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Extremal Properties of Narumi−Katayama Index of Chemical Trees

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ABSTRACT. The Narumi−Katayama index was the first topological index defined by the product of some graph theoretical quantities. It is defined as the product of deg(v) over all vertices of the graph under consideration. In this paper, the problem of computing k^{th} minimal and maximal, $1 \leq k \leq 4$, Narumi-Katayama index are considered into account. The four maximum and minimum values of these topological index were computed. This generalizes some results by Gutman and Ghorbani [10].

INTRODUCTION

Throughout this paper, all graphs under consideration will be finite, undirected, and loopless. Suppose T is such a graph with $V(T) = \{v_1, v_2, ..., v_n\}$. We denote the degree sequence of T by $d_1, d_2, \ ,d_n$, where $d_i = deg_T(v_i)$, $1 \leq i \leq n$. In this work we focus on chemical trees, the trees in which each vertex has degree at most 4. A chemical graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds.

A topological index is a number invariant under automorphisms of the graph under consideration. The Narumi−Katayama index (NK index) was the first topological index defined by the product of some graph theoretical quantities [1, 2]. It is defined as the product of d(v) over all degrees of vertices in G. In [3, 4], the authors investigated some properties of this topological index, but the main mathematical properties of NK index was reported by Klein and Rosenfeld [5]. This paper makes a new start on research about mathematical properties and chemical meaning of NK index. We encourage the interested readers to consult [6−11] and references therein for computational techniques as well as mathematical properties of this topological index.

In this paper the problem of computing k^{th}, $1 \leq k \leq 4$, minimal and maximal values of Narumi−Katayama index will be considered into account. Our notation is standard and taken from the famous book of West [12].

MAIN RESULTS

The aim of this section is to determine the first, second, third and forth maxiaml and minimal values of Narumi-Katayama index in the class of chemical trees. Gutman and Ghorbani [4] computed the first and second Narumi−Katayama index of trees. We also extend these results and calculate the third and forth maximal and minimal values of this topological index in the class of all trees. Throughout this section, for simplicity of our argument we denote $deg_G(u)$ by $d(u)$ and T_n denotes a tree or chemical tree..

Lemma 1. Let T_n be an n–vertex tree or chemical tree and T_n' is another n–vertex tree obtained from T_n by deleting a pendant vertex and appending a vertex to another pendant vertex of T_n. Then $\mathrm{NK}(T_n') \le \mathrm{NK}(T_n)$.

Proof. Suppose uv is a pendant edge of T_n, $deg(v) = 1$, $deg(u) \ge 2$ and w is a pendant vertex of T_n such that T_n' is obtained by deleting uv and appending it to w. Then $\deg_{T_n}(w) = 1 = \deg_{T_n'}(w) - 1$, $\deg_{T_n}(u) = \deg_{T_n'}(u) + 1$ and for another vertex x different from u and w, $\deg_{T_n}(x) = \deg_{T_n'}(x)$. On the other hand,

$$NK(T_n) = \prod_{x \in V(T_n)} d_{T_n}(x) = \prod_{x \neq u,w} d_{T_n}(x) \times d_{T_n}(u) \times d_{T_n}(w) = \prod_{x \neq u,w} d_{T_n}(x) \times d_{T_n}(u) \times 1,$$

$$NK(T_n') = \prod_{x \in V(T_n')} d_{T_n'}(x) = \prod_{x \neq u,w} d_{T_n'}(x) \times d_{T_n'}(u) \times d_{T_n'}(w)$$

$$= \prod_{x \neq u,w} d_{T_n}(x) \times (d_{T_n}(u) - 1) \times 2,$$

and $d(u) \le (d(u) - 1) \times 2$ if and only if $\frac{1}{2} \le 1 - \frac{1}{d(u)}$. But $d(u) \ge 2$, proving the lemma.

◄

Lemma 2. Let T be an n–vertex tree or chemical tree. Then $NK(T) \le 2^{n-2}$ with equality if and only if T is a path of length n. The second–maximal NK index is $3.\ 2^{n-4}$ and the second maximal is attained if and only if T is isomorphic to P_n^*, where P_n^* is a tree with exactly three pendant vertices. ◄

Lemma 3. Let T_n be an n–vertex tree or chemical tree containing vertices u, z such that $d_T(u) = 2$ and $d_T(z) = 2$ or 3. Suppose T_1 and T_2 are maximal subtrees of T_n containing u as a pendant vertex and $z \in V(T_2)$, Figures 1 and 2. If T_n^* is the chemical tree constructed from T_1 and T_2 by identifying u and z then $\mathrm{NK}(T_n) \ge \mathrm{NK}(T_n^*)$.

Proof. It is easy to see that $d_{T_n}(u) = 2$, $d_{T_n'}(u) = 1$, $d_{T_n'}(z) = d_{T_n}(z) + 1$ and for another arbitrary vertex x, $d_{T_n}(x) = d_{T_n'}(x)$.

Figure 1. The Chemical Tree T_n Containing a Subtree T_1.

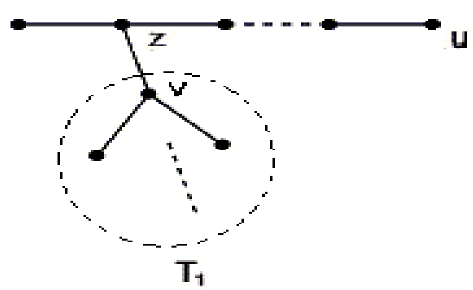


Figure 2. The Chemical Tree T_n^* Constructed from T_1 and T_2.

Therefore, $NK(T_n) = \prod_{x \in V(T_n)} d_{T_n}(x) = \prod_{x \neq u,z} d_{T_n}(x) \times d_{T_n}(u) \times d_{T_n}(z) = \prod_{x \neq u,z} d_{T_n}(x) \times d_{T_n}(z) \times 2$

and $NK(T_n^*) = \prod_{x \in V(T_n^*)} d_{T_n^*}(x) = \prod_{x \neq u,z} d_{T_n^*}(x) \times d_{T_n^*}(u) \times d_{T_n^*}(z)$

$= \prod_{x \neq u,z} d_{T_n}(x) \times (d_{T_n}(z)+1) \times 1$. On the other hand, $d(z) \times 2 > d(z)+1$ if and only if $2 > 1 + \frac{1}{d(z)}$. Since $d(z) \geq 2$, the last inequality is satisfied, proving the lemma. ◄

Lemma 4. Let T_n be an n−vertex tree or chemical tree containing vertices u and z of degree 3. We also assume that T_1, T_2 and T_3 are maximal subtrees of T_n with u as a pendant and $z \in T_3$. If T_n'' is the chemical tree constructed from T_1 and T_2 by identifying u and z then $NK(T_n) \geq NK(T_n'')$.

Proof. By our assumption $d_{T_n}(u) = 3, d_{T_n''}(u) = 2$ and $d_{T_n}(z) = 3, d_{T_n''}(u) = 4$. The degree of remaining vertices will not change. Thus,

$$NK(T_n) = \prod_{x \in V(T_n)} d_{T_n}(x) = \prod_{x \neq u,z} d_{T_n}(x) \times d_{T_n}(u) \times d_{T_n}(z) = \prod_{x \neq u,z} d_{T_n}(x) \times 3 \times 3,$$

$$NK(T_n') = \prod_{x \in V(T_n^*)} d_{T_n'}(x) = \prod_{x \neq u,z} d_{T_n'}(x) \times d_{T_n'}(u) \times d_{T_n'}(z) = \prod_{x \neq u,z} d_{T_n}(x) \times 4 \times 2.$$

which implies that $NK(T_n) \geq NK(T_n^*)$. ◄

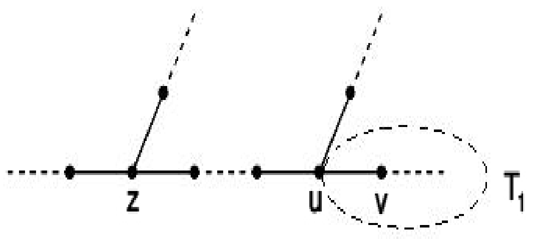


Figure 3. The Chemical Tree T_n.

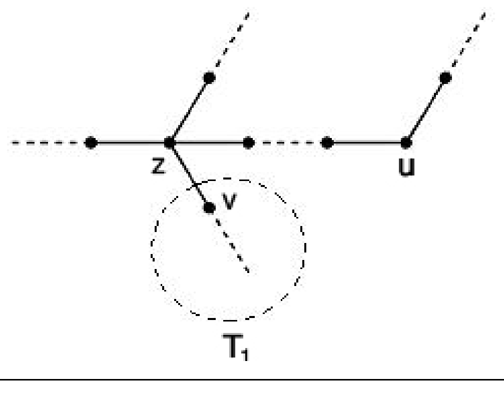


Figure 4. The Chemical Tree T_n'' Constructed from T_n.

Lemma 5. Suppose T_n and F_n are n−vertex trees (chemical trees) with r and s leaves, respectively. If $r < s$ then $NK(T_n) > NK(F_n)$. If $r = s$ and $\Delta(T_n) < \Delta(F_n)$ then $NK(T_n) > NK(F_n)$.

By Lemmas 1−5 and case by case investigation on trees and chemical trees, one can compute the first four maximum and minimum values of NK index in the classes of trees and chemical trees. Our main results are collected in the following tables:

Table 1: The first, second, third and forth Maximum of NK Index in Trees and Chemical Trees.

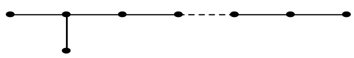
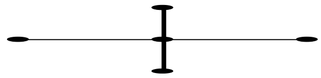
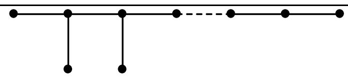
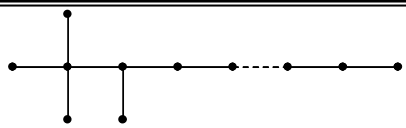
k	|V(G)|	NK Index	Trees and Chemical Trees with k^th^ Maximum NK Index.
k = 1	n = 1	0	·
k = 1	n ≥ 2	$2^{(n-2)}$	P_n
k = 2	n ≥ 4	$3 \times 2^{(n-4)}$	
k = 3	n = 5	4	
k = 3	n ≥ 6	$3^2 \times 2^{(n-6)}$	
k = 4	n ≥ 6	$2^{(n-3)}$	

Table 2: The First, Second, Third and Forth Minimum of NK Index in Trees.

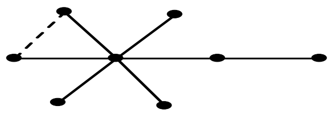
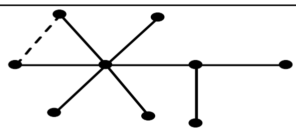
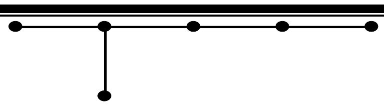
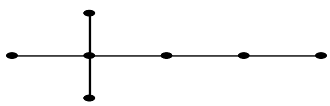
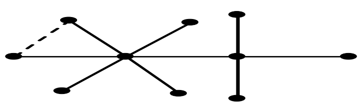
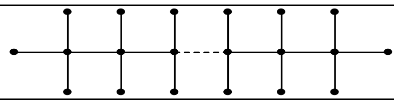
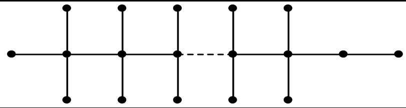
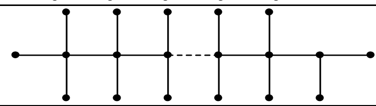
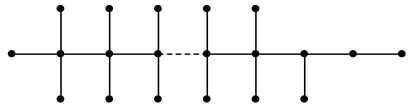
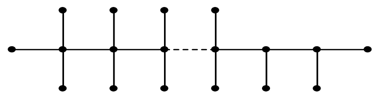
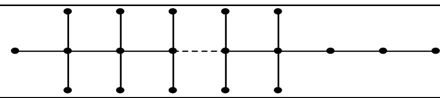
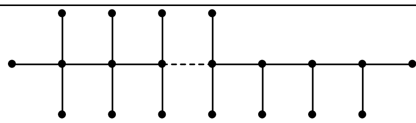
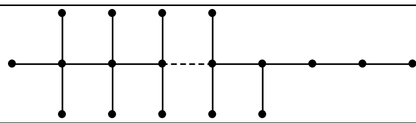
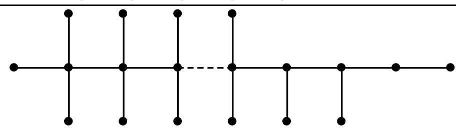
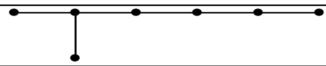
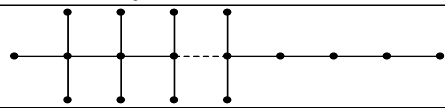
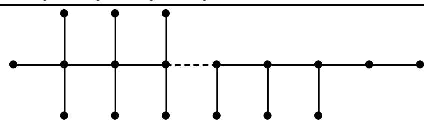
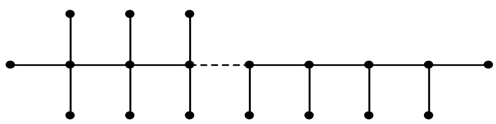
k	|V(G)|	NK Index	The k^th^ Minimumof NK Index in Trees
k = 1	n = 1	0	·
k = 1	n ≥ 2	n–1	S_n
k = 2	n ≥ 4	2(n–2)	
k = 3	n = 5	8	
k = 3	n ≥ 6	3(n–3)	
k = 4	n = 6	12	
k = 4	n = 7	16	
k = 4	n ≥ 8	4(n–4)	

Table 3: The First, Second, Third and Forth Minimum of NK Index in Chemical Trees.

k	#Vertices	NK Index	The kth Minimumof NK Index in Chemical Trees
k = 1	n = 3m+2 , m ≥ 0	4^m	
k = 1	n = 3m+3 , m ≥ 0	$2^{(2m+1)}$	
k = 1	n = 3m+1 , m ≥ 1	$3 \times 4^{(m-1)}$	
k = 2	n = 3m+2 , m ≥ 1	$3 \times 2^{(2m-1)}$	
k = 2	n = 3m+3 , m ≥ 1	$9 \times 4^{(m-1)}$	
k = 2	n = 3m+1 , m ≥ 1	4^m	
k = 3	n = 5	8	
k = 3	n = 3m+2 , m ≥ 2	$27 \times 4^{(m-2)}$	
k = 3	n = 3m+3 , m ≥ 1	3×4^m	
k = 3	n = 3m+1 , m ≥ 2	$9\times 2^{(2m-3)}$	
k = 4	n = 6	16	
k = 4	n = 7	24	
k = 4	n = 3m+2 , m ≥ 2	$2^{(2m+1)}$	
k = 4	n = 3m+3 , m ≥ 2	$27 \times 2^{(2m-3)}$	
k = 4	n = 3m+1 , m ≥ 3	$81 \times 4^{(m-3)}$	

Acknowledgement

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