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MODIFIED NARUMI–KATAYAMA INDEX

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ABSTRACT. The Narumi–Katayama index of a graph G is equal to the product of the degrees of the vertices of G. In this paper we consider a new version of the Narumi–Katayama index in which each vertex degree d is multiplied d times. We characterize the graphs extremal w.r.t. this new topological index.

1 Introduction

A topological index is a graph invariant used in structure–property correlations. Hundreds of topological indices have been introduced and studied [1], starting with the seminal work by Wiener in which he used the sum of all shortest–path distances of a (molecular) graph for modeling physical properties of alkanes [2]. The aim of this paper is to put forward a new variant of the Narumi–Katayama index. We determine its basic properties and characterize graphs extremal with respect to it.

2 Definitions and preliminaries

Our notation is standard and mainly taken from standard books of graph theory such as, e. g., [3]. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The number of vertices of G is denoted by n.

The degree d_v of a vertex $v \in V(G)$ is the number of vertices of G adjacent to v. A vertex $v \in V(G)$ is said to be isolated, pendent, or fully connected if $d_v = 0$, $d_v = 1$, or $d_v = n-1$, respectively. The n-vertex graph in which all vertices are fully connected is the complete graph K_n. The n-vertex graph with a single fully connected vertex and $n-1$ pendent vertices is the star S_n. The connected n-vertex graph with two pendent vertices and $n-2$ vertices of degree 2 is the path P_n. The connected n-vertex graph whose all vertices are of degree 2 is the cycle C_n [3].

In the 1980s, Narumi and Katayama considered the product

$$NK = NK(G) = \prod_{u \in V(G)} d_u$$

and named it "*simple topological index*" [4]. Eventually this molecular structure–descriptor was re-named as "*Narumi–Katayama index*" [5]. The properties of NK were much investigated, see [4–11].

We now propose a modified version of the Narumi–Katayama index as follows:

$$NK^* = NK^*(G) = \prod_{u \in V(G)} d_u^{d_u} .$$

3 Main Results

In this section we present the value of NK^* for several classes of graphs.

Example 1. Let S_n be the star graph on n vertices. Its central vertex has degree $n-1$ and its other vertices are pendent. This implies

$$NK^*(S_n) = (n-1)^{n-1} .$$

Example 2. Let K_n be the complete graph on n vertices. All vertices of K_n have degree $n-1$ and so $NK^*(K_n) = (n-1)^{n(n-1)}$.

Example 3. Let P_n be the path with n vertices. The pendent vertices have degree 1 and other vertices have degree two. Hence,

$$NK^*(P_n) = 2^{2(n-2)} = 4^{n-2} \ .$$

Example 4. Consider the cycle C_n with n vertices. Since its every vertex is of degree 2, then

$$NK^*(C_n) = 2^{2n} = 4^n \ .$$

Theorem 5. Let G be an arbitrary n-vertex graph. Then

$$NK^*(G) \leq NK^*(K_n)$$

with equality if and only if $G \cong K_n$.

Theorem 6.

$$NK^*(G) = \prod_{uv \in E(G)} d_u \, d_v \ .$$

Proof. For every vertex $u \in V(G)$, d_u appears d_u times in the product $\prod_{uv \in E(G)} d_u \, d_v$.

■

Theorem 7.

(a) The n-vertex tree with maximal modified Narumi–Katayama index is the star S_n . Thus, $NK^*(T) < (n-1)^{n-1}$ for any n-vertex tree T different from S_n .

(b) The n-vertex connected unicyclic graph with maximal Narumi–Katayama index is $S_n + e$, depicted in Fig. 1; $NK^*(S_n + e) = 16\,(n-1)^{n-1}$. Thus, $NK^*(U) < 16\,(n-1)^{n-1}$ for any n-vertex connected unicyclic graph U different from $S_n + e$.

(c) Among all connected bicyclic graphs on n vertices, the graph $S_n + e + e'$, depicted in Fig. 2, has the maximal modified Narumi–Katayama index; $NK^*(S_n + e + e') = 256\,(n-1)^{n-1}$. Thus, $NK^*(B) < 256\,(n-1)^{n-1}$ for any n-vertex connected bicyclic graph B different from $S_n + e + e'$.

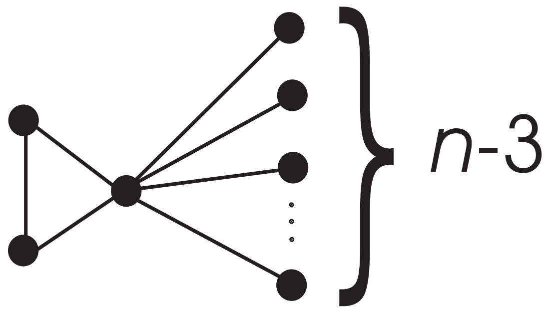

Fig. 1. The unicyclic graph $S_n + e$ with maximal NK^*-value.

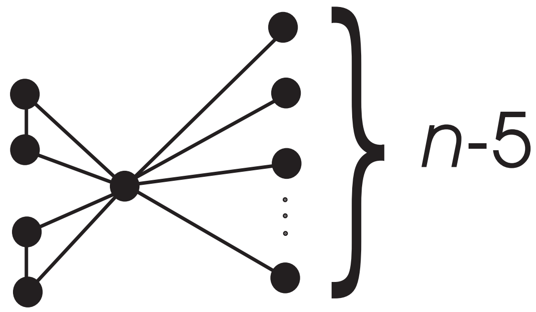

Fig. 2. The bicyclic graph $S_n + e + e'$ with maximal NK^*-value.

Theorem 8.

(a) The n-vertex tree with minimal modified Narumi–Katayama index is the path P_n. Thus, $NK^*(T) > 4^{n-2}$ for any n-vertex tree T different from P_n.

(b) The n-vertex connected unicyclic graph with minimal Narumi–Katayama index is the cycle C_n. Thus, $NK^*(U) > 4^n$ for any connected n-vertex unicyclic graph U different from C_n.

(c) Among all connected bicyclic graphs on n vertices, the graphs B_{min} whose structure is indicated in Fig. 3, have minimal modified Narumi–Katayama index; $NK^*(B_{min}) = 2^{2n+6}$. Thus, $NK^*(B) > 2^{2n+6}$ for any connected n-vertex bicyclic graph B whose structure is different from B_{min}.

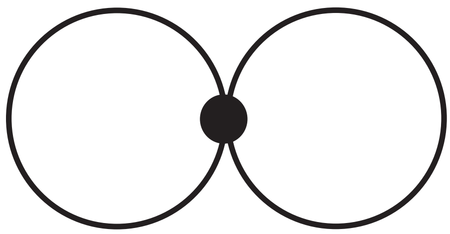

Fig. 3. The bicyclic graph B_{min} with minimal NK^*-value. Recall that there exist $\lfloor (n-3)/2 \rfloor$ distinct n-vertex bicyclic graphs of the type B_{min}.

Theorem 9.

(a) The n-vertex tree with second–maximal modified Narumi–Katayama index is the graph S_n', depicted in Fig. 4; $NK^*(S_n') = 4(n-2)^{n-2}$. Thus, $NK^*(T) < 4(n-2)^{n-2}$ for any n-vertex tree T different from S_n and S_n'.

(b) The n-vertex connected unicyclic graph with second–maximal modified Narumi–Katayama index is the graph K_n, depicted in Fig. 5; $NK^*(K_n) = 64\,(n-2)^{n-2}$. Thus, $NK^*(U) < 64\,(n-2)^{n-2}$ for any connected n-vertex unicyclic graph U different from $S_n + e$ and K_n.

(c) Among all connected bicyclic graphs on n vertices, the graph F_n, depicted in Fig. 6, has the second–maximal modified Narumi–Katayama index; $NK^*(F_n) = 2^{10}\,(n-2)^{n-2}$. Thus, $NK^*(B) < 2^{10}\,(n-2)^{n-2}$ for any connected n-vertex bicyclic graph B different from $S_n + e + e'$ and K_n.

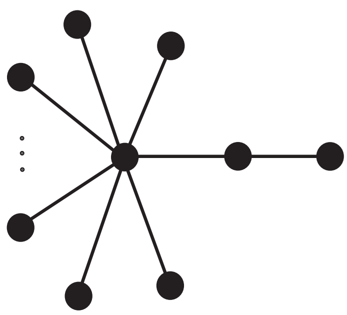

Fig. 4. The tree S_n' with second–maximal NK^*-value.

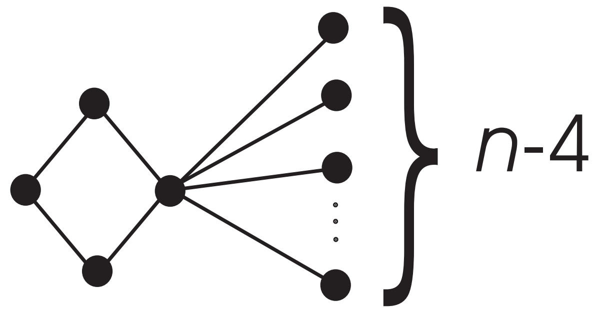

Fig. 5. The unicyclic graph K_n with second–maximal NK^*-value.

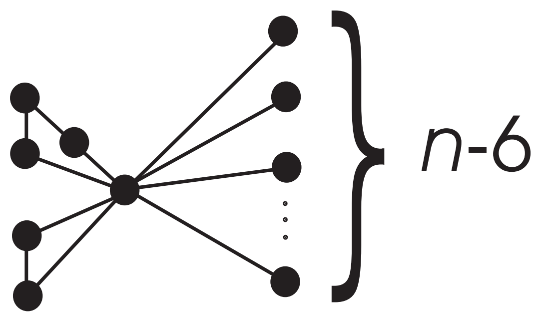

Fig. 6. The bicyclic graph F_n with second–maximal NK^*-value.

Theorem 10.

(a) The n-vertex tree with second–minimal modified Narumi–Katayama index is one of the trees $T_{a,b,c}$, depicted in Fig. 7, where $a,b,c \geq 1$ and $a+b+c=n-1$; $NK^*(T_{a,b,c}) = 27 \cdot 4^{n-4}$. Thus, $NK^*(T) > 27 \cdot 4^{n-4}$ for any n-vertex tree T different from P_n and $T_{a,b,c}$.

(b) The n-vertex connected unicyclic graph with second–minimal modified Narumi–Katayama index is the graph R_n, depicted in Fig. 8; $NK^*(R_n) = 27 \cdot 4^{n-2}$. Thus, $NK^*(T) > 27 \cdot 4^{n-2}$ for any n-vertex connected unicyclic graph U different from C_n and R_n.

(c) Among all connected bicyclic graphs on n vertices, the graphs B'_{min}, whose structure is indicated in Fig. 9 have second–minimal modified Narumi–Katayama index; $NK^*(B'_{min}) = 3^6 \cdot 4^{n-2}$. Thus, $NK^*(B) > 3^6 \cdot 4^{n-2}$ for any connected n-vertex bicyclic graph B whose structure is different from B_{min} and B'_{min}.

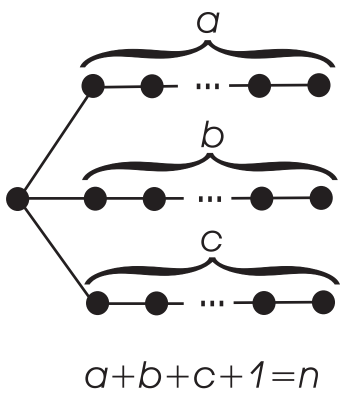

Fig. 7. The tree $T_{a,b,c}$ with second–minimal NK^*-value.

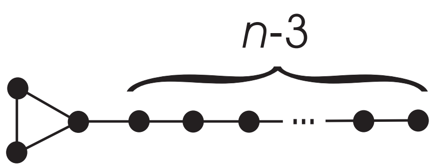

Fig. 8. The unicyclic graph R_n with second–minimal NK^*-value.

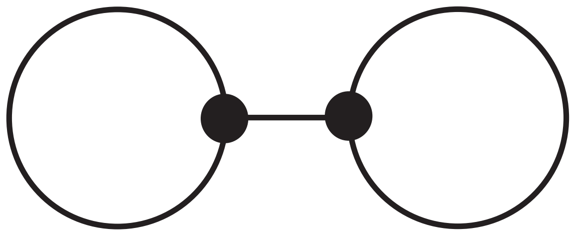

Fig. 9. The bicyclic graph B'_{min} with second–minimal NK^*-value. Recall that there exist $\lfloor (n-4)/2 \rfloor$ distinct n-vertex bicyclic graphs of the type B'_{min}.

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