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Extremal tricyclic, tetracyclic, and pentacyclic graphs with respect to the Narumi–Katayama index

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Abstract. Let G be an n-vertex graph with the vertex degree sequence d_1, d_2, $\ldots$, d_n. The Narumi–Katayama index of G is defined as $NK(G) = \prod_{i=1}^{n} d_i$. We determine eight classes of n-vertex tricyclic graphs with the first through the eighth maximal NK index, $n \geq 10$. We also identify ten classes of n-vertex tetracyclic graphs with the first through the ninth maximal NK index, $n \geq 10$, and thirteen classes of n-vertex pentacyclic graphs with the first through the twelfth maximal NK index, $n \geq 12$.

1. Introduction

In this paper, we consider only finite undirected simple graphs. Let G be such a graph with vertex set $V(G) = \{v_1, \ldots, v_n\}$. If G has exactly n vertices, m edges, and k components with $m-n+k = 3, 4, 5$, then the graph G is called *tricyclic*, *tetracyclic* and *pentacyclic*, respectively. Throughout this paper, we use the following notation: $d_1, d_2, \ldots, d_n$ denotes the degree sequence of G, where $d_i := deg_G(v_i)$. We use the symbols $\Delta(G)$ and $n_i = n_i(G)$ for the maximum degree of vertices in G and the number of vertices of degree i in G, respectively.

It is clear that $\sum_{i=1}^{\Delta(G)} n_i = |V(G)| = n$ and $\sum_{i=1}^{\Delta(G)} in_i = \sum_{i=1}^{n} d_i = 2m$, where m is the number of edges in G. The following natural question arises: what we can say about $\prod_{i=1}^{n} d_i$?

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In the 1980s, Narumi and Katayama [11] used the term *simple topological index* for this graph invariant, but nowadays researchers prefer the *Narumi–Katayama index* (NK index). Thus, $NK(G) = \prod_{i=1}^{n} d_i$. Klein and Rosenfeld [9] characterized this topological index, first, as the number of "functional" subgraphs of a certain directed graph, and, second, as a suitable weighting over a certain class of ordinary subgraph covers of the graph under consideration. They introduced the NK polynomial [10], by analogy with Hosoya Z-index and matching polynomial.

Suppose that PH is a phenylene and HS is its hexagonal squeeze. Tomović and Gutman [12] proved that the respective Narumi–Katayama indices of these molecular graphs are related as $NK(PH) = 9^{h-1}NK(HS)$, where h is the number of hexagons in PH and HS. Gutman and Ghorbani [7] obtained the maximal and minimal Narumi–Katayama index among all connected n-vertex trees, unicyclic and bicyclic graphs. Wang and Xia [13] characterized the first and second smallest Narumi–Katayama index among n-vertex unicycic graphs. Zolfi and Ashrafi [16] computed the first, second, third, and forth maximum and minimum of NK index for n-vertex trees and chemical trees. They also calculated the first ten minimum and maximum values of NK index in the classes of unicyclic and unicyclic chemical graphs [17]. In addition, they computed the first fifteen maximum values of the bicyclic graphs. You and Liu [15] determined the extremal NK index of trees and unicyclic graphs with a given diameter and the number of vertices.

Eliasi [4] applied the theory of majorization to order the first through sixth n-vertex trees, unicycic, and bicyclic graphs with respect to the NK index. Jamil et al. [8] characterized the upper and lower bounds of Narumi–Katayama index for the graphs with given order, number of pendant vertices, and cyclomatic number, and characterized the corresponding extremal graphs. Wang and Wei [14] identified the upper and lower bounds of Narumi–Katayama index for all cactus graphs and characterized the corresponding extremal graphs. Very recently Eliasi and Ghalavand [5] characterized the first through eighth maximal NK index among n-vertex trees by the theory of majorization.

Suppose that $x_1, \ldots, x_m$, $y_1, \ldots, y_m$ and k are positive integers. By the symbol $C^k(x_1^{(y_1)}, \ldots, x_m^{(y_m)})$ we denote the class of all graphs with cyclomatic number k, where y_i are vertices of degree x_i, $1 \leq i \leq m$. The set of all connected graphs with exactly n vertices and cyclomatic number i is denoted by $C^i(n)$.

Lemma 1.1. *Let $x_3, x_4, \ldots, x_m$ be nonnegative integers. Then,*

$$\frac{\prod_{i=3}^{m} i^{x_i}}{2^{\sum_{i=3}^{m} x_i(i-1)}} \leq 1.$$

Equality holds if and only if $x_i = 0$ for $i = 3, 4, \ldots, m$.

Proof. Note that

$$\begin{aligned}\ln \frac{\prod_{i=3}^{m} i^{x_i}}{2^{\sum_{i=3}^{m} x_i(i-1)}} &= \ln \prod_{i=3}^{m} i^{x_i} - \ln 2^{\sum_{i=3}^{m} x_i(i-1)} \\ &= \sum_{i=3}^{m} x_i \ln i - \sum_{i=3}^{m} x_i(i-1)\ln 2 \\ &= \sum_{i=3}^{m} x_i(\ln i - (i-1)\ln 2) \\ &= \sum_{i=3}^{m} x_i(\ln \frac{i}{2^{i-1}}) \leq 0.\end{aligned}$$

If $i \geq 3$, then $\frac{i}{2^{i-1}} < 1$ and so $\ln \frac{i}{2^{i-1}} < 0$. Therefore, the inequality holds its maximum if and only if $x_i = 0$, $3 \leq i \leq m$, proving the lemma. □

Throughout this paper, the path and complete graphs on n vertices are denoted by P_n and K_n, respectively. Other notation is standard and can be taken from standard books on graph theory.

2. Narumi–Katayama index of tricyclic graphs

The aim of this section is to determine eight classes of n-vertex tricyclic graphs with the first through the eight maximal NK index, $n \geq 10$.

Lemma 2.1. *Let G be a connected tricyclic graph with n vertices. Then, $n_1(G) = \sum_{i=3}^{\Delta(G)}(i-2)n_i - 4$ and $n_2(G) = n + 4 - \sum_{i=3}^{\Delta(G)}(i-1)n_i$.*

Proof. We note that the number of edges of G is $n+4$. Since $\sum_{i=1}^{\Delta(G)} n_i = n$ and $\sum_{i=1}^{\Delta(G)} in_i = 2|E(G)|$, we have $n_1 + n_2 + \sum_{i=3}^{\Delta(G)} n_i = n$ and $n_1 + 2n_2 + \sum_{i=3}^{\Delta(G)} in_i = 2n + 4$. By solving these equations, we obtain the result. □

Lemma 2.2. *Let G_1 and G_2 be two tricyclic graphs in $C^3(n)$. If $n_i(G_1) \geq n_i(G_2)$ for $i = 3, \ldots, n-1$, then $NK(G_1) \leq NK(G_2)$. Equality holds if and only if $n_i(G_1) = n_i(G_2)$.*

Proof. By Lemma 2.1,

$$\begin{aligned}\frac{NK(G_1)}{NK(G_2)} &= \frac{\prod_{i=1}^{n-1} i^{n_i(G_1)}}{\prod_{i=1}^{n-1} i^{n_i(G_2)}} = \frac{2^{n+4-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{n+4-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}} \\ &= \frac{2^{-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}} \qquad (1) \\ &= \frac{2^{\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}} = \frac{\prod_{i=3}^{n-1} i^{n_i(G_1)-n_i(G_2)}}{2^{\sum_{i=3}^{n-1}(n_i(G_1)-n_i(G_2))(i-1)}}.\end{aligned}$$

We now apply Lemma 1.1 and equalities (1) to prove the result. □

Lemma 2.2 implies the following two results.

Corollary 2.1. *Let G' be an n-vertex tricyclic graph, $n \geq 10$, $\Delta(G') = 3$, and $n_3(G') \geq 8$. Then, for each $G \in C^3(3^{(7)}, 2^{(n-10)}, 1^{(3)})$, we have $NK(G') < NK(G)$.*

Corollary 2.2. *Let G' be an n-vertex tricyclic graph and $\Delta(G') = 4$, where $n \geq 10$. If $n_4(G') = 1$ and $n_3(G') \geq 6$, then, for each $G \in C^3(4^{(1)}, 3^{(5)}, 2^{(n-9)}, 1^{(3)})$, we have $NK(G') < NK(G)$.*

Lemma 2.3. *Let G' be an n-vertex tricyclic graph, $\Delta(G') = 4$ and $n \geq 10$. If $n_4(G') \geq 2$ and*

$$G' \notin C^3(4^{(2)}, 24^{(n-2)}) \cup C^3(4^{(2)}, 3^{(1)}, 2^{(n-4)}, 1^{(1)}) \cup C^3(4^{(2)}, 3^{(2)}, 2^{(n-6)}, 1^{(2)}),$$

then, for each $G \in C^3(4^{(2)}, 3^{(2)}, 2^{(n-6)}, 1^{(2)})$, we have $NK(G') < NK(G)$.

Proof. Suppose that $n_4(G') \geq 3$ and $H \in C^3(4^{(3)}, 2^{(n-5)}, 1^{(2)})$. By Lemma 2.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{4^2 \times 3^2 \times 2^{n-6}}{4^3 \times 2^{n-5}} > 1.$$

The other cases can be obtained directly from Lemma 2.2. □

Lemma 2.4. *Let G' be an n-vertex tricyclic graph with maximum degree five, $n \geq 10$. If $G' \notin C^3(5^{(1)}, 3^{(1)}, 2^{(n-2)}) \cup C^3(5^{(1)}, 3^{(2)}, 2^{(n-4)}, 1^{(1)})$, then, for each $G \in C^3(5^{(1)}, 3^{(2)}, 2^{(n-4)}, 1^{(1)})$ we have $NK(G') < NK(G)$.*

Proof. Suppose that $n_5(G') \geq 2$. Choose a graph H from $C^3(5^{(2)}, 2^{(n-4)}, 1^{(2)})$. Then, by Lemma 2.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{5 \times 3^2 \times 2^{n-4}}{5^2 \times 2^{n-4}} > 1.$$

Thus, it is enough to assume that $n_5(G') = 1$. Suppose that $n_4(G') \geq 1$ and $n_3(G') \leq 1$, and choose $H \in C^3(5^{(1)}, 4^{(1)}, 2^{(n-3)}, 1^{(1)})$. Then, by Lemma 2.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{5 \times 3^2 \times 2^{n-4}}{5 \times 4 \times 2^{n-3}} > 1.$$

The other cases can be obtained directly from Lemma 2.2. □

Theorem 2.1. *Let G' be a tricyclic graph with $n \geq 10$ vertices and let $\Delta(G') \geq 6$. If $G' \notin C^3(6^{(1)}, 2^{(n-1)})$, then, for each $G \in C^3(6^{(1)}, 2^{(n-1)})$, we have $NK(G') < NK(G)$.*

Proof. We first assume that $\Delta(G') \geq 7$. Then, by Lemmas 2.1 and 1.1,

$$\begin{aligned}\frac{NK(G)}{NK(G')} &= \frac{6\times 2^{(n-1)}}{2^{n+4-\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)}\prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\ &= \frac{6\times 2^{\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)-5}}{\prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\ &= \frac{6\times 2^{n_\Delta(G')(\Delta(G')-1)-5}}{\Delta(G')^{n_\Delta(G')}} \times \frac{2^{\sum_{i=3}^{\Delta(G')-1} n_i(G')(i-1)}}{\prod_{i=3}^{\Delta(G')-1} i^{n_i(G')}} \\ &\geq \frac{6\times 2^{n_\Delta(G')(\Delta(G')-1)-5}}{\Delta(G')^{n_\Delta(G')}}.\end{aligned} \tag{2}$$

But

$$\begin{aligned}&\ln \frac{6\times 2^{n_\Delta(G')(\Delta(G')-1)-5}}{\Delta(G')^{n_\Delta(G')}} \\ &\quad = \ln 6 + n_\Delta(G')(\Delta(G')-1)\ln 2 - 5\ln 2 - n_\Delta(G')\ln\Delta(G') \\ &\quad > n_\Delta(G')(\Delta(G')-1)\ln 2 - n_\Delta(G')\ln\Delta(G') - 1.7 > 0.\end{aligned}$$

Since

$$n_\Delta(G')\ln\frac{2^{\Delta(G')-1}}{\Delta(G')} \geq \ln\frac{2^6}{7} > 1.7,$$

by (2) one has $\frac{NK(G)}{NK(G')} > 1$. In other cases, the result can be obtained by Lemma 2.2. □

In the next theorem, it is assumed that $n \geq 10$,

$G_1 \in C^3(3^{(4)}, 2^{(n-4)})$,	$G_2 \in C^3(4^{(1)}, 3^{(2)}, 2^{(n-3)})$,
$G_3 \in C^3(4^{(2)}, 2^{(n-2)})$,	$G_4 \in C^3(3^{(5)}, 2^{(n-6)}, 1^{(1)})$,
$G_5 \in C^3(5^{(1)}, 3^{(1)}, 2^{(n-2)})$,	$G_6 \in C^3(4^{(1)}, 3^{(3)}, 2^{(n-5)}, 1^{(1)})$,
$G_7 \in C^3(4^{(2)}, 3^{(1)}, 2^{(n-4)}, 1^{(1)})$,	$G_8 \in C^3(6^{(1)}, 2^{(n-1)})$,
$G_9 \in C^3(3^{(6)}, 2^{(n-8)}, 1^{(2)})$,	$G_{10} \in C^3(5^{(1)}, 3^{(2)}, 2^{(n-4)}, 1^{(1)})$,
$G_{11} \in C^3(4^{(1)}, 3^{(5)}, 2^{(n-9)}, 1^{(3)})$,	$G_{12} \in C^3(4^{(2)}, 3^{(2)}, 2^{(n-6)}, 1^{(2)})$,
$G_{13} \in C^3(3^{(7)}, 2^{(n-10)}, 1^{(3)})$,	$G_{14} \in C^3(4^{(1)}, 3^{(4)}, 2^{(n-7)}, 1^{(2)})$,

Theorem 2.2. *Let G be an n-vertex tricyclic graph outside the set $\{G_1, G_2, \ldots, G_8\}$. Then we have $NK(G_1) > NK(G_2) > NK(G_3) > NK(G_4) > NK(G_5) > NK(G_6) > NK(G_7) = NK(G_8) > NK(G)$.*

Proof. By Table 1, $NK(G_1) > NK(G_2) > NK(G_3) > NK(G_4) > NK(G_5) > NK(G_6) > NK(G_7) = NK(G_8)$. If $G \in \{G_9, \ldots, G_{14}\}$, then Table 1 gives us the result. If $\Delta(G) = 3$ and $n_3(G) \geq 8$, then the result can

TABLE 1. The tricyclic graphs.

Classes	NK Index
$C^3(3^{(4)}, 2^{(n-4)})$	$3^4 \times 2^{(n-4)}$
$C^3(3^{(5)}, 2^{(n-6)}, 1^{(1)})$	$3^5 \times 2^{(n-6)}$
$C^3(3^{(6)}, 2^{(n-8)}, 1^{(2)})$	$3^6 \times 2^{(n-8)}$
$C^3(3^{(7)}, 2^{(n-10)}, 1^{(3)})$	$3^7 \times 2^{(n-10)}$
$C^3(4^{(1)}, 3^{(2)}, 2^{(n-3)})$	$4 \times 3^2 \times 2^{(n-3)}$
$C^3(4^{(1)}, 3^{(3)}, 2^{(n-5)}, 1^{(1)})$	$4 \times 3^3 \times 2^{(n-5)}$
$C^3(4^{(1)}, 3^{(4)}, 2^{(n-7)}, 1^{(2)})$	$4 \times 3^4 \times 2^{(n-7)}$
$C^3(4^{(1)}, 3^{(5)}, 2^{(n-9)}, 1^{(3)})$	$4 \times 3^5 \times 2^{(n-9)}$
$C^3(4^{(2)}, 2^{(n-2)})$	$4^2 \times 2^{(n-2)}$
$C^3(4^{(2)}, 3^{(1)}, 2^{(n-4)}, 1^{(1)})$	$4^2 \times 3 \times 2^{(n-4)}$
$C^3(4^{(2)}, 3^{(2)}, 2^{(n-6)}, 1^{(2)})$	$4^2 \times 3^2 \times 2^{(n-6)}$
$C^3(5^{(1)}, 3^{(1)}, 2^{(n-2)})$	$5 \times 3 \times 2^{(n-2)}$
$C^3(5^{(1)}, 3^{(2)}, 2^{(n-4)}, 1^{(1)})$	$5 \times 3^2 \times 2^{(n-4)}$
$C^3(6^{(1)}, 2^{(n-1)})$	$6 \times 2^{(n-1)}$

be deduced from Corollary 2.1. Suppose that $\Delta(G) = 4$. If $n_4(G) = 1$ and $n_3(G) \geq 6$, then Corollary 2.2 gives us the result. If $n_4(G) \geq 2$, then the result follows from Lemma 2.3, and if $\Delta(G) = 5$, then the result is a consequence of Lemma 2.4. If $\Delta(G) \geq 6$, then the result follows from Theorem 2.1. In other cases, $G \in \{G_1, G_2, \ldots, G_8\}$, as desired. □

3. Narumi–Katayama index of tetracyclic graphs

The aim of this section is to determine the first through the nine maximal NK index in the class of all n-vertex tetracyclic graphs, $n \geq 10$.

Lemma 3.1. *If G is a connected tetracyclic graph with n vertices, then*

$$n_1(G) = \sum_{i=3}^{\Delta(G)} (i-2)n_i - 6 \quad \text{and} \quad n_2(G) = n + 6 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Proof. It is easy to see that $\sum_{i=1}^{\Delta(G)} n_i = n$ and $\sum_{i=1}^{\Delta(G)} in_i = 2|E(G)|$. Since $|E(G)| = n + 3$,

$$n_1 + n_2 + \sum_{i=3}^{\Delta(G)} n_i = n, \quad \text{and} \quad n_1 + 2n_2 + \sum_{i=3}^{\Delta(G)} in_i = 2n + 6,$$

proving the lemma. □

Lemma 3.2. *Let G_1 and G_2 be two tetracyclic graphs in $C^4(n)$. If $n_i(G_1) \geq n_i(G_2)$, $3 \leq i \leq n-1$, then $NK(G_1) \leq NK(G_2)$. The equality holds if and only if $n_i(G_1) = n_i(G_2)$, where $3 \leq i \leq n-1$.*

Proof. By Lemma 3.1, we have

$$\frac{NK(G_1)}{NK(G_2)} = \frac{\prod_{i=1}^{n-1} i^{n_i(G_1)}}{\prod_{i=1}^{n-1} i^{n_i(G_2)}} = \frac{2^{n+6-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{n+6-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}}$$
$$= \frac{2^{-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}}$$
$$= \frac{2^{\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}} = \frac{\prod_{i=3}^{n-1} i^{n_i(G_1)-n_i(G_2)}}{2^{\sum_{i=3}^{n-1}(n_i(G_1)-n_i(G_2))(i-1)}}.$$

Now Lemma 1.1 gives us the result. □

Lemma 3.2 implies the following three results.

Corollary 3.1. *Let G' be a tetracyclic graph with $n \geq 10$ vertices, $\Delta(G') = 3$, and $n_3(G') \geq 9$. Then, for each $G \in C^4(3^{(8)}, 2^{(n-10)}, 1^{(2)})$, we have $NK(G') < NK(G)$.*

Corollary 3.2. *Let G' be a tetracyclic graph with $n \geq 10$ vertices and $\Delta(G') = 4$. If $n_4(G') = 1$ and $n_3(G') \geq 7$, then, for each $G \in C^4(4^{(1)}, 3^{(6)}, 2^{(n-9)}, 1^{(2)})$, we have $NK(G') < NK(G)$.*

Corollary 3.3. *Let G' be an n-vertex tetracyclic graph with $\Delta(G') = 4$ and $n \geq 10$. If $n_4(G') = 2$ and $n_3(G') \geq 5$, then, for each $G \in C^4(4^{(2)}, 3^{(4)}, 2^{(n-8)}, 1^{(2)})$, we have $NK(G') < NK(G)$.*

Lemma 3.3. *Let G' be an n-vertex tetracyclic graph, where $\Delta(G') = 4$ and $n \geq 10$. If $n_4(G') \geq 3$ and*

$$G' \notin C^4(4^{(3)}, 2^{(n-3)}) \cup C^4(4^{(3)}, 3^{(1)}, 2^{(n-5)}, 1^{(1)}) \cup C^4(4^{(3)}, 3^{(2)}, 2^{(n-7)}, 1^{(2)}),$$

then, for each $G \in C^4(4^{(3)}, 3^{(2)}, 2^{(n-7)}, 1^{(2)})$, we have $NK(G') < NK(G)$.

Proof. Suppose that $n_4(G') \geq 4$ and choose a graph H in $C^4(4^{(4)}, 2^{(n-6)}, 1^{(2)})$. Then, by Lemma 3.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{4^3 \times 3^2 \times 2^{n-7}}{4^4 \times 2^{n-6}} > 1.$$

On other cases, the result can be obtained from Lemma 3.2. □

Lemma 3.4. *Let G' be an n-vertex tetracyclic graph, where $\Delta(G') = 5$, and $n \geq 10$. If $G' \notin C^4(5^{(1)}, 3^{(3)}, 2^{(n-4)}) \cup C^4(5^{(1)}, 3^{(4)}, 2^{(n-6)}, 1^{(1)}) \cup C^4(5^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-3)})$, then, for each $G \in C^4(5^{(1)}, 3^{(4)}, 2^{(n-6)}, 1^{(1)})$, we have $NK(G') < NK(G)$.*

Proof. We first assume that $n_5(G') \geq 2$. Choose an $H \in C^4(5^{(2)}, 2^{(n-2)})$. Then, by Lemma 3.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{5 \times 3^4 \times 2^{n-6}}{5^2 \times 2^{n-2}} > 1.$$

If $n_5(G') = 1$ and $n_4(G') = 1$, then

$$C^4(5^{(1)}, 4^{(1)}, 3^{(2)}, 2^{(n-5)}, 1^{(1)}).$$

Hence, by Lemma 3.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{5 \times 3^4 \times 2^{n-6}}{5 \times 4 \times 3^2 \times 2^{n-5}} > 1.$$

We now assume that $n_5(G') = 1$, $n_4(G') \geq 2$, and choose a graph H in the set

$$C^4(5^{(1)}, 4^{(2)}, 2^{(n-4)}, 1^{(1)}).$$

Then, by Lemma 3.2,

$$\frac{NK(G)}{NK(G')} \geq \frac{NK(G)}{NK(H)} = \frac{5 \times 3^4 \times 2^{n-6}}{5 \times 4^2 \times 2^{n-4}} > 1.$$

In other cases, the result can be obtained by Lemma 3.2. □

Theorem 3.1. *Let G' be an n-vertex tetracyclic graph with $n \geq 10$ vertices, and let $\Delta(G') \geq 6$. If $G' \notin C^4(6^{(1)}, 3^{(2)}, 2^{(n-3)})$, then, for each $G \in C^4(6^{(1)}, 3^{(2)}, 2^{(n-3)})$, we have $NK(G') < NK(G)$.*

Proof. Our main proof will consider the following three cases.

(1) Suppose that $\Delta(G') \geq 8$. Then, by Lemma 3.1 and Lemma 1.1,

$$\begin{aligned}\frac{NK(G)}{NK(G')} &= \frac{6 \times 3^2 \times 2^{(n-3)}}{2^{n+6-\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)} \prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\ &= \frac{54 \times 2^{\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)-9}}{\prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\ &= \frac{54 \times 2^{n_\Delta(G')(\Delta(G')-1)-9}}{\Delta(G')^{n_\Delta(G')}} \times \frac{2^{\sum_{i=3}^{\Delta(G')-1} n_i(G')(i-1)}}{\prod_{i=3}^{\Delta(G')-1} i^{n_i(G')}} \\ &\geq \frac{54 \times 2^{n_\Delta(G')(\Delta(G')-1)-9}}{\Delta(G')^{n_\Delta(G')}}.\end{aligned} \tag{3}$$

On the other hand, since $n_\Delta(G') \ln \frac{2^{\Delta(G')-1}}{\Delta(G')} \geq \ln \frac{2^7}{8} > 2.25$, we get

$$\begin{aligned}\ln \frac{54 \times 2^{n_\Delta(G')(\Delta(G')-1)-9}}{\Delta(G')^{n_\Delta(G')}} &= \ln 54 + n_\Delta(G')(\Delta(G')-1)\ln 2 \\ &\quad - 9\ln 2 - n_\Delta(G') \ln \Delta(G')\end{aligned}$$

$$> n_\Delta(G')(\Delta(G')-1)\ln 2 - n_\Delta(G')\ln\Delta(G') - 2.25 > 0.$$

We now apply (3) to prove that $\frac{NK(G)}{NK(G')} > 1$.

(2) Let $\Delta(G') = 7$. By Lemma 3.2, there exists a graph H in $C^4(7^{(1)}, 3^{(1)}, 2^{(n-2)}) \cup C^4(7^{(1)}, 4^{(1)}, 2^{(n-3)}, 1^{(1)}) \cup C^4(7^{(1)}, 5^{(1)}, 2^{(n-4)}, 1^{(2)}) \cup C^4(7^{(1)}, 6^{(1)}, 2^{(n-5)}, 1^{(3)}) \cup C^4(7^{(2)}, 2^{(n-6)}, 1^{(4)})$. Hence, $NK(G') \le NK(H) < NK(G)$ which proves the assertion .

(3) Let $\Delta(G') = 6$. By Lemma 3.2, there exists a graph H such that

$$\begin{aligned} H \in\ & C^4(6^{(1)}, 3^{(3)}, 2^{(n-5)}, 1^{(1)}) \cup C^4(6^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-4)}, 1^{(1)}) \\ & \cup C^4(6^{(1)}, 4^{(2)}, 2^{(n-5)}, 1^{(2)}) \cup C^4(6^{(1)}, 5^{(1)}, 3^{(1)}, 2^{(n-5)}, 1^{(2)}) \\ & \cup C^4(6^{(1)}, 5^{(1)}, 4^{(1)}, 2^{(n-6)}, 1^{(3)}) \cup C^4(6^{(1)}, 5^{(2)}, 2^{(n-7)}, 1^{(4)}) \\ & \cup C^4(6^{(2)}, 3^{(1)}, 2^{(n-6)}, 1^{(3)}) \cup C^4(6^{(2)}, 4^{(1)}, 2^{(n-7)}, 1^{(4)}) \\ & \cup C^4(6^{(2)}, 5^{(1)}, 2^{(n-8)}, 1^{(5)}) \cup C^4(6^{(3)}, 2^{(n-9)}, 1^{(6)}). \end{aligned}$$

Thus, $NK(G') \le NK(H) < NK(G)$. □

In the following theorem, it is assumed that $n \ge 10$ and

$$\begin{array}{ll} H_1 \in C^4(3^{(6)}, 2^{(n-6)}), & H_2 \in C^4(4^{(1)}, 3^{(4)}, 2^{(n-5)}), \\ H_3 \in C^4(4^{(2)}, 3^{(2)}, 2^{(n-4)}), & H_4 \in C^4(3^{(7)}, 2^{(n-8)}, 1^{(1)}), \\ H_5 \in C^4(5^{(1)}, 3^{(3)}, 2^{(n-4)}), & H_6 \in C^4(4^{(3)}, 2^{(n-3)}), \\ H_7 \in C^4(4^{(1)}, 3^{(5)}, 2^{(n-7)}, 1^{(1)}), & H_8 \in C^4(5^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-3)}), \\ H_9 \in C^4(4^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)}), & H_{10} \in C^4(6^{(1)}, 3^{(2)}, 2^{(n-3)}), \\ H_{11} \in C^4(3^{(8)}, 2^{(n-10)}, 1^{(2)}), & H_{12} \in C^4(5^{(1)}, 3^{(4)}, 2^{(n-6)}, 1^{(1)}), \\ H_{13} \in C^4(4^{(3)}, 3^{(1)}, 2^{(n-5)}, 1^{(1)}), & H_{14} \in C^4(4^{(1)}, 3^{(6)}, 2^{(n-9)}, 1^{(2)}), \\ H_{15} \in C^4(4^{(2)}, 3^{(4)}, 2^{(n-8)}, 1^{(2)}), & H_{16} \in C^4(4^{(3)}, 3^{(2)}, 2^{(n-7)}, 1^{(2)}). \end{array}$$

Theorem 3.2. *Let H be a tetracyclic graph with $n \ge 10$ vertices, except from the graphs $H_1, H_2, \ldots, H_{10}$. Then, $NK(H_1) > NK(H_2) > NK(H_3) > NK(H_4) > NK(H_5) > NK(H_6) > NK(H_7) > NK(H_8) > NK(H_9) = NK(H_{10}) > NK(H)$.*

Proof. From Table 2, $NK(H_1) > NK(H_2) > NK(H_3) > NK(H_4) > NK(H_5) > NK(H_6) > NK(H_7) > NK(H_8) > NK(H_9) = NK(H_{10})$. If $H \in \{H_{11}, \ldots, H_{16}\}$, then Table 2 gives us the result. If $\Delta(H) = 3$ and $n_3(H) \ge 9$, then the result follows from Corollary 3.1.

Suppose that $\Delta(H) = 4$. If $n_4(H) = 1$ and $n_3(H) \ge 7$, then the result follows from Corollary 3.2. If $n_4(H) = 2$ and $n_3(H) \ge 5$, then our result is a consequence of Corollary 3.3. Moreover, if $n_4(H) \ge 3$, then Lemma 3.3 completes the proof.

Table 2. The tetracyclic graphs.

Classes	NK Index
$C^4(3^{(6)}, 2^{(n-6)})$	$3^6 \times 2^{(n-6)}$
$C^4(3^{(7)}, 2^{(n-8)}, 1^{(1)})$	$3^7 \times 2^{(n-8)}$
$C^4(3^{(8)}, 2^{(n-10)}, 1^{(2)})$	$3^8 \times 2^{(n-10)}$
$C^4(4^{(1)}, 3^{(4)}, 2^{(n-5)})$	$4 \times 3^4 \times 2^{(n-5)}$
$C^4(4^{(1)}, 3^{(5)}, 2^{(n-7)}, 1^{(1)})$	$4 \times 3^5 \times 2^{(n-7)}$
$C^4(4^{(1)}, 3^{(6)}, 2^{(n-9)}, 1^{(2)})$	$4 \times 3^6 \times 2^{(n-9)}$
$C^4(4^{(2)}, 3^{(2)}, 2^{(n-4)})$	$4^2 \times 3^2 \times 2^{(n-4)}$
$C^4(4^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$	$4^2 \times 3^3 \times 2^{(n-6)}$
$C^4(4^{(2)}, 3^{(4)}, 2^{(n-8)}, 1^{(2)})$	$4^2 \times 3^4 \times 2^{(n-8)}$
$C^4(4^{(3)}, 2^{(n-3)})$	$4^3 \times 2^{(n-3)}$
$C^4(4^{(3)}, 3^{(1)}, 2^{(n-5)}, 1^{(1)})$	$4^3 \times 3 \times 2^{(n-5)}$
$C^4(4^{(3)}, 3^{(2)}, 2^{(n-7)}, 1^{(2)})$	$4^3 \times 3^2 \times 2^{(n-7)}$
$C^4(5^{(1)}, 3^{(3)}, 2^{(n-4)})$	$5 \times 3^3 \times 2^{(n-4)}$
$C^4(5^{(1)}, 3^{(4)}, 2^{(n-6)}, 1^{(1)})$	$5 \times 3^4 \times 2^{(n-6)}$
$C^4(5^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-3)})$	$5 \times 4 \times 3 \times 2^{(n-3)}$
$C^4(6^{(1)}, 3^{(2)}, 2^{(n-3)})$	$6 \times 3^2 \times 2^{(n-3)}$

If $\Delta(H) = 5$, then Lemma 3.4 gives us the result. For $\Delta(H) \geq 6$, we apply Theorem 3.1. For other cases, we note that H is included in the set $\{H_1, H_2, \dots, H_{10}\}$. □

4. Narumi–Katayama index of pentacyclic graphs

The aim of this section is to determine the first through the twelfth maximal NK index in the class of all n-vertex pentacyclic graphs, $n \geq 12$.

Lemma 4.1. *Let G be a connected pentacyclic graph with n vertices. Then*

$$n_1(G) = \sum_{i=3}^{\Delta(G)} (i-2)n_i - 8 \ \text{ and } \ n_2(G) = n + 8 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Proof. It is easy to see that $\sum_{i=1}^{\Delta(G)} n_i = n$ and $\sum_{i=1}^{\Delta(G)} in_i = 2|E(G)|$. Since G is a pentacyclic graph with n vertices, $|E(G)| = n + 4$. Therefore,

$$n_1 + n_2 + \sum_{i=3}^{\Delta(G)} n_i = n \ \text{ and } \ n_1 + 2n_2 + \sum_{i=3}^{\Delta(G)} in_i = 2n + 8,$$

proving the result. □

Lemma 4.2. *Let G_1 and G_2 be two pentacyclic graphs in $C^5(n)$. If $n_i(G_1) \geq n_i(G_2)$, $3 \leq i \leq n-1$, then $NK(G_1) \leq NK(G_2)$. Equality holds if and only if $n_i(G_1) = n_i(G_2)$, where $i = 3, 4, \ldots, n-1$.*

Proof. By Lemma 4.1,

$$\frac{NK(G_1)}{NK(G_2)} = \frac{\prod_{i=1}^{n-1} i^{n_i(G_1)}}{\prod_{i=1}^{n-1} i^{n_i(G_2)}} = \frac{2^{n+8-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{n+8-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}}$$
$$= \frac{2^{-\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{-\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}}$$
$$= \frac{2^{\sum_{i=3}^{n-1} n_i(G_2)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_1)}}{2^{\sum_{i=3}^{n-1} n_i(G_1)(i-1)} \prod_{i=3}^{n-1} i^{n_i(G_2)}} = \frac{\prod_{i=3}^{n-1} i^{n_i(G_1)-n_i(G_2)}}{2^{\sum_{i=3}^{n-1}(n_i(G_1)-n_i(G_2))(i-1)}}.$$

Now Lemma 1.1 gives us the result. □

Lemma 4.2 implies the following three results.

Corollary 4.1. *Let G' be an n-vertex pentacyclic graph. Assume that $n \geq 14$, $\Delta(G') = 3$, and $n_3(G') \geq 12$. Then, for each $G \in C^5(3^{(11)}, 2^{(n-14)}, 1^{(3)})$, we have $NK(G') < NK(G)$.*

Corollary 4.2. *Let G' be an n-vertex pentacyclic graph, where $\Delta(G') = 4$, and let $n \geq 12$. If $n_4(G') = 1$ and $n_3(G') \geq 9$, then, for each $G \in C^5(4^{(1)}, 3^{(8)}, 2^{(n-11)}, 1^{(2)})$, we have $NK(G') < NK(G)$.*

Corollary 4.3. *Let G' be a pentacyclic graph, where $\Delta(G') = 4$, and let $n \geq 12$. If $n_4(G') = 2$ and $n_3(G') \geq 7$, then, for each $G \in C^5(4^{(2)}, 3^{(6)}, 2^{(n-10)}, 1^{(2)})$, we have $NK(G') < NK(G)$.*

Lemma 4.3. *Let G' be a pentacyclic graph, where $\Delta(G') = 4$, and let $n \geq 12$. If $n_4(G') \geq 3$ and $G' \notin C^5(4^{(3)}, 3^{(2)}, 2^{(n-5)}) \cup C^5(4^{(4)}, 2^{(n-4)}) \cup C^5(4^{(3)}, 3^{(3)}, 2^{(n-7)}, 1^{(1)})$, then, for each $G \in C^5(4^{(3)}, 3^{(3)}, 2^{(n-7)}, 1^{(1)})$, we have $NK(G') < NK(G)$.*

Proof. Suppose that $n_4(G') \geq 4$. Then, by Lemma 4.2, there exists a graph H in $C^5(4^{(4)}, 3^{(1)}, 2^{(n-6)}, 1^{(1)}) \cup C^5(4^{(5)}, 2^{(n-7)}, 1^{(2)})$. Thus, $NK(G') \leq NK(H) < NK(G)$, as desired. In other cases, the result follows from Lemma 4.2. □

Lemma 4.4. *Let G' be a pentacyclic graph, where $\Delta(G') = 5$, and let $n \geq 12$. If $n_5(G') = 1$ and $G' \notin C^5(5^{(1)}, 3^{(5)}, 2^{(n-6)}) \cup C^5(5^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-5)}) \cup C^5(5^{(1)}, 3^{(6)}, 2^{(n-8)}, 1^{(1)})$, then, for each $G \in C^5(5^{(1)}, 3^{(6)}, 2^{(n-8)}, 1^{(1)})$, we have $NK(G') < NK(G)$.*

Proof. Suppose that $n_3(G') < 6$. By Lemma 4.2, there exists a graph H such that

$$H \in C^5(5^{(1)}, 4^{(2)}, 3^{(3)}, 2^{(n-8)}, 1^{(2)}) \cup C^5(5^{(1)}, 4^{(3)}, 3^{(2)}, 2^{(n-9)}, 1^{(3)})$$

$$\cup\, C^5(5^{(1)}, 4^{(4)}, 3^{(1)}, 2^{(n-10)}, 1^{(4)}) \cup C^5(5^{(1)}, 4^{(5)}, 2^{(n-11)}, 1^{(5)}).$$

So, $NK(G') \leq NK(H) < NK(G)$, as desired. In other cases, the result follows from Lemma 4.2. □

Lemma 4.5. *Let G' be an n-vertex pentacyclic graph, where $\Delta(G') = 5$, and $n \geq 12$. If $n_5(G') \geq 2$ and $G' \notin C^5(5^{(2)}, 3^{(2)}, 2^{(n-4)}) \cup C^5(5^{(2)}, 4^{(1)}, 2^{(n-3)}) \cup C^5(5^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$, then, for each $G \in C^5(5^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$, we have $NK(G') < NK(G)$.*

Proof. Suppose that $n_5(G') \geq 3$. If H is a graph in $C^5(5^{(3)}, 3^{(1)}, 2^{(n-6)}, 1^{(2)}) \cup C^5(5^{(3)}, 4^{(1)}, 2^{(n-7)}, 1^{(3)}) \cup C^5(5^{(4)}, 2^{(n-8)}, 1^{(4)})$, then, by Lemma 4.2, $NK(G') \leq NK(H) < NK(G)$. In the case when $n_5(G') = 2$ and $n_3(G') < 3$, we choose the graph H in $C^5(5^{(2)}, 4^{(1)}, 3^{(1)}, 2^{(n-5)}, 1^{(1)}) \cup C^5(5^{(2)}, 4^{(2)}, 2^{(n-6)}, 1^{(2)})$. Then, by Lemma 4.2, $NK(G') \leq NK(H) < NK(G)$. Finally, in other cases, we apply Lemma 4.2 to complete our argument. □

Theorem 4.1. *Let G' be an n-vertex pentacyclic graph with $n \geq 12$ vertices and $\Delta(G') \geq 6$. If*

$$G' \notin C^5(8^{(1)}, 3^{(2)}, 2^{(n-3)}) \cup C^5(7^{(1)}, 3^{(3)}, 2^{(n-4)}) \cup C^5(6^{(1)}, 3^{(4)}, 2^{(n-5)}) \cup C^5(6^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)}) \cup C^5(6^{(2)}, 2^{(n-2)}),$$

then, for each $G \in C^5(6^{(2)}, 2^{(n-2)})$, we have $NK(G') < NK(G)$.

Proof. We consider five cases as follows.

(1) $\Delta(G') \geq 10$. By Lemmas 4.1 and 1.1,

$$\begin{aligned}
\frac{NK(G)}{NK(G')} &= \frac{6^2 \times 2^{(n-2)}}{2^{n+8-\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)} \prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\
&= \frac{36 \times 2^{\sum_{i=3}^{\Delta(G')} n_i(G')(i-1)-10}}{\prod_{i=3}^{\Delta(G')} i^{n_i(G')}} \\
&= \frac{36 \times 2^{n_\Delta(G')(\Delta(G')-1)-10}}{\Delta(G')^{n_\Delta(G')}} \times \frac{2^{\sum_{i=3}^{\Delta(G')-1} n_i(G')(i-1)}}{\prod_{i=3}^{\Delta(G')-1} i^{n_i(G')}} \\
&\geq \frac{36 \times 2^{n_\Delta(G')(\Delta(G')-1)-10}}{\Delta(G')^{n_\Delta(G')}}.
\end{aligned} \tag{4}$$

On the other hand, since $n_\Delta(G') \ln \frac{2^{\Delta(G')-1}}{\Delta(G')} \geq \ln \frac{2^9}{10} > 3.35$,

$$\begin{aligned}
\ln \frac{36 \times 2^{n_\Delta(G')(\Delta(G')-1)-10}}{\Delta(G')^{n_\Delta(G')}} &= \ln 36 + n_\Delta(G')(\Delta(G')-1)\ln 2 \\
&\quad - 10\ln 2 - n_\Delta(G')\ln \Delta(G') \\
&> n_\Delta(G')(\Delta(G')-1)\ln 2
\end{aligned}$$

$$- n_\Delta(G') \ln \Delta(G') - 3.35 > 0.$$

We now apply (4) to prove $\frac{NK(G)}{NK(G')} > 1$.

(2) $\Delta(G') = 9$. By Lemma 4.2, there exists a graph H in the set $C^5(9^{(1)}, 3^{(1)}, 2^{(n-2)}) \cup C^5(9^{(1)}, 4^{(1)}, 2^{(n-3)}, 1^{(1)}) \cup C^5(9^{(1)}, 5^{(1)}, 2^{(n-4)}, 1^{(2)}) \cup C^5(9^{(1)}, 6^{(1)}, 2^{(n-5)}, 1^{(3)}) \cup C^5(9^{(1)}, 7^{(1)}, 2^{(n-6)}, 1^{(4)}) \cup C^5(9^{(1)}, 8^{(1)}, 2^{(n-7)}, 1^{(5)}) \cup C^5(9^{(2)}, 2^{(n-8)}, 1^{(6)})$ such that $NK(G') \le NK(H) < NK(G)$, as desired.

(3) $\Delta(G') = 8$. Again by Lemma 4.2, there exists a graph H in the set

$$\begin{aligned}
&C^5(8^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-4)}, 1^{(1)}) \cup C^5(8^{(1)}, 5^{(1)}, 3^{(1)}, 2^{(n-5)}, 1^{(2)})\\
&\quad \cup C^5(8^{(1)}, 6^{(1)}, 3^{(1)}, 2^{(n-6)}, 1^{(3)}) \cup C^5(8^{(1)}, 7^{(1)}, 3^{(1)}, 2^{(n-7)}, 1^{(4)})\\
&\quad \cup C^5(8^{(2)}, 3^{(1)}, 2^{(n-8)}, 1^{(5)}) \cup C^5(8^{(1)}, 4^{(2)}, 2^{(n-5)}, 1^{(2)})\\
&\quad \cup C^5(8^{(1)}, 5^{(1)}, 4^{(1)}, 2^{(n-6)}, 1^{(3)}) \cup C^5(8^{(1)}, 6^{(1)}, 4^{(1)}, 2^{(n-7)}, 1^{(4)})\\
&\quad \cup C^5(8^{(1)}, 7^{(1)}, 4^{(1)}, 2^{(n-8)}, 1^{(5)}) \cup C^5(8^{(2)}, 4^{(1)}, 2^{(n-9)}, 1^{(6)})\\
&\quad \cup C^5(8^{(1)}, 5^{(2)}, 2^{(n-7)}, 1^{(4)}) \cup C^5(8^{(1)}, 6^{(1)}, 5^{(1)}, 2^{(n-8)}, 1^{(5)})\\
&\quad \cup C^5(8^{(1)}, 7^{(1)}, 5^{(1)}, 2^{(n-9)}, 1^{(6)}) \cup C^5(8^{(2)}, 5^{(1)}, 2^{(n-10)}, 1^{(7)})\\
&\quad \cup C^5(8^{(1)}, 6^{(2)}, 2^{(n-9)}, 1^{(6)}) \cup C^5(8^{(1)}, 7^{(1)}, 6^{(1)}, 2^{(n-10)}, 1^{(7)})\\
&\quad \cup C^5(8^{(2)}, 6^{(1)}, 2^{(n-11)}, 1^{(8)}) \cup C^5(8^{(1)}, 7^{(2)}, 2^{(n-11)}, 1^{(8)})\\
&\quad \cup C^5(8^{(2)}, 7^{(1)}, 2^{(n-12)}, 1^{(9)}) \cup C^5(8^{(3)}, 2^{(n-13)}, 1^{(10)}),
\end{aligned}$$

such that $NK(G') \le NK(H) < NK(G)$, which completes the proof of this part.

(4) $\Delta(G') = 7$. Apply Lemma 4.2 to prove that there exists a graph H such that

$$\begin{aligned}
H \in\ &C^5(7^{(1)}, 4^{(1)}, 3^{(2)}, 2^{(n-5)}, 1^{(1)}) \cup C^5(7^{(1)}, 5^{(1)}, 3^{(2)}, 2^{(n-6)}, 1^{(2)})\\
&\cup C^5(7^{(1)}, 6^{(1)}, 3^{(2)}, 2^{(n-7)}, 1^{(3)}) \cup C^5(7^{(2)}, 3^{(2)}, 2^{(n-8)}, 1^{(4)})\\
&\cup C^5(7^{(1)}, 4^{(2)}, 3^{(1)}, 2^{(n-6)}, 1^{(2)}) \cup C^5(7^{(1)}, 5^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-7)}, 1^{(3)})\\
&\cup C^5(7^{(1)}, 6^{(1)}, 4^{(1)}, 3^{(1)}, 2^{(n-8)}, 1^{(4)}) \cup C^5(7^{(2)}, 4^{(1)}, 3^{(1)}, 2^{(n-9)}, 1^{(5)})\\
&\cup C^5(7^{(1)}, 5^{(2)}, 3^{(1)}, 2^{(n-8)}, 1^{(4)}) \cup C^5(7^{(1)}, 6^{(1)}, 5^{(1)}, 3^{(1)}, 2^{(n-9)}, 1^{(5)})\\
&\cup C^5(7^{(2)}, 5^{(1)}, 3^{(1)}, 2^{(n-10)}, 1^{(6)}) \cup C^5(7^{(1)}, 6^{(2)}, 3^{(1)}, 2^{(n-10)}, 1^{(6)})\\
&\cup C^5(7^{(2)}, 6^{(1)}, 3^{(1)}, 2^{(n-11)}, 1^{(7)}) \cup C^5(7^{(3)}, 3^{(1)}, 2^{(n-12)}, 1^{(8)})\\
&\cup C^5(7^{(1)}, 4^{(3)}, 2^{(n-7)}, 1^{(3)}) \cup C^5(7^{(1)}, 5^{(1)}, 4^{(2)}, 2^{(n-8)}, 1^{(4)})\\
&\cup C^5(7^{(1)}, 6^{(1)}, 4^{(2)}, 2^{(n-9)}, 1^{(5)}) \cup C^5(7^{(2)}, 4^{(2)}, 2^{(n-10)}, 1^{(6)})
\end{aligned}$$

$$\cup C^5(7^{(1)},5^{(2)},4^{(1)},2^{(n-9)},1^{(5)}) \cup C^5(7^{(1)},6^{(1)},5^{(1)},4^{(1)},2^{(n-10)},1^{(6)})$$
$$\cup C^5(7^{(2)},5^{(1)},4^{(1)},2^{(n-11)},1^{(7)}) \cup C^5(7^{(1)},6^{(2)},4^{(1)},2^{(n-11)},1^{(7)})$$
$$\cup C^5(7^{(2)},6^{(1)},4^{(1)},2^{(n-12)},1^{(8)}) \cup C^5(7^{(3)},4^{(1)},2^{(n-13)},1^{(9)})$$
$$\cup C^5(7^{(1)},5^{(3)},2^{(n-10)},1^{(6)}) \cup C^5(7^{(1)},6^{(1)},5^{(2)},2^{(n-11)},1^{(7)})$$
$$\cup C^5(7^{(2)},5^{(2)},2^{(n-12)},1^{(8)}) \cup C^5(7^{(1)},6^{(2)},5^{(1)},2^{(n-12)},1^{(8)})$$
$$\cup C^5(7^{(2)},6^{(1)},5^{(1)},2^{(n-13)},1^{(9)}) \cup C^5(7^{(3)},5^{(1)},2^{(n-14)},1^{(10)})$$
$$\cup C^5(7^{(1)},6^{(3)},2^{(n-13)},1^{(9)}) \cup C^5(7^{(2)},6^{(2)},2^{(n-14)},1^{(10)})$$
$$\cup C^5(7^{(3)},6^{(1)},2^{(n-15)},1^{(11)}) \cup C^5(7^{(4)},2^{(n-16)},1^{(12)}),$$

and $NK(G') \leq NK(H) < NK(G)$.

(5) $\Delta(G') = 6$. If $n_6(G') \geq 2$, then the result follows from Lemma 4.2. If $n_6(G') = 1$, then, by Lemma 4.2, there exists a graph H such that

$$H \in C^5(6^{(1)},5^{(1)},3^{(3)},2^{(n-7)},1^{(2)}) \cup C^5(6^{(2)},3^{(3)},2^{(n-8)},1^{(3)})$$
$$\cup C^5(6^{(1)},4^{(2)},3^{(2)},2^{(n-7)},1^{(2)}) \cup C^5(6^{(1)},5^{(1)},4^{(1)},3^{(2)},2^{(n-8)},1^{(3)})$$
$$\cup C^5(6^{(2)},4^{(1)},3^{(2)},2^{(n-9)},1^{(4)}) \cup C^5(6^{(1)},5^{(2)},3^{(2)},2^{(n-9)},1^{(4)})$$
$$\cup C^5(6^{(2)},5^{(1)},3^{(2)},2^{(n-10)},1^{(5)}) \cup C^5(6^{(3)},3^{(2)},2^{(n-11)},1^{(6)})$$
$$\cup C^5(6^{(1)},4^{(3)},3^{(1)},2^{(n-8)},1^{(3)}) \cup C^5(6^{(1)},5^{(1)},4^{(2)},3^{(1)},2^{(n-9)},1^{(4)})$$
$$\cup C^5(6^{(2)},4^{(2)},3^{(1)},2^{(n-10)},1^{(5)}) \cup C^5(6^{(1)},5^{(2)},4^{(1)},3^{(1)},2^{(n-10)},1^{(5)})$$
$$\cup C^5(6^{(2)},5^{(1)},4^{(1)},3^{(1)},2^{(n-11)},1^{(6)}) \cup C^5(6^{(3)},4^{(1)},3^{(1)},2^{(n-12)},1^{(7)})$$
$$\cup C^5(6^{(1)},5^{(3)},3^{(1)},2^{(n-11)},1^{(6)}) \cup C^5(6^{(2)},5^{(2)},3^{(1)},2^{(n-12)},1^{(7)})$$
$$\cup C^5(6^{(3)},5^{(1)},3^{(1)},2^{(n-13)},1^{(8)}) \cup C^5(6^{(4)},3^{(1)},2^{(n-14)},1^{(9)})$$
$$\cup C^5(6^{(1)},4^{(4)},2^{(n-9)},1^{(4)}) \cup C^5(6^{(1)},5^{(1)},4^{(3)},2^{(n-10)},1^{(5)})$$
$$\cup C^5(6^{(2)},4^{(3)},2^{(n-11)},1^{(6)}) \cup C^5(6^{(1)},5^{(2)},4^{(2)},2^{(n-11)},1^{(6)})$$
$$\cup C^5(6^{(2)},5^{(1)},4^{(2)},2^{(n-12)},1^{(7)}) \cup C^5(6^{(3)},4^{(2)},2^{(n-13)},1^{(8)})$$
$$\cup C^5(6^{(1)},5^{(3)},4^{(1)},2^{(n-12)},1^{(7)}) \cup C^5(6^{(2)},5^{(2)},4^{(1)},2^{(n-13)},1^{(8)})$$
$$\cup C^5(6^{(3)},5^{(1)},4^{(1)},2^{(n-14)},1^{(9)}) \cup C^5(6^{(4)},4^{(1)},2^{(n-15)},1^{(10)})$$
$$\cup C^5(6^{(1)},5^{(4)},2^{(n-13)},1^{(8)}) \cup C^5(6^{(2)},5^{(3)},2^{(n-14)},1^{(9)})$$
$$\cup C^5(6^{(3)},5^{(2)},2^{(n-15)},1^{(10)}) \cup C^5(6^{(4)},5^{(1)},2^{(n-16)},1^{(11)})$$
$$\cup C^5(6^{(5)},2^{(n-17)},1^{(12)}),$$

and $NK(G') \leq NK(H) < NK(G)$. This completes the proof. □

TABLE 3. The pentacyclic graphs.

Classes	NK Index
$C^5(3^{(8)}, 2^{(n-8)})$	$3^8 \times 2^{(n-8)}$
$C^5(3^{(9)}, 2^{(n-10)}, 1^{(1)})$	$3^9 \times 2^{(n-10)}$
$C^5(3^{(10)}, 2^{(n-12)}, 1^{(2)})$	$3^{10} \times 2^{(n-12)}$
$C^5(3^{(11)}, 2^{(n-14)}, 1^{(3)})$	$3^{11} \times 2^{(n-14)}$
$C^5(4^{(1)}, 3^{(6)}, 2^{(n-7)})$	$4 \times 3^6 \times 2^{(n-7)}$
$C^5(4^{(1)}, 3^{(7)}, 2^{(n-9)}, 1^{(1)})$	$4 \times 3^7 \times 2^{(n-9)}$
$C^5(4^{(1)}, 3^{(8)}, 2^{(n-11)}, 1^{(2)})$	$4 \times 3^8 \times 2^{(n-11)}$
$C^5(4^{(2)}, 3^{(4)}, 2^{(n-6)})$	$4^2 \times 3^4 \times 2^{(n-6)}$
$C^5(4^{(2)}, 3^{(5)}, 2^{(n-8)}, 1^{(1)})$	$4^2 \times 3^5 \times 2^{(n-8)}$
$C^5(4^{(2)}, 3^{(6)}, 2^{(n-10)}, 1^{(2)})$	$4^2 \times 3^6 \times 2^{(n-10)}$
$C^5(4^{(3)}, 3^{(2)}, 2^{(n-5)})$	$4^3 \times 3^2 \times 2^{(n-5)}$
$C^5(4^{(4)}, 2^{(n-4)})$	$4^4 \times 2^{(n-4)}$
$C^5(4^{(3)}, 3^{(3)}, 2^{(n-7)}, 1^{(1)})$	$4^3 \times 3^3 \times 2^{(n-7)}$
$C^5(5^{(1)}, 3^{(5)}, 2^{(n-6)})$	$5 \times 3^5 \times 2^{(n-6)}$
$C^5(5^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-5)})$	$5 \times 4 \times 3^3 \times 2^{(n-5)}$
$C^5(5^{(1)}, 3^{(6)}, 2^{(n-8)}, 1^{(1)})$	$5 \times 3^6 \times 2^{(n-8)}$
$C^5(5^{(2)}, 3^{(2)}, 2^{(n-4)})$	$5^2 \times 3^2 \times 2^{(n-4)}$
$C^5(5^{(2)}, 4^{(1)}, 2^{(n-3)})$	$5^2 \times 4 \times 2^{(n-3)}$
$C^5(5^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$	$5^2 \times 3^3 \times 2^{(n-6)}$
$C^5(6^{(2)}, 2^{(n-2)})$	$6^2 \times 2^{(n-2)}$
$C^5(8^{(1)}, 3^{(2)}, 2^{(n-3)})$	$8 \times 3^2 \times 2^{(n-3)}$
$C^5(7^{(1)}, 3^{(3)}, 2^{(n-4)})$	$7 \times 3^3 \times 2^{(n-4)}$
$C^5(6^{(1)}, 3^{(4)}, 2^{(n-5)})$	$6 \times 3^4 \times 2^{(n-5)}$
$C^5(6^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$	$6 \times 4 \times 3^3 \times 2^{(n-6)}$

Suppose $n \geq 14$ and choose the graphs $F_1, \ldots, F_{24}$ such that

$F_1 \in C^5(3^{(8)}, 2^{(n-8)})$, $F_2 \in C^5(4^{(1)}, 3^{(6)}, 2^{(n-7)})$,
$F_3 \in C^5(4^{(2)}, 3^{(4)}, 2^{(n-6)})$, $F_4 \in C^5(3^{(9)}, 2^{(n-10)}, 1^{(1)})$,
$F_5 \in C^5(5^{(1)}, 3^{(5)}, 2^{(n-6)})$, $F_6 \in C^5(4^{(3)}, 3^{(2)}, 2^{(n-5)})$,
$F_7 \in C^5(4^{(1)}, 3^{(7)}, 2^{(n-9)}, 1^{(1)})$, $F_8 \in C^5(5^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-5)})$,
$F_9 \in C^5(4^{(4)}, 2^{(n-4)})$, $F_{10} \in C^5(4^{(2)}, 3^{(5)}, 2^{(n-8)}, 1^{(1)})$,
$F_{11} \in C^5(6^{(1)}, 3^{(4)}, 2^{(n-5)})$, $F_{12} \in C^5(3^{(10)}, 2^{(n-12)}, 1^{(2)})$,
$F_{13} \in C^5(5^{(1)}, 3^{(6)}, 2^{(n-8)}, 1^{(1)})$, $F_{14} \in C^5(3^{(11)}, 2^{(n-14)}, 1^{(3)})$,
$F_{15} \in C^5(4^{(1)}, 3^{(8)}, 2^{(n-11)}, 1^{(2)})$, $F_{16} \in C^5(4^{(2)}, 3^{(6)}, 2^{(n-10)}, 1^{(2)})$,
$F_{17} \in C^5(4^{(3)}, 3^{(3)}, 2^{(n-7)}, 1^{(1)})$, $F_{18} \in C^5(5^{(2)}, 3^{(2)}, 2^{(n-4)})$,
$F_{19} \in C^5(5^{(2)}, 4^{(1)}, 2^{(n-3)})$, $F_{20} \in C^5(5^{(2)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$,

$F_{21} \in C^5(6^{(2)}, 2^{(n-2)})$, $F_{22} \in C^5(8^{(1)}, 3^{(2)}, 2^{(n-3)})$,
$F_{23} \in C^5(7^{(1)}, 3^{(3)}, 2^{(n-4)})$, $F_{24} \in C^5(6^{(1)}, 4^{(1)}, 3^{(3)}, 2^{(n-6)}, 1^{(1)})$.

Theorem 4.2. *Let F be a pentacyclic graph with $n \geq 12$ vertices, except from the graphs $F_1, F_2, \ldots, F_{13}$. Then, $NK(F_1) > NK(F_2) > NK(F_3) > NK(F_4) > NK(F_5) > NK(F_6) > NK(F_7) > NK(F_8) > NK(F_9) > NK(F_{10}) = NK(F_{11}) > NK(F_{12}) > NK(F_{13}) > NK(F)$.*

Proof. From Table 3, $NK(F_1) > NK(F_2) > NK(F_3) > NK(F_4) > NK(F_5) > NK(F_6) > NK(F_7) > NK(F_8) > NK(F_9) > NK(F_{10}) = NK(F_{11}) > NK(F_{12}) > NK(F_{13})$. If $F \in \{F_{14}, \ldots, F_{24}\}$, then Table 3 gives us the result. If $\Delta(F) = 3$ and $n_3(F) \geq 12$, then the result follows from Corollary 4.1. Suppose that $\Delta(F) = 4$. If $n_4(F) = 1$ and $n_3(F) \geq 9$, then Corollary 4.2 gives us the result. If $n_4(F) = 2$ and $n_3(F) \geq 7$, then the result is a consequence of Corollary 4.3. If $n_4(F) \geq 3$, then it is enough to apply Lemma 4.3. Suppose that $\Delta(F) = 5$. If $n_5(F) = 1$, then Lemma 4.4 proves the result, and if $n_5(F) \geq 2$, then we apply Lemma 4.5. If $\Delta(F) \geq 6$, then the result follows from Theorem 4.1. In other cases, F is a member of the set $\{F_1, F_2, \ldots, F_{13}\}$, which completes the proof. □

5. Concluding remarks

In this paper, the Narumi–Katayama index of simple graphs was considered. We determined eight classes of n-vertex tricyclic graphs with the first through the eighth maximal NK index, $n \geq 10$, ten classes of n-vertex tetracyclic graphs with the first through the ninth maximal NK index, $n \geq 10$, and thirteen classes of n-vertex pentacyclic graphs with the first through the twelfth maximal NK index, $n \geq 12$.

Let d_1, d_2, $\ldots$, d_n be the vertex degree sequence of an n-vertex simple graph G. The following inequality (for any n positive numbers) is known:

$$\frac{1}{n}\sum_{j=1}^{n} d_j \geq \Big(\prod_{j=1}^{n} d_i\Big)^{\frac{1}{n}} = [NK(G)]^{\frac{1}{n}}.$$

The equality holds if and only if $d_1 = d_2 = \ldots = d_n$, that is, when G is a regular graph. Hence, one can derive another index, evaluating the degree of regularity of an arbitrary simple graph:

$$reg(G) := \frac{n^n NK(G)}{(2m)^n} \leq 1.$$

Since for two simple graphs G_1 and G_2, with the same values of n and m, we have $reg(G_1) \geq reg(G_2)$ if and only if $NK(G_1) \geq NK(G_2)$, the $NK(G)$ can itself evaluate the regularity of G. The "regularity" is the antipode of "irregularity", which, in our terms, can be determined as

$$irr(G) := 1 - reg(G). \tag{5}$$

In the literature, also other irregularity indices are known, where $irr(G)$ denotes some other parameter than (5). Disregarding what $irr(G)$ may precisely mean in [1, 2, 3, 6], the role of the irregularity of a graph G (which may also apply to $NK(G)$!) is by now a subject seriously studied in the literature. In particular [1], its relation to the spectra of graphs has been studied, and so on. Thus, it is a good research problem for future to obtain this relationship.

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