EXTREMAL DEGREE-PRODUCT INDICES OF GRAPHS WITH FIXED NUMBER OF PENDANT VERTICES AND CYCLOMATIC NUMBER

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ABSTRACT: The Narumi-Katayama index \( NK(G) \) and first multiplicative Zagreb index \( \prod_1(G) \) of a graph \( G \) are defined as the product of the degrees of the vertices of \( G \) and the product of square of the degrees of the vertices of \( G \), respectively. The second multiplicative Zagreb index is defined as \( \prod_2(G) = \prod_{u \in E(G)} d(u)d(v) \). In this paper, we compute the extremal \( NK(G) \), \( \prod_1(G) \) and \( \prod_2(G) \) for the graphs with given order, number of pendant vertices and cyclomatic number.

1 INTRODUCTION

In this paper we are concerned with simple connected graphs. Let \( G \) be such a graph with vertex set \( V(G) \) and edge set \( E(G) \). The number of vertices and edges of \( G \) are denoted by \( n \) and \( m \), respectively. In a graph \( G \) the number of independent cycles is called its cyclomatic number, denoted by \( \gamma \). For connected graphs, the cyclomatic number is equal to \( \gamma = m - n + 1 \). Recall that graphs with \( \gamma = 0, 1, 2 \) are referred to as trees, unicyclic graphs, and bicyclic graphs, respectively. Let \( v \in V(G) \) then the degree of \( v \), denoted as \( d(v) \), is the number of vertices of \( G \) adjacent to \( v \). A vertex \( v \) with \( d(v) = 1 \) is called a pendant vertex. A graph with \( n \) vertices and \( n_1 \) pendant vertices will be said to be an \( (n, n_1) \)-graph [2].

In 1984, Narumi and Katayama [6] established a definition “simple topological index”:

\[
NK(G) = \prod_{v \in V(G)} d(v)
\]

In recent works on this graph invariant [1, 4, 10], the name Narumi-Katayama index is being used. In [13] You and Liu deduced extremal \( NK(G) \) of trees, unicyclic graphs with given diameter and vertices and the minimal \( NK(G) \) of bicyclic graphs with given vertices was obtained.

The vertex-degree-based graph invariants

\[
M_1(G) = \sum_{v \in V(G)} d(v)^2
\]

\[
M_2(G) = \sum_{u \in E(G)} d(u)d(v)
\]

are known under the name first and second Zagreb index, respectively. They have been conceived in the 1970s and found considerable applications in chemistry [7, 11]. The Zagreb indices were subject to a large number of mathematical studies, of which we mention only a few newest [3, 5, 14]. Todeschini et al. [8, 9] have recently proposed to consider the multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to
\[ \prod_1(G) = \prod_{v \in V(G)} d(v)^2 \]
\[ \prod_2(G) = \prod_{uv \in E(G)} d(u) d(v) = \prod_{v \in V(G)} d(v) d(v) \]

The properties of these “multiplicative Zagreb indices” have not been studied so far, and the present work is an attempt to contribute towards their better understanding.

In [2], I. Gutman et al. computed the minimal first Zagreb index of graphs with fixed number of pendant vertices. In this paper we determine the extremal values of the Narumi-Katayama, first Zagreb and second Zagreb indices of connected \((n, n_1)\)-graphs with fixed cyclomatic number and show that these bounds are tight. For other notation in this paper we refer [12].

2 EXTREMAL \((n, n_1)\)-GRAPHS RELATIVELY TO NARUMI-KATAYAMA INDEX

We need the following well-known property.

**Lemma 2.1** Let \(n, r, x_1, x_2, \ldots, x_n\) be positive integers such that \(x_i \geq r\) and
\[
\sum_{i=1}^{n} x_i = a \geq rn.
\]

Then \(\prod_{i=1}^{n} x_i\) is minimum if and only if there exists an index \(i, 1 \leq i \leq n\) such that \(x_i = a - (n-1)r\) and \(x_j = r\) for every \(j \neq i\) and it is maximum if and only if \(x_1, \ldots, x_n\) are almost equal, i.e.,
\[
\max\{x_1, \ldots, x_n\} - \min\{x_1, \ldots, x_n\} \leq 1.
\]

Since in a connected graph a non-pendant vertex has at least degree 2 and \(NK(G) = \prod_{x \in V(G), d(x) \geq 2} d(x)\), by Lemma 2.1 we have the following consequence:

**Corollary 2.2** If \(G\) is a connected graph of order \(n\) and size \(m\) with \(n_1\) pendant vertices \((n > n_1)\) then
\[
NK(G) \geq 2^{n-n_1-1}(2m - 2n + n_1 + 2).
\]
This bound is achieved if \(G\) has one vertex of degree \(2m - 2n + n_1 + 2\) and all other non-pendant vertices are of degree 2.

Let \(G\) be a connected \((n, n_1)\)-graph with cyclomatic number \(\gamma\). If \(\gamma = 0\) then \(G\) is a tree and \(2 \leq n_1 \leq n-1\). Otherwise we suppose that \(0 \leq n_1 \leq n-1\). We define the auxiliary quantities \(t, n_t\) and \(n_{t+1}\) as:
\[
t = \left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 1, \quad n_t = (n - n_1) \left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor - n_1 - 2(\gamma - 1),
\]
\[
n_{t+1} = n - (n - n_1) \left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 2(\gamma - 1).
\]

Recall that \(\left\lfloor x \right\rfloor\) is the greatest integer that is not greater then \(x\), or the integer part of \(x\).
Theorem 2.3 Let $G$ be a connected $(n,n_1)$-graph with cyclomatic number $\gamma$. Then

$$2^{n-n_1-1}(2\gamma+n_1) \leq NK(G) \leq \left( \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor +1 \right)^{n_1} \left( \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor +2 \right)^{n_1+1}.$$ 

(a) For trees ($\gamma = 0$) both lower and upper bounds are reached.

(b) For $\gamma \geq 1$ lower bound can be attained for $n \geq 2\gamma + n_1 +1$ and upper bound for $n \geq 3\gamma + n_1$.

**Proof.** Lower bound. A graph with $n$ vertices and cyclomatic number $\gamma$ has size $m = n + \gamma - 1$, so by Corollary 2.2, we have

$$NK(G) \geq 2^{n-n_1-1}(2\gamma+n_1).$$

To see that this bound can be reached for $\gamma = 0$ consider a path with $n-n_1+1$ vertices and add $n_1-1$ pendant vertices, all adjacent to a unique end vertex of this path.

For $\gamma > 0$ take $\gamma$ cycles, having together $n-n_1$ vertices and a unique common vertex. Then all $n_1$ remaining vertices are joined each by an edge to this common vertex. It follows that $n \geq 2\gamma + n_1 +1$, and equality holds when all $\gamma$ cycles have a length equal to 3. Figures 1, 3 and 5 illustrate graphs having minimum $NK$ index for $n = 22, n_1 = 13$ and $\gamma = 0, 1, 2$.

Upper bound. By Lemma 2.1 $NK(G)$ will be maximum if $G$ has $n_1$ ($0 < n_1 \leq n-n_1$) non-pendant vertices of degree $t$ and $n_{t+1} = n-n_1-n_t$ non-pendant vertices of degree $t+1$, then

$$NK(G) \leq t^{n_1}(t+1)^{n_1+1}.$$  

(1)

As a graph of order $n$ with cyclomatic number $k$ has size $n + \gamma - 1$, we can write:

$$n_1 + t n_t + (t+1)(n-n_1-n_t) = 2(n + \gamma -1),$$

(2)

which yields

$$t(n-n_1)-n_t = n + 2(\gamma -1),$$

(3)

or

$$t - \frac{n_t}{n-n_1} = \frac{n + 2(\gamma -1)}{n-n_1}.  

Taking integer parts,

$$\left\lfloor t - \frac{n_t}{n-n_1} \right\rfloor = \left\lfloor \frac{n + 2(\gamma -1)}{n-n_1} \right\rfloor.$$ 

Since $t$ is a positive integer, we obtain

$$t-1 = \left\lfloor \frac{n + 2(\gamma -1)}{n-n_1} \right\rfloor,$$

or

$$t = \left\lfloor \frac{n + 2(\gamma -1)}{n-n_1} \right\rfloor +1.$$  

(4)

From equations (3) and (4),

$$\left(n-n_1\right)\left\lfloor \frac{n + 2(\gamma -1)}{n-n_1} \right\rfloor + n - n_1 - n_t = n + 2(\gamma -1),$$

which gives
\[ n_t = (n-n_1) \left[ \frac{n+2(\gamma-1)}{n-n_1} \right] - n_1 - 2(\gamma-1). \]

As \( n_{t+1} = n - n_1 - n_t \), we get:

\[ n_{t+1} = n + 2(\gamma-1) - (n-n_1) \left[ \frac{n+2(\gamma-1)}{n-n_1} \right]. \]

From equations (1) and (4) we deduce:

\[ NK(G) \leq \left( \left[ \frac{n+2(\gamma-1)}{n-n_1} \right] + 1 \right)^{n_t} \left( \left[ \frac{n+2(\gamma-1)}{n-n_1} \right] + 2 \right)^{n_{t+1}}, \]

as required.

For \( \gamma = 0 \) the upper bound can be reached. To see this consider a path \( P_{n-n_1} \) with \( n-n_1 \) vertices. Now add the remaining \( n_1 \) pendant vertices using the following algorithm: join each new vertex sequentially, to a vertex of \( P_{n-n_1} \), having minimum degree. Initially, all vertices have degrees 1 and 2 and after that we obtain, by construction, a tree with \( n_1 \) pendant vertices and non-pendant vertices having almost equal degrees.

For \( \gamma > 0 \) take \( \gamma \) vertex disjoint cycles containing together \( n-n_1 \) vertices and joined by edges, such that by contracting each cycle to a vertex yields a path with \( \gamma \) vertices. Then join each new vertex sequentially, to a vertex on the cycles, having minimum degree. Initially all degrees are 2 and 3 and after that we obtain, by construction, almost equal degrees for non-pendant vertices. We have \( n \geq 3\gamma + n_1 \), and equality holds when all vertex disjoint cycles have a length equal to 3. Figures 2, 4 and 6 illustrate graphs having maximum \( NK \) index for \( n = 22, n_1 = 13 \) and \( \gamma = 0,1,2 \).

Figure 1: Tree with \( n = 22 \) and \( n_1 = 13 \) having minimal NK index.

Figure 2: Tree with \( n = 22 \) and \( n_1 = 13 \) having maximal NK index.
Figure 3: Unicyclic graph with $n = 22$ and $n_t = 13$ having minimal NK index.

Figure 4: Unicyclic graph with $n = 22$ and $n_t = 13$ having maximal NK index.

Figure 5: Bicyclic graph with $n = 22$ and $n_t = 13$ having minimal NK index.
3 Extremal \((n, n_1)\)-graphs relatively to Multiplicative Zagreb indices

Since \(\prod_1(G) = NK(G)^2\), Theorem 2.3 implies the following corollary.

**Corollary 3.1** Let \(G\) be a connected \((n, n_1)\)-graph with cyclomatic number \(\gamma\). Then

\[
4^{n-n_1-1}(2\gamma + n_1)^2 \leq \prod_1(G) \leq \left(\frac{n+2(\gamma-1)}{n-n_1} + 1\right)^{2n_1} \left(\frac{n+2(\gamma-1)}{n-n_1} + 2\right)^{2n_1+1}.
\]

(a) For trees \((\gamma = 0)\) both lower and upper bounds are reached.
(b) For \(\gamma \geq 1\) lower bound can be attained for \(n \geq 2\gamma + 1 + n_1\) and upper bound for \(n \geq 3\gamma + n_1\).

Some extremal properties of the second multiplicative Zagreb index in some families of graphs are deduced below. First we need the following property:

**Lemma 3.2** Function \(\phi(x) = \frac{x^x}{(x-1)^{x-1}}\) is increasing for \(x \geq 2\).

**Proof.** We get

\[
\phi'(x) = \frac{x^x (x-1)^{x-1} (\ln x - \ln (x-1))}{(x-1)^{2(x-1)}} > 0,
\]

therefore \(\phi\) is increasing for \(x \geq 2\). \(\square\)

Let \(\Gamma_{n,n_1}\) be the family of connected graphs with order \(n\) and \(n_1\) pendant vertices.

We define a family of trees of order \(n\) with \(n_1\) pendant vertices, denoted \(T^*_{n,n_1}\) as the set of trees of order \(n\) consisting of \(n_1\) paths having a common end vertex. Note that \(T^*_{n,2} = \{P_3\}\).

**Theorem 3.3** Let \(T\) be a tree in \(\Gamma_{n,n_1}\), where \(n \geq n_1 \geq 2\); then

\[
\prod_2(T) \leq n_1^{n_1} 4^{n-n_1-1}
\]

and the equality holds if and only if \(T \in T^*_{n,n_1}\).
Proof. We shall prove this result by induction on $n + n_1$. Let $f(n, n_1) = n_1^{n_1} 4^{n-n_1-1}$. If $n_1 = 2$ and $n \geq n_1$, then $T \cong P_n$ and by direct calculation $\prod_2(P_n) = 4^{n-2}$ and this equals $f(n, 2)$, hence the property is verified.

Let $n_1 \geq 3$ and suppose that the result is true for any tree of order $n'$ with $n_1'$ pendant vertices such that $7 \leq n' + n_1' < n + n_1$. Let $T$ be a tree in $\Gamma_{n, n_1}$ and $x$ be a pendant vertex of $T$. If $xy \in E(T)$, suppose that $d(y) = a$. We shall consider two cases: 1) $a = 2$ and 2) $a \geq 3$.

1) In this case $T - x$ has order $n - 1$ and $n_1$ pendant vertices, hence $\prod_2(T) = 2^2 \prod_2(T - x)$ and by the induction hypothesis $\prod_2(T - x) \leq f(n - 1, n_1)$ and the equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1}$. It follows that $\prod_2(T) \leq f(n, n_1)$ and the equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$.

2) $T - x$ having order $n - 1$ and $n_1 - 1$ pendant vertices, we have

$$\prod_2(T) = \frac{a^a}{(a-1)^{a-1}} \prod_2(T - x).$$

By our supposition of induction,

$$\prod_2(T) \leq \frac{a^a}{(a-1)^{a-1}} f(n - 1, n_1 - 1).$$

Equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1-1}$. The last inequality may be written

$$\prod_2(T) \leq \frac{a^a}{(a-1)^{a-1}} \frac{(n_1 - 1)^{n_1 - 1}}{n_1^{n_1}} f(n, n_1).$$

By Lemma 3.1, $\phi(x)$ is an increasing function, so $\frac{a^a}{(a-1)^{a-1}}$ is maximum for maximum value of $a$ and in the set of trees with $n_1$ pendant vertices the maximum degree of a vertex is $n_1$, so

$$\prod_2(T) \leq f(n, n_1).$$

Equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$ since $d(y) = n_1$ only if $x$ is adjacent to the unique vertex in $T - x$ of degree $n_1 - 1$.

We define a family of unicyclic graphs of order $n$ with $n_1$ pendant vertices, denoted $\mathcal{U}^*_{n,n_1}$, as the set of unicyclic graphs of order $n$ consisting of a cycle $C_p$ ($p \geq 3$) and $n_1$ paths having a common end vertex which lies on $C_p$.

Theorem 3.4 Let $U$ be a unicyclic graph in $\Gamma_{n,n_1}$ such that $n > n_1 \geq 0$; then

$$\prod_2(U) \leq (n_1 + 2)^{n_1 + 2} 4^{n-n_1-1}$$

and the equality holds if and only if $U \in \mathcal{U}^*_{n,n_1}$.

Proof. We shall prove this result also by induction on $n + n_1$. Let $g(n, n_1) = (n_1 + 2)^{n_1 + 2} 4^{n-n_1-1}$. If $n_1 = 0$, then $U \cong C_n$ and by direct calculation $\prod_2(C_n) = 4^n = g(n, 0)$. 

Proof. We shall prove this result by induction on $n + n_1$. Let $f(n, n_1) = n_1^{n_1} 4^{n-n_1-1}$. If $n_1 = 2$ and $n \geq n_1$, then $T \cong P_n$ and by direct calculation $\prod_2(P_n) = 4^{n-2}$ and this equals $f(n, 2)$, hence the property is verified.

Let $n_1 \geq 3$ and suppose that the result is true for any tree of order $n'$ with $n_1'$ pendant vertices such that $7 \leq n' + n_1' < n + n_1$. Let $T$ be a tree in $\Gamma_{n, n_1}$ and $x$ be a pendant vertex of $T$. If $xy \in E(T)$, suppose that $d(y) = a$. We shall consider two cases: 1) $a = 2$ and 2) $a \geq 3$.

1) In this case $T - x$ has order $n - 1$ and $n_1$ pendant vertices, hence $\prod_2(T) = 2^2 \prod_2(T - x)$ and by the induction hypothesis $\prod_2(T - x) \leq f(n - 1, n_1)$ and the equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1}$. It follows that $\prod_2(T) \leq f(n, n_1)$ and the equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$.

2) $T - x$ having order $n - 1$ and $n_1 - 1$ pendant vertices, we have

$$\prod_2(T) = \frac{a^a}{(a-1)^{a-1}} \prod_2(T - x).$$

By our supposition of induction,

$$\prod_2(T) \leq \frac{a^a}{(a-1)^{a-1}} f(n - 1, n_1 - 1).$$

Equality holds if and only if $T - x \in \mathcal{T}^*_{n-1,n_1-1}$. The last inequality may be written

$$\prod_2(T) \leq \frac{a^a}{(a-1)^{a-1}} \frac{(n_1 - 1)^{n_1 - 1}}{n_1^{n_1}} f(n, n_1).$$

By Lemma 3.1, $\phi(x)$ is an increasing function, so $\frac{a^a}{(a-1)^{a-1}}$ is maximum for maximum value of $a$ and in the set of trees with $n_1$ pendant vertices the maximum degree of a vertex is $n_1$, so

$$\prod_2(T) \leq f(n, n_1).$$

Equality holds if and only if $T \in \mathcal{T}^*_{n,n_1}$ since $d(y) = n_1$ only if $x$ is adjacent to the unique vertex in $T - x$ of degree $n_1 - 1$.

We define a family of unicyclic graphs of order $n$ with $n_1$ pendant vertices, denoted $\mathcal{U}^*_{n,n_1}$, as the set of unicyclic graphs of order $n$ consisting of a cycle $C_p$ ($p \geq 3$) and $n_1$ paths having a common end vertex which lies on $C_p$.

Theorem 3.4 Let $U$ be a unicyclic graph in $\Gamma_{n,n_1}$ such that $n > n_1 \geq 0$; then

$$\prod_2(U) \leq (n_1 + 2)^{n_1 + 2} 4^{n-n_1-1}$$

and the equality holds if and only if $U \in \mathcal{U}^*_{n,n_1}$.

Proof. We shall prove this result also by induction on $n + n_1$. Let $g(n, n_1) = (n_1 + 2)^{n_1 + 2} 4^{n-n_1-1}$. If $n_1 = 0$, then $U \cong C_n$ and by direct calculation $\prod_2(C_n) = 4^n = g(n, 0)$. 

Let \( n_1 \geq 1 \) and suppose that the result is true for any unicyclic graph of order \( n' \) with \( n_1 \) pendant vertices, such that \( 4 \leq n' + n_1 < n + n_1 \). As before, let \( U \) be a unicyclic graph in \( \Gamma_{n,n_1} \) and \( x \) a pendant vertex of \( U \). If \( y \) is adjacent to \( x \) in \( U \), let \( d(y) = a \). We shall consider two cases:  
1) \( a = 2 \) and 2) \( a \geq 3 \). 

1) In this case \( U-x \) is unicyclic, has order \( n-1 \) and \( n_1 \) pendant vertices, hence \( \prod_2(U) = 2^2 \prod_2(U-x) \) and by the induction hypothesis \( \prod_2(U-x) \leq g(n-1,n_1) \) and the equality holds if and only if \( U-x \in U_{n-1,n_1}^* \). It follows that \( \prod_2(U) \leq g(n,n_1) \) and the equality holds if and only if \( U \in U_{n,n_1}^* \).

2) \( U-x \) having order \( n-1 \) and \( n_1-1 \) pendant vertices, we get

\[
\prod_2(U) = \frac{a^a}{(a-1)^{a-1}} \prod_2(U-x).
\]

By induction hypothesis,

\[
\prod_2(U) \leq \frac{a^a}{(a-1)^{a-1}} g(n-1,n_1-1),
\]

and equality holds if and only if \( U \in U_{n-1,n_1-1}^* \). We deduce

\[
\prod_2(U) \leq \frac{a^a}{(a-1)^{a-1}} \frac{(n_1+1)^{n_1+1}}{(n_1+2)^{n_1+2}} g(n,n_1).
\]

By Lemma 3.1, \( \phi(x) \) is strictly increasing in \( a \) and in the set of unicyclic graphs with \( n_1 \) pendant vertices the maximum degree of a vertex is \( n_1 + 2 \), so

\[
\prod_2(U) \leq g(n,n_1).
\]

Equality holds if and only if \( U \in U_{n,n_1}^* \) since \( d(y) = n_1 + 2 \) only if \( x \) is adjacent to the unique vertex in \( U-x \) of degree \( n_1 + 1 \), which is common to the cycle and \( n_1 - 1 \) pendant paths.

In a similar way we can generalize this result for a given cyclomatic number \( \gamma \geq 2 \) for every \( n \geq 3\gamma + n_1 \) as follows: Let \( G_{n,n_1,\gamma} \) be the set of connected graphs of order \( n \), having \( n_1 \) pendant vertices and cyclomatic number \( \gamma \), consisting of \( \gamma \) cycles having a common vertex \( w \) and \( n_1 \) paths having an end vertex in \( w \). If \( G \) is a connected graph of order \( n \), having \( n_1 \) pendant vertices and cyclomatic number \( \gamma \), then

\[
\prod_2(G) \leq (n_1 + 2\gamma)^{n_1+2\gamma} 4^{n-n_1-1}
\]

and the equality holds if and only if \( G \in G_{n,n_1,\gamma}^* \).

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