\]

By \((\star 1)\), we have

\[
\frac{d[\ln(\prod_1'(x))]}{dx} = (2x + k - n) \cdot \ln 2 + \frac{1}{2} [(2x + 1)\ln(k + x - 1) - (2n - 2k - 2x - 1)\ln(n - x - 1)] + [\frac{x}{(k+x-1)} - \frac{(n-k-x)/(n-x-1)}{(n-x-1)}] + k[(\ln(n + k + x - 2) - \ln(2n - x - 2)) + \ln \left( \frac{x}{n+k+x-2} - \frac{n-k-x}{2(n-x-2)} \right)].
\]

Below, we need to prove that, given numbers \( k \geq 1 \) and \( n \geq 3 \), all of the following are negative for any \( 1 \leq x < \frac{n - k}{2} \):

\[
\Delta_1 = (2x + k - n)\ln 2,
\]

\[
\Delta_2 = (2x - 1)\ln(k + x - 1) - (2n - 2k - 2x - 1)\ln(n - x - 1),
\]

\[
\Delta_3 = (2n - 2k - 2x + 1)\ln(n - x - 1) + 2x - 1).
\]

\[
\Delta_4 = (2n - 2k - 2x + 1)\ln(n - x - 1) + 2x - 1).
\]
\[ \Delta_3 = \frac{n(n-1)}{(k+2)} - \frac{n(n-k)(n-k-1)}{(n-1)} , \]
\[ \Delta_4 = \ln(n+k+x-2) - \ln(2n-x-2) , \]
\[ \Delta_5 = \frac{x}{n+k+x-2} - \frac{n-k-x}{2n-x-2} . \]

(1) Since \( 1 \leq x < \frac{2n-k}{2} \), \( 2x+k-n < 0 \). Then \( \Delta_1 < 0 \).

(2) Since \( 1 \leq x < \frac{2n-k}{2} \), \( n-k > 2x \) and \( n-x-1 > x+k-1 \). Then
\[ (n-x-1)^{2n-2k-2x-1} = (n-x-1)^{2(n-k)-2x-1} > (n-x-1)^{2x-2x-1} = (n-x-1)^{2x-1} > (x+k-1)^{2x-1} \]

which implies that \( \frac{(x+k-1)^{2x-1}}{(n-x-1)^{2x-1}} < 1 \), that is \( \Delta_2 < 0 \).

(3) Since \( 1 \leq x < \frac{2n-k}{2} \), \( x < n-k-x \). Let us consider
\[ f(x) = \frac{x(x-1)}{k+x-1} . \]
Then the function \( f(x) \) is increasing for \( 1 \leq x < \frac{2n-k}{2} \) and \( k \geq 1 \). Thus,
\[ \Delta_3 = \frac{x(x-1)}{(k+2)} - \frac{n(n-k)(n-k-1)}{(n-1)} = \frac{x(x-1)}{(k+2)} - \frac{x(n-k-1)(n-k)}{(n-1)} = f(x) - f(n-k-x) < 0 . \]

(4) Since \( 1 \leq x < \frac{2n-k}{2} \), \( n+k+x-2 < 2n-x-2 \). Then \( \frac{n+k+x-2}{2n-x-2} < 1 \), which implies
\[ \ln \frac{n+k+x-2}{2n-x-2} < 0 , \]
that is,
\[ \Delta_4 < 0 . \]

(5) Since \( 1 \leq x < \frac{2n-k}{2} \), \( n-k-2x > 0 \). By Proposition 2.3,
\[ \Delta_5 = \frac{x}{n+k+x-2} - \frac{n-k-x}{2n-x-2} = \frac{x}{n+k+x-2} - \frac{x(n-k-2x)}{n+k+x-2 + (n-k-2x)} , \]
implying
\[ \Delta_5 < 0 . \]

Up to now, we have proved that for any \( 1 \leq x < \frac{2n-k}{2} \),
\[ \frac{d[\ln(vi(x))]}{dx} < 0 . \]

Now we only need to clarify that for an integer \( \frac{n-k}{2} \geq 2 \),
\[ \Pi'_i[(G(\frac{n-k}{2}, K, \frac{n-k}{2})) < \Pi'_i(G(1, K, n-k-1)) . \]

In fact, since \( \frac{n-k}{2} \) is a positive integer, \( n, k \) have the same parity. Since \( 1 \leq k \leq n-4 \), then \( n+k-2 \leq 2n-6 \), \( \frac{3n+k-4}{2} \leq 2n-6, n+k-1 \leq 2n-5 \) and \( 2 \leq n-k-2 \leq n-3 \). Since \( n \geq 5 \), \( 2n-4 \geq 6 \).

By (1), we have
\[ \Pi'_i(G(1, K, n-k-1)) = [2(n-1)]^{(\frac{n-k-1}{2})} \cdot [2(n-2)]^{\frac{(n-3)(n-k-2)}{2}} \cdot [n+k-1]^k \cdot [2n-3]^{(n-k-1)} \]
and
\[ \Pi'_i(G(\frac{n-k}{2}, K, \frac{n-k}{2})) = [2(n-1)]^{(\frac{n-k-1}{2})} \cdot [n+k-2]^{\frac{(n+3)(n-k-2)}{2}} \cdot [\frac{3n+k-4}{2}]^{(n-k)}. \]
Immediately, we have
\[
\prod_1^n(G(1, K_t, n - k - 1))
\quad \frac{\prod_1^n(G(\frac{n-k}{2}, K_t, \frac{n-k}{2})]}{
\prod_1^n(G(\frac{n-k}{2}, K_t, \frac{n-k}{2})])}
\]
\[
= \frac{(2n - 4)k(2n - 3)}{(n + k - 2)^k} \cdot (2n - 3)^{k(n-k)} \cdot (n + k - 1)^k \cdot (2n - 4)^{n-k^2/4} \cdot (2n - 3)^k \cdot (2n - 4)^{n-k^2}
\]
\[
> \frac{(n + k - 1)^k}{(2n - 3)^k} \cdot (2n - 4)^{n-k^2/4} > 1.
\]

Now, we want to prove \(\frac{(n + x - 1)^x}{(2n - 3)^x} > 1\). Let
\[
h(x) = \frac{(n + x - 1)^x}{(2n - 3)^x} > 1
\]
with \(x \in [1, n - 4]\) and \(n \geq 4\). After a simple calculation, we have
\[
\frac{d\ln[h(x)]}{dx} = \ln(n + x - 1) - \ln(2n - 3) + \left[\frac{x}{x + (n - 1)} - (n - x - 2)\ln \sqrt{2n - 4}\right]
\]
Since \(n \geq 5\) and \(1 \leq x \leq n - 4\), we have
\[
\ln(n + x - 1) < \ln(2n - 3),
\]
\[
\frac{x}{x + (n - 1)} < 1 < 2 \cdot \ln \sqrt{6} < (n - x - 2) \cdot \ln \sqrt{2n - 4}.
\]
Therefore, \(\frac{d\ln[h(x)]}{dx} < 0\), implying that \(h(x)\) is strictly decreasing in \(1 \leq x \leq n - 4\). Then by Proposition 2.4, we have
\[
\prod_1^n(G(1, K_t, n - k - 1)) \prod_1^n(G(\frac{n-k}{2}, K_t, \frac{n-k}{2})) > 1.
\]
Hence, Claim 1 holds. □

Similarly, with respect to \(\prod_2^n(G)\), its corresponding function is \(f(x, y) = (x + y)^{x+y}\). After calculation, we obtain that
\[
\prod_2^n(G) = \prod_{\forall u \in E(G)} [d_G(u) + d_G(v)]^{[d_G(u) + d_G(v)]}^{1/2}
\]
\[
= [2(k + j - 1)]^{2(k+j-1) \frac{n-k-j}{2}} \cdot [2(n - 1)]^{2(n-1) \frac{k-j}{2}} \cdot [2(n - j - 1)]^{2(n-j-1) \frac{n-k-j}{2}} \cdot [n + k + j - 2]^{(n+k+j-2)k(n-k-j)}
\]
\[
\prod_2^n(G(\frac{n-k}{2}, K_t, \frac{n-k}{2})) < \prod_2^n(G(1, K_t, n - k - 1)).
\]

Claim 2. For the class of the graphs \(G = G(j, K_t, n - k - j)\) with given \(n \geq 3\) and \(k \geq 1\), we have \(\prod_2^n(G)\) is a strictly decreasing discrete function with respect to the variable \(j\), where \(1 \leq j < \frac{n-k}{2}\). Furthermore, if \(\frac{n-k}{2} \geq 2\) is an integer, then \(\prod_2^n(G(\frac{n-k}{2}, K_t, \frac{n-k}{2})) \prod_2^n(G(1, K_t, n - k - 1)).
\]

Proof of Claim 2.
Since \(\prod_2^n(G) > 0\) for \(1 \leq j \leq \frac{n-k}{2}\), \(\ln[\prod_2^n(G)]\) has the same monotonicity as \(\prod_2^n(G)\).
Define the corresponding real function
\[
\prod_2^n(x) = [2(k + x - 1)]^{2(k+x-1) \frac{n-k-j}{2}} \cdot [2(n - 1)]^{2(n-1) \frac{k-j}{2}} \cdot [2(n - x - 1)]^{2(n-x-1) \frac{n-k-j}{2}} \cdot [n + k + j - 2]^{(n+k+j-2)k(n-k-j)}
\]
\[ k + x - 2)^{(n+k+1-2)\cdot x^k} : [2n - x - 2]^{(2n-x-2)\cdot k(n-k-x)} \quad (\ast 2) \]

with respect to one variable \( x \) in the interval \([1, \frac{n-k}{2}]\). By Derivative Theory of a function with one variable, we only need to prove that

\[
\frac{d[\ln(1_{2}^{n}(x))]}{dx} < 0.
\]

By (\ast 2) we have

\[
\frac{d[\ln(1_{2}^{n}(x))]}{dx} = \ln 2 \cdot \left[ (x(x-1) - (n-k-x)(n-k-x-1)) + [(2x-1)(k+x-1) - (n-x-1)(2n-2k-2x-1)] + \\
[(2x-1)(k+x-1)\ln(k+x-1) - (2n-2k-2x-1)(n-x-1)\ln(n-x-1)] + \\
[k((n+k+x-2)\ln(n+k+x-2) - (2n-x-2)\ln(2n-x-2)) + \\
(x(1 + \ln(n+k+x-2)) - (n-k-x)(1 + \ln(2n-x-2)))].
\]

Below, we need to prove all of the following are non-positive for any \( 1 \leq x < \frac{n-k}{2} \) and given numbers \( k \geq 1 \) and \( n \geq 2 \) as follows.

\[ \Delta_1 = x(x-1) - (n-k-x)(n-k-x-1), \]
\[ \Delta_2 = (2x-1)(k+x-1) - (n-x-1)(2n-2k-2x-1), \]
\[ \Delta_3 = (x(x-1)[1 + \ln(k+x-1)]) - (n-k-x)(n-k-x-1)[1 + \ln(n-x-1)], \]
\[ \Delta_4 = (n+k+x-2)[n+k+x-2] - (2n-x-2)[2n-x-2], \]
\[ \Delta_5 = x[1 + \ln(n+k+x-2)] - (n-k-x)[1 + \ln(2n-x-2)]. \]

(1) Let us consider \( f(x) = x(x-1) - (n-k-x)(n-k-x-1) \) and \( g(x) = (2x-1)(k+x-1) \) with respect to \( x \). They are both increasing functions for \( 1 \leq x < \frac{n-k}{2} \) and \( n-k-x > x \). Then

\[ \Delta_{11} = x(x-1) - (n-k-x)(n-k-x-1) = f(x) - f(n-k-x) < 0, \]
\[ \Delta_{12} = (2x-1)(k+x-1) - [2(n-k-x) - 1][k + (n-k-x) - 1] = g(x) - g(n-k-x) < 0. \]

(2) Since \( 1 \leq x < \frac{n-k}{2}, x < n-k-x \). Consider a function

\[ f(x) = (2x-1)(k+x-1)\ln(k+x-1). \]

It is obvious that \( f(x) \) is strictly increasing for \( 1 \leq x < \frac{n-k}{2} \) and \( k \geq 1 \). Thus,

\[ \Delta_2 = (2x-1)(k+x-1)\ln(k+x-1) - [2(n-k-x) - 1][k + (n-k-x) - 1] : \ln[k + (n-k-x)] = f(x) - f(n-k-x) < 0. \]

(3) Let \( f(x) = x(x-1)[1 + \ln(k+x-1)] \). It is obvious that \( f(x) \) is strictly increasing for \( 1 \leq x < \frac{n-k}{2} \) and \( k \geq 1 \). Since \( 1 \leq x < \frac{n-k}{2}, x < n-k-x \). Thus,

\[ \Delta_3 = x(x-1)[1 + \ln(k+x-1)] - (n-k-x)(n-k-x-1)[1 + \ln(n-x-1)] = f(x) - f(n-k-x) < 0. \]

(4) Since \( 1 \leq x < \frac{n-k}{2}, k+x < n-x \). Let

\[ f(x) = (n+k+x-2)\ln(n+k+x-2). \]

It is obvious that \( f(x) \) is increasing for \( 1 \leq x < \frac{n-k}{2} \). Then

\[ \Delta_4 = (n+k+x-2)\ln(n+k+x-2) - (2n-x-2)\ln(2n-x-2) = f(k+x) - f(n-x) < 0. \]

(5) Since \( 1 \leq x < \frac{n-k}{2} \), we have \( 2x < n-k \) and \( k+x < n-x \). Then
\[\Delta_5 = x[1 + \ln(n + k + x - 2)] - (n - k - x)[1 + \ln(2n - x - 2)]\]
\[< x[1 + \ln(n + k + x - 2)] - (2x - x)[1 + \ln(x + k + n - 2)] = 0.\]

Up to now, we have proved that for any \(1 \leq x < \frac{n-k}{x},\)
\[\frac{d[\ln(\prod_n^k(x))]}{dx} < 0.\]

Now we only need to clarify that for an integer \(\frac{n-k}{x} \geq 2,\)
\[\prod_n^k(G(\frac{n-k}{x}, K_n, \frac{n-k}{x})) < \prod_n^k(G(1, K_n, n - k - 1)).\]

In fact, since \(n, k\) have the same parity, \(\frac{n-k}{x}\) is a positive integer. Since \(1 \leq k \leq n - 4, 4 \leq n - k \leq n - 1,\)
\(3 \leq n-k-1 \leq n-2, 2 \leq n-k-2 \leq n-3, n \leq n-k-1 \leq 2n-5, n-1 \leq n+k-2 \leq 2n-6,\)
\[\frac{3n-3}{2} \leq \frac{3n+k-4}{2} \leq 2n-4.\]

For the convenience of writing, let \(F(x) = x^n.\) It is a strictly increasing function on \(x \in [5, +\infty)\) and \(F'(x) = (1 + x)F(x).\) By (*)2, we have
\[\prod_n^k(G(1, K_n, n - k - 1))\]
\[= [F(2(n - 1))]^{(n-1)} \cdot [F(2(n - 2))]^{(n-2)} \cdot [F(n + k - 1)]^k \cdot [F(2n - 3)]^{k(n-k-1)}.\]
and
\[\prod_n^k(G(\frac{n-k}{x}, K_n, \frac{n-k}{x}))\]
\[= [F(2(n - 1))]^{(n-1)} \cdot [F(n + k - 2)]^{(n-2)} \cdot [F(3n+k-4)]^{k(n-k)}.\]

Immediately, we have
\[\prod_n^k(G(1, K_n, n - k - 1))\]
\[\frac{\prod_n^k(G(\frac{n-k}{x}, K_n, \frac{n-k}{x}))}{\prod_n^k(G(1, K_n, n - k - 1))}\]
\[= \frac{[F(2(n - 2))]^{(n-1)[(n-2)(n-1)]}}{[F(3n+k-4)]^{k(n-k)}} \cdot \frac{[F(n + k - 1)]^k}{[F(n + k - 2)]^{(n-1)(n-k)+1}} \cdot [F(2n - 3)]^{k(n-k-1)}\]
\[> [F(2n - 4)]^{(n-1)[(n-2)(n-1)]} \cdot [F(n + k - 2)]^{k(n-1)} \cdot [F(2n - 3)]^{k(n-k-1)}\]
\[= [F(2n - 4)]^{(n+2)(n-4) + 3(n-4)-3(n-4)+2} \cdot [F(n + k - 2)]^{2k(n-2)+2n+k+2} \cdot [F(2n - 3)]^{k(n-k-1)}.\]

Now, we want to prove that
\[F(2n - 4)]^{(n+2)(n-4) + 3(n-4)-3(n-4)+2} \cdot [F(n + k - 2)]^{2k(n-2)+2n+k+2} \cdot [F(2n - 3)]^{k(n-k-1)} > 1.\]

Let
\[g(x) = [F(2n - 4)]^{(n+2)(n-4) + 3(n-4)-3(n-4)+2} \cdot [F(n + x - 2)]^{2k(n-2)+2n+k+2} \cdot [F(2n - 3)]^{k(n-k-1)},\]
with \(x \in [1, n - 4]\) and \(n \geq 5.\) After a simple calculation, we have
\[\frac{d[\ln(g(x))]}{dx} = \frac{-4n+6x+3}{2} \cdot \ln F(2n - 4) + \frac{x-x^1}{2} \cdot \ln F(n + x - 2) + \frac{1}{4}[2(x + n) - (n - x)^2] \cdot [1 + \ln(n + x - 2)] + (n - 2x - 1) \cdot \ln F(2n - 3)\]
\[< \frac{(-4n+6x+3)+(n-x)+1+(n-2x-1)}{2} \cdot \ln F(2n - 3) + \frac{2(x+n) - (n-x)^2}{4} \cdot [1 + \ln(n + x - 2)]\]
\[= \frac{-(n-x-2)}{2} \cdot \ln F(2n - 3) + \frac{x+n}{2} \cdot [1 + \ln(n + x - 2)] - \frac{(n-x)^2}{4} \cdot [1 + \ln(n + x - 2)]\]
\[< \frac{(n-x-2)(2n-3)}{2} \ln(2n - 3) + \frac{x+n}{2} \ln(n + x - 2) + \frac{2(x+n) - (n-x)^2}{4}\]
Then it is easy to check that $\pi(\pi(G) - 1)$ is very easy to check that $\pi(\pi(G) - 1)$ is strictly increasing in $[1, n - 4]$, and $-n + x + 3 < -1$ and $\pi(\pi(G) - 1) > n - 6$ when $n \geq 5$.

Therefore, $\frac{d[\ln[\pi(G)]]}{dx} < 0$, implying that $\pi(x)$ is strictly decreasing in $1 \leq x \leq n - 4$. Then

$$
(F(2n - 4))^{\frac{3(n - 2)}{4}} \cdot (F(n + k - 2))^{\frac{3(n - k)}{4}} \cdot (F(2n - 3))^{\frac{3(n - k + 1)}{4}}
$$

> $\pi(n - 4) = (F(2n - 4))^{\frac{3(n - 2)}{4}} \cdot (F(n - 6))^{\frac{3(n - 2)}{4}} \cdot (F(2n - 3))^{\frac{3(n - 2)}{4}} > 1.$

Hence, Claim 2 holds. □

By Claims 1 and 2, we can recursively use this process from $j$ to $j - 1$, and obtain that

$$
\pi_i'(G(j, K_k, n - k - j)) < \pi_i'(G(j - 1, K_k, n - k - j + 1)) < \pi_i'(G(j - 2, K_k, n - k - j + 2)) < \\
\cdots < \pi_i'(G(1, K_k, n - k - 1)).
$$

Therefore, $\pi_i'(G(j, K_k, n - k - j)) < \pi_i'(G(1, K_k, n - k - 1))$ for any $2 \leq j \leq \frac{n - 2}{2}$ and $i = 1, 2$.

Thus, we complete the proof. □

Now, we give a lemma related to the minimum values of the modified Zagreb indices of graphs.

**Lemma 2.8.** Let $G$ be a connected graph with $u \in V(G)$ such that $d_G(u) = 1$ and $uv \in E(G)$. If $d_G(u) \geq 3$, then we can find a connected graph $G'$ such that $\pi_i'(G') < \pi_i'(G)$ with $i = 1, 2$

**Proof.** Choose a vertex $w \in N(v) - \{u\}$ and construct a connected graph $G'$ by deleting $uw$ and adding $uw$. Then it is easy to check that $\pi_i'(G') < \pi_i'(G)$ with $i = 1, 2$ holds. □

3. Proofs of the main results

We now turn to prove our main results in this section.

**Proof of Theorem 1.1**

Note that the degree sequence of $K_n^k$ is $k, n - 2, n - 2, \ldots, n - 2, n - 1, n - 1, \ldots, n - 1$. By the definitions of $\pi_i'(G)$, $\pi_i'(G)$ and routine calculations, we have

$$
\pi_i'(K_n^k) = 2^{\frac{2(n - 1)k}{3} \cdot (n - 2)} \cdot (n - 1)^{\frac{2(n - 1)k}{3} \cdot (n - 2)} \cdot (n + k - 1)^{k \cdot (n - 3)k}(n + k - 1)^k,
$$

$$
\pi_i'(K_n^k) = 2^{\frac{2(n - 1)k}{3} \cdot (n - 2)} \cdot (n - 1)^{\frac{2(n - 1)k}{3} \cdot (n - 2)} \cdot (n + k - 1)^{k \cdot (n - 3)k}(n + k - 1)^k.
$$

It suffices to prove that $\pi_i'(G) \leq \pi_i'(K_n^k)$ and $\pi_i'(G) \leq \pi_i'(K_n^k)$, and the equalities hold if and only if $G \cong K_n^k$.

If $k = n - 1$, then $G \cong K_n^k$, and the theorem is true. Below, we assume $1 \leq k \leq n - 2$ and then choose a graph $G_1(G_2)$ such that $\pi_i'(G_1)$ and $\pi_i'(G_2)$ respectively is maximal.

Since $G \cong K_n^k$ for $i = 1, 2$, then $G_i$ has a vertex cut set of size $k$. Let $V_i = \{v_{1i}, v_{2i}, \ldots, v_{ki}\}$ be the cut vertex set of $G_i$. Let $\omega(G_i - V_i)$ denote the number of components of $G_i - V_i$. By Lemma 2.5 and the choice of $G_i$, it is very easy to check that $\omega(G_i - V_i) = 2$ and the induced subgraphs of $V(G_1) \cup V_i$ and $V(G_2) \cup V_i$ in $G_i$ are
complete subgraphs for $i = 1, 2$. Thus, we obtain that $G_{11}, G_{1}[V_1]$ and $G_{22}$ are complete subgraphs of $G_i$. Let $G_{11} = K_v$ and $G_{22} = K_{V_2}$. Then we have $G_i = K_v \oplus K_v \oplus K_{V_i}$ which is a type of $G(j, K_v, n - k - j)$. Without loss of generality, assume that $n' \leq n''$. Then $1 \leq n' \leq \frac{n}{2}$. By Lemma 2.7, we have a new graph $G_i = K_v \oplus K_v \oplus K_{n-k-1}$ in $\mathcal{V}_n^k$ such that $\prod_i(G_i) \geq \prod_i(G_{11})$ and equality holds if and only if $G_i = K_v \oplus K_v \oplus K_{n-k-1} = K_n^k$ for $i = 1, 2$. Hence the proof of Theorem 1.1 is complete.

Since $K_n^k \in \mathcal{E}_n^k \subset \mathcal{V}_n^k$, then the following result is an immediate consequence.

**Theorem 3.1.** Let $G$ be a graph in $\mathcal{E}_n^k$. Then
\[
\prod_1(G) \leq \prod_1(K_n^k) \quad \text{and} \quad \prod_2(G) \leq \prod_2(K_n^k),
\]
where the equalities hold if and only if $G \cong K_n^k$, and
\[
\prod_1(K_n^k) = 2^{\frac{(k-1)(k-2)}{2}} \cdot (n - 1)^{(k-1)} \cdot (n - 2)^{(n-k)} \cdot (n + k - 1)^k,
\]
\[
\prod_2(K_n^k) = 2^{(n-1)(k-1)+n(n-2)(n-k-1)(n-k-2)} \cdot (n-1)^{(k-1)} \cdot (n-2)^{(n-k)} \cdot (n+1)^{k(n-k-1)} \cdot (n+k-1)^{(n-k)}.
\]

**Proof of Theorem 1.2**

Since we consider the minimal values of the modified first and second Zagreb indices of graphs $G$ in $\mathcal{V}_n^k$, by Proposition 2.2(ii), $k = 1$ and $G$ contains no cycles. Thus $G$ must be a tree with $n$ vertices. By Lemma 2.6 and routine calculations, we have
\[
\prod_1(P_n) = 9 \cdot 4^{n-3} \quad \text{and} \quad \prod_2(P_n) = 729 \cdot 256^{n-3}.
\]

We only need to prove that for any tree $T_n$ in $\mathcal{V}_n^k$, if $T_n \neq P_n$, then there exists a tree $T'_n$ such that $\prod_1(T'_n) < \prod_1(T_n)$ for $i = 1, 2$. Since $T_n \neq P_n$, then there exists a vertex $w$ in $T_n$ such that $d_T(w) \geq 3$ and $T_n$ has at least three vertices, $x_1, y_1, z_1$ such that $d_T(x_1) = d_T(y_1) = d_T(z_1) = 1$. Let $x_1x_2$, $y_1y_2$, and $z_1z_2$ be three edges of $T_n$. Applying Lemma 2.8, we may assume that $d_{T_n}(x_2) = d_{T_n}(y_2) = d_{T_n}(z_2) = 2$.

Choose a path $P = x_1x_2 \cdots x_k$ in $T_n$ such that $d_T(x_i) = 2$ for $1 \leq i \leq k$ and $d_T(x_k) \geq 3$. If $d_T(x_k) \geq 4$, then set $T'_n = T - x_kx_1 + x_kx_2 + y_ky_1$ and we can get $d_{T}(x_k) = d_{T}(y_k) = d_{T}(z_k) = 1$. Let $x_1x_2, y_1y_2, z_1z_2$ be three edges of $T_n$. Applying Lemma 2.8, we may assume that $d_{T'_n}(x_2) = d_{T'_n}(y_2) = d_{T'_n}(z_2) = 2$.

Choose a path $P = x_1x_2 \cdots x_k$ in $T_n$ such that $d_T(x_i) = 2$ for $1 \leq i \leq k$ and $d_T(x_k) \geq 3$. If $d_T(x_k) \geq 4$, then set $T'_n = T - x_kx_1 + x_kx_2 + y_ky_1$ and we can get $d_{T}(x_k) = d_{T}(y_k) = d_{T}(z_k) = 1$. Let $x_1x_2, y_1y_2, z_1z_2$ be three edges of $T_n$. Applying Lemma 2.8, we may assume that $d_{T'_n}(x_2) = d_{T'_n}(y_2) = d_{T'_n}(z_2) = 2$.

Note that $d_{T_n}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_k, x_1, y_1, z_1\}$, we can easily check that $\prod_i(T'_n) < \prod_i(T_n)$ for $i = 1, 2$. Hence, we may assume that $d_{T'_n}(w) = 3$.

Let $(w_1, w_2) = N_{T_n}(x_1) - \{x_k\}$. We now show that $d_{T_n}(w) = 2$ for $i = 1, 2$. In fact, by Lemma 2.8, we may assume that $d_{T_n}(w) \geq 2$ for $i = 1, 2$. If $d_{T_n}(w) \geq 3$, set $T_n = T - x_1x_2 + x_1x_3$, where $x_1$ and $x_3$ are in the different components of $T_n - x_1x_2$. Then $T_n$ is a tree and $d_{T_n}(x_1) = d_{T_n}(x_3) = 1$, $d_{T_n}(w_1) + d_{T_n}(w_2) = 2$, $d_{T_n}(x_2) = 2$. Noting that $d_{T_n}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_1, x_2, x_3, w_1, w_2\}$, we can deduce that $\prod_i(T'_n) < \prod_i(T_n)$ for $i = 1, 2$. Hence we may assume that $d_{T_n}(w) = 2$ for $i = 1, 2$.

Note that $d_{T_n}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_1, x_2, x_3, w_1, w_2\}$, we can deduce that $\prod_i(T'_n) < \prod_i(T_n)$ for $i = 1, 2$. Hence the proof of Theorem 1.2 is complete.

Note that $P_n \in \mathcal{E}_n^k \subset \mathcal{V}_n^k$, then the following theorem is obvious.

**Theorem 3.2.** Let $G$ be a graph in $\mathcal{E}_n^k$. Then
\[
\prod_1(G) \geq 9 \cdot 4^{n-3} \text{ and } \prod_2(G) \geq 729 \cdot 256^{n-3},
\]
where the equalities hold if and only if $G \cong P_n$. 

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