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On the Extremal Narumi-Katayama Index of Graphs

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Abstract. The Narumi-Katayama index of a graph G, denoted by $NK(G)$, is defined as $\prod_{i=1}^{n} deg(v_i)$. In this paper, we determine the extremal $NK(G)$ of trees, unicyclic graphs with given diameter and vertices. Moreover, the second and third minimal $NK(G)$ of unicyclic graphs with given vertices and the minimal $NK(G)$ of bicyclic graphs with given vertices are obtained.

1. Introduction

Let G be a simple graph with the vertex set $V(G)$ and edge set $E(G)$. A connected graph G with n vertices is a tree (unicyclic or bicyclic graph) if $|E(G)| = n - 1$ ($|E(G)| = n$ or $|E(G)| = n + 1$). Denote by $deg(v_i)$ or d_i the degree of vertex v_i. The distance between two vertices is defined as the length of a shortest path between them. The diameter of G is the maximum distance over all pairs of vertices u and v of G. In 1984, Narumi and Katayama [1] proposed a definition "simple topological index":

$$NK(G) = \prod_{i=1}^{n} deg(v_i).$$

On this graph invariant, several works [2,3,4,5,6] are reported and the name "Narumi-Katayama index" is used.

In [6], I. Gutman et al. considered the problem of extremal Narumi-Katayama index and offered a few results filling the gap. For graphs without isolated vertices, I. Gutman et al. [6] presented the minimal, second-minimal and third-minimal (maximal, second-maximal, and third-maximal, resp.) NK-values and extremal graphs. Moreover, the maximal (second-maximal) Narumi-Katayama index of n-vertex tree (unicyclic graph) is determined [6]. And the maximal Narumi-Katayama index of n-vertex bicyclic graphs is given. For connected n-vertex graphs, the minimal and second minimal Narumi-Katayama index are showed [6]. Consequently, the second-minimal Narumi-Katayama index among n-vertex trees and the minimal Narumi-Katayama index among n-vertex unicyclic graphs are presented [6].

In this paper, we determine the extremal $NK(G)$ of trees, unicyclic graphs with given diameter and vertices. Moreover, the second and third minimal $NK(G)$ of unicyclic graphs with given vertices and the minimal $NK(G)$ of bicyclic graphs with given vertices are obtained.

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2. The minimal Narumi-Katayama index of trees and unicyclic graphs with given diameter

Lemma 2.1 *Operation A: For an edge uv of Graph G, let u be a vertex with all adjacency vertices are pendent vertices except a vertex v. If all pendent edges incident with u are grafted to v, then the resulting graph* G^* *(Fig. 1) satisfies* $NK(G) > NK(G^*)$.

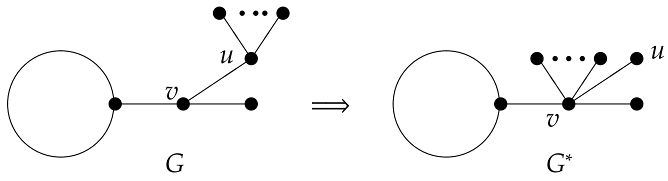

Figure 1: Operation A

Proof. By the definition of NK-index,

$$NK(G) - NK(G^*) = \prod_{v_i \in V(G)\setminus\{u,v\}} deg(v_i) \cdot [deg_G(u) \cdot deg_G(v) - 1 \cdot (deg_G(u) + deg_G(v) - 1)]$$
$$= \prod_{v_i \in V(G)\setminus\{u,v\}} deg(v_i) \cdot (deg_G(u) - 1) \cdot (deg_G(v) - 1) > 0.$$

Hence the result holds. □

Lemma 2.2 *Operation B: Let G be a connected graph. For a cut vertex v of G (we say v is an root of G), if* T_1 *is a tree branch of G including v (see Fig. 2), we transform* T_1 *to the star with same order* $S_{|T_1|}$ *and obtain* G^**, then* $NK(G) \geq NK(G^*)$*, with the equality holds if and only if* $T_1 \cong S_{|T_1|}$.

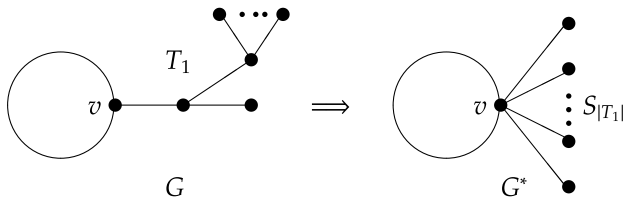

Figure 2: Operation B

Proof. T_1 is a tree including vertex v. By the definition of NK-index and repeating the operation in Lemma 2.1,

$$NK(G) = \prod_{v_i \in V(G)\setminus T_1} deg(v_i) \cdot \prod_{v_i \in T_1} deg(v_i) \geq \prod_{v_i \in V(G)\setminus T_1} deg(v_i) \cdot \prod_{v_i \in S_{|T_1|}} deg(v_i) = NK(G^*).$$

Obviously, the equality holds if and only if $T_1 \cong S_{|T_1|}$. □

Lemma 2.3 *Operation C: Let* S_{k+1} *and* S_{l+1} *be two stars rooted in u and v, respectively. If all edges incident to v are grafted to u with* $d(u) \geq d(v)$*, denoted by the resulting graph* G^* *(Fig. 3), then* $NK(G) > NK(G^*)$.

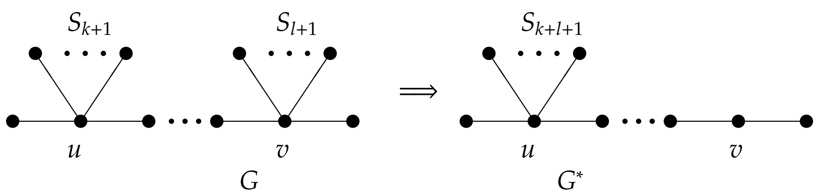

Figure 3: Operation C

Proof. By the definition of NK-index, then

$$NK(G) - NK(G^*) = \prod_{v_i \in V(G)\setminus\{u,v\}} deg(v_i) \cdot [deg_G(u) \cdot deg_G(v) - (deg_G(u) + l) \cdot (deg_G(v) - l)]$$
$$= \prod_{v_i \in V(G)\setminus\{u,v\}} deg(v_i) \cdot l \cdot [deg_G(u) - deg_G(v) + l].$$

Since $deg_G(u) \geq deg_G(v)$ and $l \geq 1$, $NK(G) - NK(G^*) > 0$.
Hence the result follows. □

Theorem 2.4 *Let T be a tree with given diameter d and n vertices. Then $NK(T) \geq NK(T_1^*)$, where $T_1^* \in \mathcal{T}_d^{1,*}$ and $\mathcal{T}_d^{1,*}$ (Fig. 4) is the set of trees with given diameter d and S_{n-d} rooted in the diametral path excepting the two end vertices.*

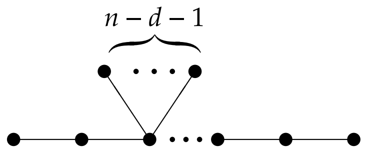

Figure 4: A tree T_1^* in $\mathcal{T}_d^{1,*}$

Proof. For a tree T with given diameter d, choose a diametral path $P_{d+1} = v_1 \cdots v_{d+1}$, and replace tree branches rooted in $v_2, \ldots, v_d$ by stars, then graft two stars to a star. Repeat the operations B and C. By Lemmas 2.2 and 2.3, the result follows. □

Theorem 2.5 *Let T be a tree with given diameter d, n vertices and $T \notin \mathcal{T}_d^{1,*}$. Then $NK(T) \geq NK(T_2^*)$, where $T_2^* \in \mathcal{T}_d^{2,*}$ and $\mathcal{T}_d^{2,*}$ (Fig. 5) is the set of trees with given diameter d and in the diametral path, S_{n-d-1} and a vertex are rooted in two different vertices.*

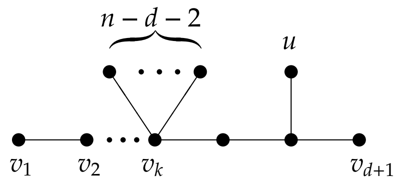

Figure 5: A tree T_2^* in $\mathcal{T}_d^{2,*}$

Proof. Similar to the proof in Theorem 2.4, by repeating operations in Lemmas 2.2 and 2.3, the NK-index of T is decreasing. Note that $T \notin \mathcal{T}_d^{1,*}$, in the diametral path $v_1v_2 \cdots v_{d+1}$, the star S_{n-d-1} is rooted in a vertex v_k. The only one remaining vertex u is adjacent to v_i ($i = 2, \ldots, d, i \neq k$) or one of pendent vertices of S_{n-d-1}. The resulting graphs are denoted by T_2^* and T_3^*. By direct calculations, $NK(T_3^*) = 2^{d-1} \cdot (n-d) > NK(T_2^*) = 3 \cdot 2^{d-3} \cdot (n-d)$.
Hence $NK(T) \geq NK(T_2^*)$. □

Lemma 2.6 [7] *Let G be a connected unicyclic graph with at least one pendent vertex, and the diameter of G be D. If $d(u, v) = D$, where $u, v \in V(G)$, then u or v should be a pendent vertex.*

Theorem 2.7 *Let $U \ncong C_n$ be a unicyclic graph with given diameter d and n vertices. Then $NK(U) \geq NK(U_j^*) = NK(U^{**})$, where U_j^* ($j = 2, \ldots, \lfloor \frac{d+1}{2} \rfloor$) is a unicyclic graph with diameter d, S_{n-d-2} and C_3 rooted in the same vertex of the diametral path $v_1v_2 \cdots v_dv_{d+1}$ except two end vertices. U_2^* and U^{**} are depicted in Figure 6.*

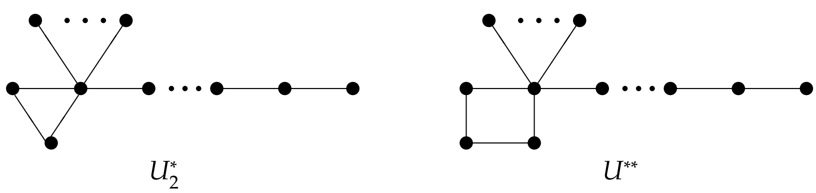

Figure 6: U_2^* and U^{**} (diameter d)

Proof. By Lemma 2.6, for $U \ncong C_n$, one of endpoints in a diametral path of unicyclic graph is a pendent vertex. There are two cases:

Case 1: A diametral path has an endpoint in the cycle.

For a unicyclic graph U, let a diametral path be $u_1u_2 \cdots u_kv_1v_2 \cdots v_l$ (without loss of generation, let $k \geq l$), where $v_1, v_2, \ldots, v_l$ are the vertices in the cycle with $k+l = d+1$. T_{u_i} $(i = 2, \ldots, k)$ are the tree branches rooted in u_i with $max\{(u_2, v)|v \in V(T_{u_2})\} \leq 1, \ldots, max\{(u_k, v)|v \in V(T_{u_k})\} \leq d-(k-1)$.

If U_1 is obtained from U by transforming the branches in Path $u_2 \cdots u_kv_1$ and the cycle to stars, by Lemma 2.2, then $NK(U) \geq NK(U_1)$. If the graph U_1 is transformed to U_2, where U_2 is the unicyclic graph that a star rooted in u_i of Path $u_2 \cdots u_k$, a star rooted in v_1 and a star rooted in v_i of the cycle, by Lemma 2.3, then $NK(U_1) \geq NK(U_2)$.

By repeating Operation C in Lemma 2.3, the graph U_3, U_4 and U_5 are obtained.

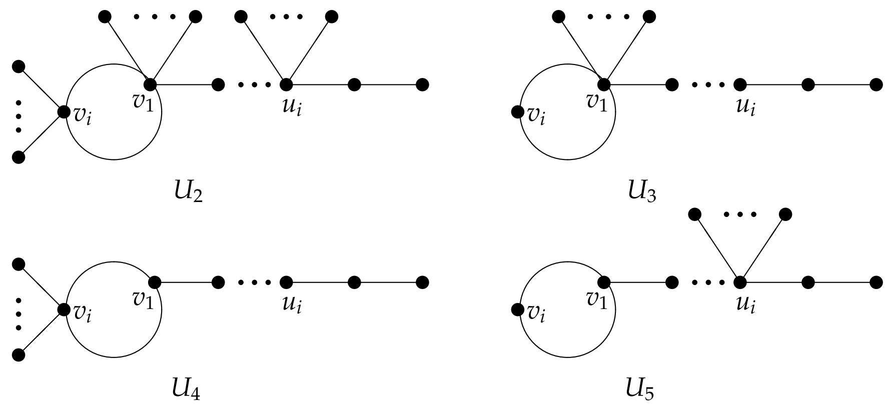

Figure 7: $U_i, i = 2, 3, 4, 5$.

Note that $NK(U_2) \geq NK(U_3)$ and $NK(U_2) \geq NK(U_4) = NK(U_5)$.

By direct calculation,

$$NK(U_3) - NK(U_4) = \prod_{v \in V(U_3)\setminus\{v_i, v_1\}} deg(v) \cdot [2 \cdot deg_{U_3}(v_1) - 3 \cdot (2 + deg_{U_3}(v_1) - 3)]$$

$$= \prod_{v \in V(U_3)\setminus\{v_i, v_1\}} deg(v) \cdot (3 - deg_{U_3}(v_1)) \leq 0.$$

If $deg_{U_3}(v_1) = 3$, then $U_3 \cong U_4$.

If $deg_{U_3}(v_1) > 3$, then $NK(U_3) \leq NK(U_4) \leq NK(U_2) \leq NK(U_1) \leq NK(U)$.

For even positive integer l, the graph U_3 consists of a path with length $d - \frac{l}{2}$, a cycle C_l and a star $S_{n-d-\frac{l}{2}+1}$ rooted in the same endpoint of the path.

$NK(U_3) = 2^{d-2+\frac{l}{2}} \cdot (n - d - \frac{l}{2} + 3)$.

Let $f(l) = 2^{d-2+\frac{l}{2}}(n - d - \frac{l}{2} + 3)$. Then $f'(l) = \dfrac{1}{2} \cdot 2^{d-2+\frac{l}{2}}[(n - d - \dfrac{l}{2} + 3)ln2 - 1] > 0$. $f(l)$ is an increasing function in l. Then $f(l) \geq f(4) = 2^d(n - d + 1)$ for $l \geq 4$, i.e., U^{**} attains the minimal NK-index.

For odd positive integer l, the graph U_3 consists of a path with length $d - \frac{l-1}{2}$, a cycle C_l and a star $S_{n-d-\frac{l-1}{2}}$ rooted in the same endpoint of the path.

$NK(U_3) = 2^{d+\frac{l-3}{2}} \cdot (n - d - \frac{l-5}{2})$.

Let $h(l) = 2^{d+\frac{l-3}{2}}(n - d - \frac{l-5}{2})$. Obviously, $h(l)$ is an increasing function in l. Then $h(l) \geq h(3) = 2^d(n - d + 1)$ for $l \geq 3$, i.e., U_2^* attains the minimal NK-index.

Case 2: Two endpoints of each diametral path are pendent vertices.

In order to decrease the NK-value of U, we can transform a unicyclic graph U to U_6, where a star S' and a unicyclic graph U' are rooted in v and w of a diametral path. By Lemma 2.2, $NK(U) \geq NK(U_6)$.

By transforming tree branches to stars in U' and grafting stars to a star, we obtain the graphs U_7 and U_8.

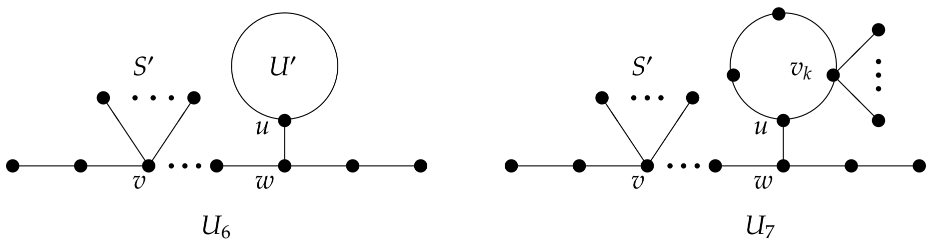

Figure 8: U_6 and U_7

By Lemmas 2.2 and 2.3, $NK(U_6) \geq NK(U_7)$, $NK(U_6) \geq NK(U_8)$ and

$NK(U_7) - NK(U_8) = \prod_{v \in V(U_7) \setminus \{v_k, u\}} deg(v)[3 \cdot deg_{U_7}(v_k) - 2 \cdot (deg_{U_7}(v_k) + 1)] > 0.$

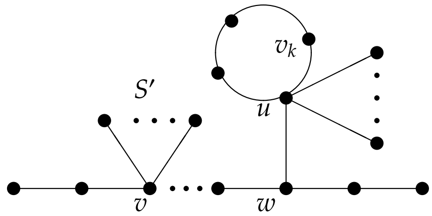

Figure 9: U_8

Let U_9 be the unicyclic graph obtained by adding a pendent vertex at w, and identifying u with w from U_8.

Then $NK(U_9) - NK(U_8) = \prod_{v \in V(U_8) \setminus \{u, w\}} deg(v)[deg_{U_8}(u) + 2 - 3 \cdot deg_{U_8}(u)] < 0.$

Let U_{10} (U_{11}) be the unicyclic graph obtained by grafting all pendent edges of vertex v (u) to vertex u (v) from U_9. Then $NK(U_{10}) - NK(U_9) = \prod_{x \in V(U_9) \setminus \{u, v\}} deg(x)[2 \cdot (deg_{U_9}(u) + deg_{U_9}(v) - 2) - deg_{U_9}(u) \cdot deg_{U_9}(v)] < 0.$ Obviously, $NK(U_{10}) \leq NK(U_{11})$.

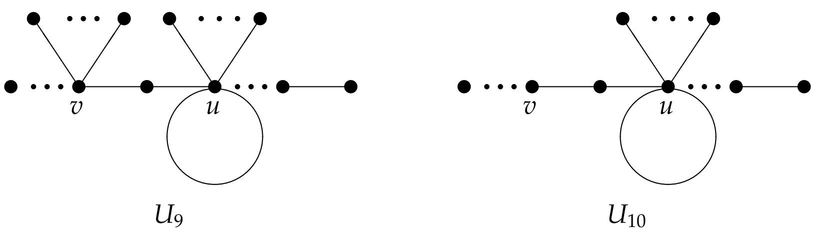

Figure 10: U_9 and U_{10}

Hence $NK(U_{10}) \leq NK(U_9) \leq NK(U_8) \leq NK(U_7) \leq NK(U_6) \leq NK(U)$.

The graph U_{10} consists of a path with length d, a cycle C_l with $l \leq d$ and a star $S_{n-d-l+1}$ rooted in the same vertex of the path except two end vertices.

And $NK(U_{10}) = 2^{d-2} \cdot 2^{l-1} \cdot (n - d - l + 4) = 2^{d+l-3} \cdot (n - d - l + 4)$.

Let $g(l) = 2^{d+l-3}(n - d - l + 4)$. Then $g'(l) = 2^{d+l-3}[(n - d - l + 4)ln2 - 1] > 0$. $g(l)$ is an increasing function in l. Then $g(l) \geq g(3) = 2^d(n - d + 1)$ for $l \geq 3$, i.e., U_j^* attains the minimal NK-index.

By above discussions, $NK(U) \geq NK(U_j^*) = NK(U^{**}) = 2^d(n - d + 1)$. □

Let $f(x) = 2^x(n - x + 1)$. Then $f'(x) = 2^x[ln2 \cdot (n - x + 1) - 1] > 0$. $f(x)$ is an increasing function in x. Then $f(x) \geq f(2)$, i.e., the following corollary holds:

Corollary 2.8 [6] *Among all connected n-vertex unicyclic graphs, the graph Y_n (Fig. 11)* has minimal Narumi-Katayama index (equal to $4(n - 1)$). This graph is unique.

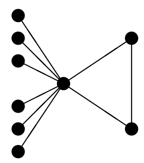

Figure 11: Y_n

3. The second and third minimal Narumi-Katayama index of unicyclic graphs

In [6], the minimal Narumi-Katayama index of unicyclic graphs is presented. In this section, we discuss the second and third minimal Narumi-Katayama index of unicyclic graphs.

Theorem 3.1 *Let $U \ncong Y_n$. U_i^* $(i = 3, 4, 5)$ is a unicyclic graph with n vertices and given cycle length k, where U_i^* $(i = 3, 4, 5)$ are depicted in Fig. 12.*

Then $NK(U) \geq NK(U_5^*) > NK(U_3^*) > NK(U_4^*)$.

Proof. Let C_k be the cycle of unicyclic graph U. In order to decrease NK-index, by Lemma 2.2, we can change the tree branches rooted in the cycle C_k to stars. By Operation C of Lemma 2.3, the Narumi-Katayama index is strictly decreasing. Repeated Operations B and C, then U_3^* is obtained.

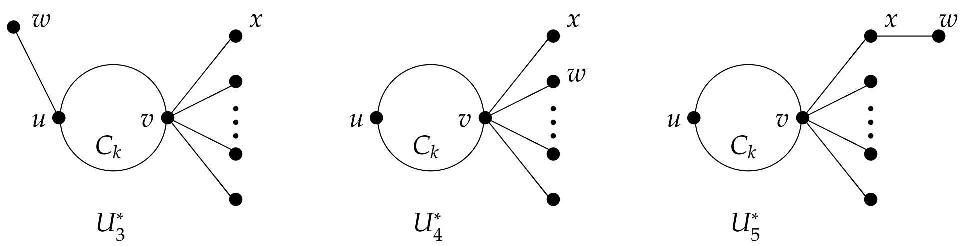

Figure 12: U_i^* $(i = 3, 4, 5)$

Let $U_4^* = U_3^* - uw + vw$, $U_5^* = U_3^* - uw + xw$. $NK(U_3^*) - NK(U_4^*) = \prod_{v_i \in V(U_3^*) \backslash \{u,v\}} deg(v_i)[3 \cdot deg_{U_3^*}(v) - 2 \cdot (deg_{U_3^*}(v) + 1)] > 0$. $NK(U_3^*) - NK(U_5^*) = \prod_{v_i \in V(U_3^*) \backslash \{u,x\}} deg(v_i)[3 \cdot 1 - 2 \cdot 2] < 0$.

Then $NK(U_4^*) < NK(U_3^*) < NK(U_5^*) \leq NK(U)$. □

Lemma 3.2 *Let U be a unicyclic graph with the cycle C_k and other vertices are pendent vertices. U' is the unicyclic graph obtained by deleting a 2-degree vertex and adding a pendent vertex of C_k. Then $NK(U) > NK(U')$.*

Proof. Let u, v be a 2-degree and a vertex of C_k.

$$NK(U) - NK(U') = \prod_{v_i \in V(U) \backslash \{u,v\}} deg(v_i) \cdot [2 \cdot deg_U(v) - 1 \cdot (deg_U(v) + 1)] > 0.$$

Hence $NK(U) > NK(U')$. □

By Theorem 3.1 and Lemma 3.2, the following result holds:

Theorem 3.3 *Let $U \ncong Y_n$. W_n and M_n are the unicyclic graphs U_5^* and U_3^* in the case $k = 3$. Then $NK(U) > NK(W_n) > NK(M_n)$.*

4. The minimal Narumi-Katayama index of bicyclic graphs

Bicyclic graphs are divided into three types:

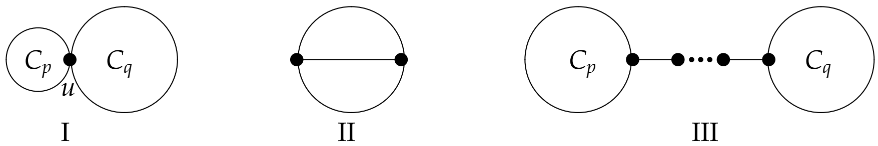

Figure 13: I, II and III-type bicyclic graphs

Lemma 4.1 *Let B be a I-type bicyclic graph with the cycles C_p, C_q and n vertices. Then $NK(B) \geq NK(B_4^*)$ (B_4^* is depicted in Fig. 14), where C_p and C_q have a common vertex u, and the other vertices are pendent vertices attached in u.*

Proof. For a bicyclic graph B with the cycles C_p and C_q, the other vertices consist of some tree branches rooted in C_p, C_q and vertex u. By Lemma 2.2, if these tree branches are transformed into stars, then Narumi-Katayama index is decreasing. Then we can obtain B_1^*. And $NK(B) \geq NK(B_1^*)$.

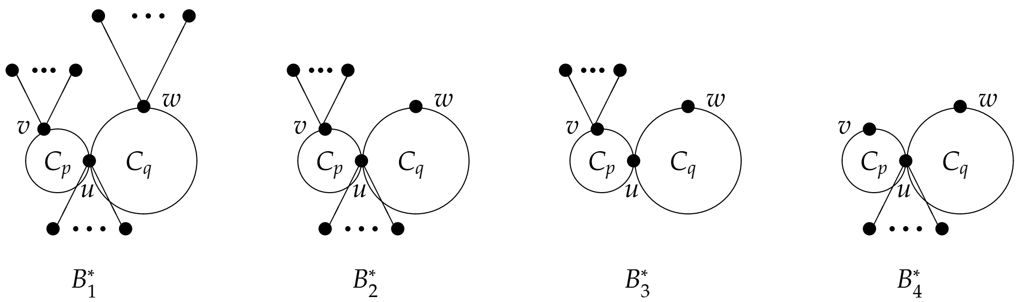

Figure 14: B_i^* $(i = 1, 2, 3, 4)$

Let B_2^* be the graph obtained by grafting all pendent edges incident with w to v from B_1^*. Then $NK(B_1^*) - NK(B_2^*) = \prod_{v_i \in V(B_1^*)\setminus\{v,w\}} deg(v_i) \cdot [deg_{B_1^*}(v) \cdot deg_{B_1^*}(w) - 2 \cdot (deg_{B_1^*}(v) + deg_{B_1^*}(w) - 2)] > 0$ for $deg_{B_1^*}(v) > 2$ and $deg_{B_1^*}(w) > 2$. If $deg_{B_1^*}(v) = 2$ or $deg_{B_1^*}(w) = 2$, then $B_1^* \cong B_2^*$.

Let B_3^* (B_4^*) be the graph obtained by grafting all pendent edges incident with u (v) to v (u) from B_2^*.

$$\begin{aligned} NK(B_2^*) - NK(B_4^*) &= \prod_{v_i \in V(B_2^*)\setminus\{u,v\}} deg(v_i) \cdot [deg_{B_2^*}(u) \cdot deg_{B_2^*}(v) - 2 \cdot (deg_{B_2^*}(v) + deg_{B_2^*}(u) - 2)] \\ &= \prod_{v_i \in V(B_2^*)\setminus\{u,v\}} deg(v_i) \cdot [(deg_{B_2^*}(u) - 2) \cdot (deg_{B_2^*}(v) - 2)]. \end{aligned}$$

If $deg_{B_2^*}(v) = 2$, then $B_2^* \cong B_4^*$. If $deg_{B_2^*}(v) > 2$, then $NK(B_2^*) > NK(B_4^*)$.

$$\begin{aligned} NK(B_3^*) - NK(B_4^*) &= \prod_{v_i \in V(B_3^*)\setminus\{u,v\}} deg(v_i) \cdot [4 \cdot deg_{B_3^*}(v) - 2 \cdot (deg_{B_3^*}(v) + 2)] \\ &= \prod_{v_i \in V(B_3^*)\setminus\{u,v\}} deg(v_i) \cdot [2 \cdot (deg_{B_3^*}(v) - 2)]. \end{aligned}$$

If $deg_{B_3^*}(v) = 2$, then $B_3^* \cong B_4^*$. If $deg_{B_3^*}(v) > 2$, then $NK(B_3^*) > NK(B_4^*)$.

Combining above discussions, we have:

(1) If $deg_{B_2^*}(v) = 2$, then $B_2^* \cong B_3^* \cong B_4^*$.

(2) If $deg_{B_2^*}(v) > 2$, then $NK(B_2^*) > NK(B_4^*)$ and $NK(B_3^*) > NK(B_4^*)$.

Hence $NK(B) \geq NK(B_4^*)$. □

Lemma 4.2 *For a bicyclic graph B_4^*, the minimal Narumi-Katayama index is attained when there are $n - 5$ pendent vertices, denoted by $B_4^*(3, 3, n - 5)$.*

Proof. Suppose there are k 2-degree vertices in B_4^*. Then $NK(B_4^*) = 2^k \cdot (n-k+3)$. Let $f(k) = 2^k(n-k+3)$. Since $f'(k) = 2^k[(n-k+3)ln2-1] > 0$, $f(k)$ is an increasing function in k. Then $f(k) \geq f(4)$ for $k \geq 4$, i.e., when $p = 3$, $q = 3$ and $n-5$ vertices are pendent vertices, i.e., $B_4^*(3,3,n-5)$ attains the minimal NK-value. □

Lemma 4.3 *Let B be a II-type bicyclic graph. Then $NK(B) \geq NK(B_5^*)$, where B_5^* is depicted in Figure 15.*

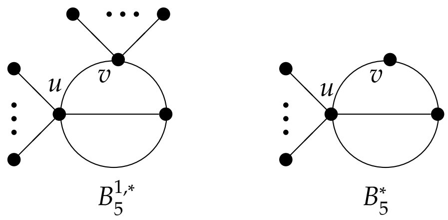

Figure 15: $B_5^{1,*}$ and B_5^*

Proof. Let B be a II-type bicyclic graph. In order to decrease $NK(B)$, by repeating operations in Lemmas 2.2 and 2.3, we can obtain the bicyclic graph $B_5^{1,*}$ and $NK(B) \geq NK(B_5^{1,*})$.

Let $B_5^{2,*}$ (B_5^*) be the graph obtained by grafting all pendent vertices of vertex u (v) to v (u) from $B_5^{1,*}$. By Lemma 2.2, $NK(B_5^{1,*}) \geq NK(B_5^{2,*})$ and $NK(B_5^{1,*}) \geq NK(B_5^*)$.

$$NK(B_5^*) - NK(B_5^{2,*}) = \prod_{v_i \in V(B_5^{1,*})\setminus\{u,v\}} deg(v_i) \cdot [2 \cdot (deg_{B_5^{1,*}}(u) + deg_{B_5^{1,*}}(v) - 2) - 3 \cdot (deg_{B_5^{1,*}}(v) + deg_{B_5^{1,*}}(u) - 3)].$$

If $deg_{B_5^{1,*}}(u) = 3$ and $deg_{B_5^{1,*}}(v) = 2$, then $B_5^{2,*} \cong B_5^*$.

Otherwise, $NK(B_5^*) \leq NK(B_5^{2,*}) \leq NK(B_5^{1,*}) \leq NK(B)$. □

Lemma 4.4 *For a bicyclic graph B_5^*, the minimal Narumi-Katayama index is attained when there are $n-4$ pendent vertices, denoted by $B_5^*(n-4)$.*

Proof. Suppose there are k 2-degree vertices in B_5^*. Then $NK(B_5^*) = (n-k+1) \cdot 2^k \cdot 3$. Let $f(k) = 3 \cdot 2^k(n-k+1)$. Since $f'(k) = 3 \cdot 2^k[(n-k+1)ln2-1] > 0$, $f(k)$ is an increasing function in k. Then $f(k) \geq f(2)$ for $k \geq 2$, i.e., when $B_5^* \cong B_5^*(n-4)$, $NK(B_5^*(n-4))$ attains the minimal value. □

Lemma 4.5 *Let B be a III-type bicyclic graph with n vertices. Then $NK(B) \geq NK(B_6^*)$, where B_6^* is depicted in Figure 16.*

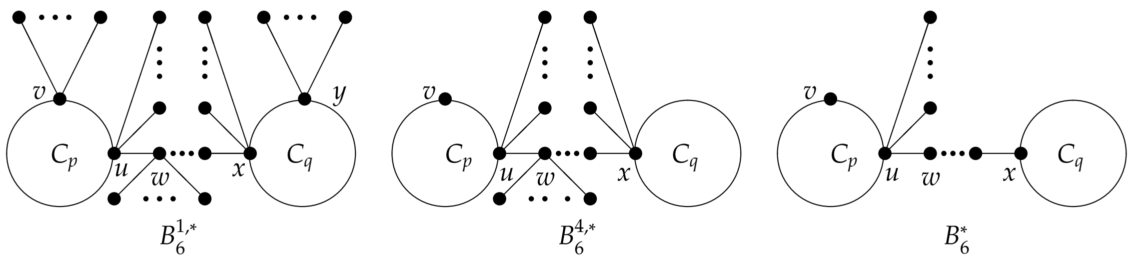

Figure 16: $B_6^{1,*}$, $B_6^{4,*}$ and B_6^*

Proof. For a III-type bicyclic graph B, similar to the proof of Lemma 4.3, and repeating the operations in Lemmas 2.2 and 2.3, we can obtain the bicyclic graph $B_6^{1,*}$ with $NK(B) \geq NK(B_6^{1,*})$.

Let $B_6^{2,*}$ ($B_6^{3,*}$) be the graph obtained by grafting all pendent vertices of vertex u (v) to v (u) from $B_6^{1,*}$. Since $deg_{B_6^{1,*}}(u) \geq 3$ and $deg_{B_6^{1,*}}(v) \geq 3$,

$$NK(B_6^{1,*}) - NK(B_6^{2,*}) = \prod_{v_i \in V(B_6^{1,*})\setminus\{u,v\}} deg(v_i) \cdot [deg_{B_6^{1,*}}(u) deg_{B_6^{1,*}}(v) - 3 \cdot (deg_{B_6^{1,*}}(v) + deg_{B_6^{1,*}}(u) - 3)] \geq 0;$$

$$NK(B_6^{2,*}) - NK(B_6^{3,*}) = \prod_{v_i \in V(B_6^{2,*}) \setminus \{u,v\}} deg(v_i) \cdot [deg_{B_6^{2,*}}(v) \cdot 3 - 2 \cdot (deg_{B_6^{2,*}}(v) - 2 + 3)] \geq 0.$$

Then $NK(B_6^{1,*}) \geq NK(B_6^{2,*}) \geq NK(B_6^{3,*})$.

Similarly, by grafting all pendent vertices of vertex y to x from $B_6^{3,*}$, we obtain the graph $B_6^{4,*}$ and $NK(B_6^{3,*}) \geq NK(B_6^{4,*})$.

Let $B_6^{5,*}$ be the graph obtained by grafting all pendent vertices of vertex x to u from $B_6^{4,*}$.

$$NK(B_6^{4,*}) - NK(B_6^{5,*}) = \prod_{v_i \in V(B_6^{4,*}) \setminus \{u,x\}} deg(v_i) \cdot [deg_{B_6^{4,*}}(u) deg_{B_6^{4,*}}(x) - 3 \cdot (deg_{B_6^{4,*}}(u) + deg_{B_6^{4,*}}(x) - 3)] \geq 0.$$

Then $NK(B_6^{4,*}) \geq NK(B_6^{5,*})$.

Let $B_6^{6,*}$ (B_6^*) be the graph obtained by grafting all pendent vertices of vertex u (w) to w (u) from $B_6^{5,*}$.

$$NK(B_6^{5,*}) - NK(B_6^{6,*}) = \prod_{v_i \in V(B_6^{5,*}) \setminus \{u,w\}} deg(v_i) \cdot [deg_{B_6^{5,*}}(u) deg_{B_6^{5,*}}(w) - 3 \cdot (deg_{B_6^{5,*}}(u) + deg_{B_6^{5,*}}(w) - 3)] \geq 0;$$

$$NK(B_6^{6,*}) - NK(B_6^{*}) = \prod_{v_i \in V(B_6^{6,*}) \setminus \{u,w\}} deg(v_i) \cdot [3 \cdot deg_{B_6^{6,*}}(w) - 2 \cdot (deg_{B_6^{6,*}}(w) - 2 + 3)] \geq 0.$$

Then $NK(B_6^{5,*}) \geq NK(B_6^{6,*}) \geq NK(B_6^*)$.

Hence $NK(B) \geq NK(B_6^{1,*}) \geq NK(B_6^{2,*}) \geq NK(B_6^{3,*}) \geq NK(B_6^{4,*}) \geq NK(B_6^{5,*}) \geq NK(B_6^{6,*}) \geq NK(B_6^*)$. □

Lemma 4.6 *For a bicyclic graph B_6^*, the minimal Narumi-Katayama index is attained when $p = 3$, $q = 3$ and other vertices are pendent vertices, denoted by $B_6^*(3, 3, n-6)$.*

Proof. Suppose there are k 2-degree vertices in B_6^*. Then $NK(B_6^*) = (n-k+1) \cdot 2^k \cdot 3$. By the proof of Lemma 4.4, $NK(B_6^*)$ is increasing in k. For $k \geq 4$, i.e., when $p = 3$, $q = 3$ and $n-6$ vertices are pendent vertices, i.e., $NK(B_6^*(3, 3, n-6))$ attains the minimal value. □

Theorem 4.7 *Let B a bicyclic graph with n vertices. Then $NK(B) \geq NK(B_5^*(n-4))$. The equality holds if and only if $B \cong B_5^*(n-4)$.*

Proof. For a bicyclic graph B, B belongs to one of three types of bicyclic graphs. By Lemmas 4.1-4.6, B attains the minimum NK-value in $B_4^*(3, 3, n-5)$, $B_5^*(n-4)$ or $B_6^*(3, 3, n-6)$. By direct calculations, $NK(B_4^*(3, 3, n-5)) = 2^4 \cdot (n-1)$, $NK(B_5^*(n-4)) = 2^2 \cdot 3 \cdot (n-1)$, and $NK(B_6^*(3, 3, n-6)) = 3 \cdot 2^4 \cdot (n-3)$. Then $NK(B_4^*(3, 3, n-5)) > NK(B_5^*(n-4))$ and $NK(B_6^*(3, 3, n-6)) > NK(B_5^*(n-4))$.

Then $NK(B) > NK(B_5^*(n-4))$ if $B \ncong B_5^*(n-4)$.

Hence $NK(B) \geq NK(B_5^*(n-4))$. □

References

[1] H. Narumi, M. Katayama, Simple topological index, A newly devised index characterizing the topological nature of sturctural isomers of saturated hydrocarbons, Memoirs of the Faculty of Engineering, Hokkaido University 16 (1984) 209–214.

[2] D.J. Klein, V.R. Rosenfeld, The degree-product index of Narumi and Katayama, MATCH Communications in Mathematical and in Computer Chemistry 64 (2010) 607–618.

[3] D.J. Klein, V.R. Rosenfeld, The Narumi-Katayama degree-product index and the degree-product polynomial, in: I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors-Theory and Applications II, Univ. Kragujevac, Kragujevac, 2010.

[4] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, 2009.

[5] Ž. Tomović, I. Gutman, Narumi-Katayama index of phenylenes, Journal of The Serbian Chemical Society 66 (2001) 243–247.

[6] I. Gutman, M. Ghorbani, Some properties of the Narumi-Katayama index, Applied Mathematics Letters 25 (2012) 1435–1438.

[7] M. Zhang, B. Liu, On the Randić index and diameter, MATCH Communications in Mathematical and in Computer Chemistry 64 (2010) 433–442.