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 $\prod_2(G) = \prod_{uv \in E(G)} d(u)d(v)$. 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 γ . 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

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

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

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

$$\begin{aligned}\prod_1(G) &= \prod_{v \in V(G)} d(v)^2 \\ \prod_2(G) &= \prod_{uv \in E(G)} d(u)d(v) = \prod_{v \in V(G)} d(v)^{d(v)}\end{aligned}$$

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 $n, r, x_1, x_2, \dots, x_n$ 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 $x_1, \dots, x_n$ are almost equal, i.e., $\max\{x_1, \dots, x_n\} - \min\{x_1, \dots, x_n\} \leq 1$.

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 γ . 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:

$$\begin{aligned}t &= \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 1, & n_t &= (n-n_1) \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor - n_1 - 2(\gamma-1), \\ n_{t+1} &= n - (n-n_1) \left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 2(\gamma-1).\end{aligned}$$

Recall that $\lfloor x \rfloor$ is the greatest integer that is not greater than x , or the integer part of x .

Theorem 2.3 Let G be a connected (n, n_1) -graph with cyclomatic number γ . Then

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

(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 $n \geq 3\gamma + n_1$.

Proof. Lower bound. A graph with n vertices and cyclomatic number γ 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 γ 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 $n \geq 2\gamma + 1 + n_1$, and equality holds when all γ 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_t ($0 < n_t \leq n - n_1$) non-pendant vertices of degree t and $n_{t+1} = n - n_1 - n_t$ non-pendant vertices of degree $t + 1$, then

$$NK(G) \leq t^{n_t} (t+1)^{n_{t+1}}. \quad (1)$$

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

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

which yields

$$t(n - n_1) - n_t = n + 2(\gamma - 1), \quad (3)$$

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

$$t = \left\lfloor \frac{n + 2(\gamma - 1)}{n - n_1} \right\rfloor + 1. \quad (4)$$

From equations (3) and (4),

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

which gives

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

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

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

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

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

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 γ 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 γ 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 $n_1 = 13$ having minimal NK index.

Figure 4: Unicyclic graph with $n = 22$ and $n_1 = 13$ having maximal NK index.

Figure 5: Bicyclic graph with $n = 22$ and $n_1 = 13$ having minimal NK index.

Figure 6: Bicyclic graph with $n = 22$ and $n_1 = 13$ having maximal 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 γ . Then*

$$4^{n-n_1-1}(2\gamma+n_1)^2 \leq \prod_1(G) \leq \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 1 \right)^{2n_t} \left(\left\lfloor \frac{n+2(\gamma-1)}{n-n_1} \right\rfloor + 2 \right)^{2n_{t+1}}.$$

(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 ϕ is increasing for $x \geq 2$. $\square$

Let Γ_{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 $T_{n, 2}^* = \{P_2\}$.

Theorem 3.3 *Let T be a tree in Γ_{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 Γ_{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 $T - x \in T_{n-1, n_1}^*$. It follows that $\prod_2(T) \leq f(n, n_1)$ and the equality holds if and only if $T \in T_{n, n_1}^*$.

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 $T - x \in T_{n-1, n_1-1}^*$. 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 $T \in T_{n, n_1}^*$ 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 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 Γ_{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 $U \in U_{n, n_1}^*$.

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 Γ_{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 γ , consisting of γ 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 γ , 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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References

- [1] I. Gutman, M. Ghorbani, Some properties of the Narumi-Katayama index, *Applied Mathematics Letters*, **25**(2012) 1435-1438.
- [2] I. Gutman, M. K. Jamil, N. Akhter, Graphs with fixed number of pendant vertices and minimal first Zagreb index, *Trans Comb.*, **4**(2015) 29-34.
- [3] B. Horoldagva, S.G. Lee, Comparing Zagreb indices for connected graphs, *Discr. Appl. Math.*, **158** (2010) 1073-1078.
- [4] D. J. Klein, V. R. Rosenfeld, The degree-product index of Narumi and Katayama. *MATCH Commun. Math. Comput. Chem.*, **64**(2010) 607-618.
- [5] M. Khalifeh, H. Yousefi Azari, A.R. Ashrafi, The first and second Zagreb indices of graph operations. *Discr. Appl. Math.*, **157** (2009) 804-811.
- [6] H. Narumi, M. Katayama, Simple topological index, A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Memoirs of the Faculty of Engineering*, Hokkaido University **16** (1984) 209-214.
- [7] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta*, **76** (2003) 113-124.
- [8] R. Todeschini, D. Ballabio, V. Consonni, Novel molecular descriptors based on functions of new vertex degrees. In: *Novel molecular structure descriptors - Theory and applications I*. (I. Gutman, B. Furtula, eds.), pp. 73-100. Kragujevac: Univ. Kragujevac 2010.
- [9] R. Todeschini, V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees. *MATCH Commun. Math. Comput. Chem.*, **64** (2010) 359-372.
- [10] Ž. Tomović, I. Gutman, Narumi-Katayama index of phenylenes, *J. Serb. Chem. Soc.*, **66** (2001) 243-247.
- [11] N. Trinajstić, S. Nikolić, A. Miličević, I. Gutman, On Zagreb indices. *Kemija u industriji*, **59** (2010) 577-589 (in Croatian).
- [12] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 2001.
- [13] Z. You, B. Liu, On the extremal Narumi-Katayama index of graphs, *Filomat*, **28**(2014) 523-529.
- [14] Q. Zhao, S. Li, On the maximum Zagreb index of graphs with k cut vertices. *Acta Appl. Math.*, **111** (2010) 93-106.