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Research Paper

On Extremal Values Of Total Structure Connectivity and Narumi-Katayama Indices on the Class of all Unicyclic and Bicyclic Graphs

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Abstract

The total structure connectivity and Narumi-Katayama indices of a simple graph G are defined as $TS(G) = \prod_{u\in V(G)} \frac{1}{\sqrt{d_u}}$ and $NK(G) = \prod_{u\in V(G)} d_u$ respectively, where d_u represents the degree of vertex u in G. In this paper, we determine the extremal values of total structure connectivity index on the class of unicyclic and bicyclic graphs and characterize the corresponding extremal graphs. In addition, we determine the bicyclic graphs extremal with respect to the Narumi-Katayama index.

1 Introduction

Topological indices are molecular descriptors calculated from the molecular graph of a chemical compound. There is a strong correlation between the structural properties of a chemical compound and its topological indices [1–6].

Let G be a graph with the vertex set $V(G)$ and edge set $E(G)$. If $u \in V(G)$, then the degree of u is the number of edges incident with u and it is denoted by $d_G(u) = d_u$. A vertex $v \in V(G)$ is said to be a pendant, whenever $d_v = 1$. If G has n vertices, then the n-tuple $D = (d_1, d_2, \ldots, d_n)$ of vertex degrees is called the degree sequence of G, where $d_1 \geq d_2 \geq ... \geq d_n$. Let G be a simple graph with p vertices and q edges. If G has n components, then $\gamma = \gamma(G) = q - p + n$ is called the cyclomatic number of G. If G is a connected graph and $\gamma(G) = 0$, then G is called a tree. Graphs with $\gamma = 1, 2$ are called unicyclic and bicyclic, respectively. In this paper, all graphs are simple and connected. In addition, the path and the cycle with n vertices are indicated by P_n and C_n, respectively.

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One of the oldest topological indices is the Zagreb index first introduced in [7], when Gutman and Trinajstic studied the relation between $\pi-$electron energy and molecule structure (see also [8]). The total structure connectivity index of a simple graph G is defined in [9] as

$$TS(G) = \prod_{v \in V(G)} \frac{1}{\sqrt{d_v}}.$$

In 1984, Narumi and Katayama [10] introduced the simple topological index by

$$N = NK(G) = \prod_{v \in V(G)} d_v.$$

This index was called the Narumi-Katayama index in later works [11, 12]. In 2017, Bozovic et al. [13] used graph transformations and obtained extremal values of some topological indices on unicyclic and bicyclic graphs. In [14], we determined extremal values of the inverse degree and the forgotten indices on the class of all unicyclic graphs. In this paper, we use some graph transformations and obtain extremal values of the total structure connectivity index on the class of all unicyclic and bicyclic graphs. Moreover, in [15] You and Liu determined the minimal Narumi-Katayama index of bicyclic graphs. Here, we use a different method and obtain the maximum and minimum values of the Narumi-Katayama index on the class of all bicyclic graphs with n vertices.

2 Some graph transformations and their affection on the total structure connectivity and the Narumi-Katayama indices

Let G be a graph, $V_1 \subseteq V(G)$ and $E_1 \subseteq E(G)$. The subgraph of G obtained by removing the vertices of V_1 and the edges incident with them is denoted by $G - V_1$. Similarly, the subgraph of G obtained by deleting the edges of E_1 is denoted by $G - E_1$. Let $a, b \in V(G)$, $V_1 = \{a\}$ and $E_1 = \{ab\}$. Then the subgraphs $G - V_1$ and $G - E_1$ will be written as $G - a$ and $G - ab$, respectively. In addition, $G \cdot ab$ is a graph, obtained from G by the contraction of edge ab onto vertex a. Finally, if a, b are nonadjacent vertices of G, then $G + ab$ is the graph obtain from G by adding an edge ab.

Theorem 2.1. *Let G and $\widetilde{G}$ be two graphs and $V(G) = V(\widetilde{G}) = V$. Suppose that $u, v \in V(G)$, where $d_G(u) = m$, $d_G(v) = n$, $d_{\widetilde{G}}(u) = m + k$ and $d_{\widetilde{G}}(v) = n - k$, for some $k \geq 0$. If $d_G(a) = d_{\widetilde{G}}(a)$ for each $a \in V \setminus \{u, v\}$, then the following statements hold:*
(i) $k = 0$ or $k = n - m$ if and only if $TS(\widetilde{G}) = TS(G)$,
(ii) $k < n - m$ if and only if $TS(\widetilde{G}) < TS(G)$,
(iii) $k > n - m$ if and only if $TS(\widetilde{G}) > TS(G)$.

Proof. We set $W = V - \{u, v\}$. Then $d_G(a) = d_{\widetilde{G}}(a)$, for each $a \in W$. Now, by the definition of the total structure connectivity index, we have

$$\begin{aligned}\frac{TS(G)}{TS(\widetilde{G})} &= \frac{\prod_{a\in V(G)}\frac{1}{\sqrt{d_a}}}{\prod_{a\in V(\widetilde{G})}\frac{1}{\sqrt{d_a}}} = \frac{\frac{1}{\sqrt{d_G(u)}}\times\frac{1}{\sqrt{d_G(v)}}}{\frac{1}{\sqrt{d_{\widetilde{G}}(u)}}\times\frac{1}{\sqrt{d_{\widetilde{G}}(v)}}}\\ &= \frac{\frac{1}{\sqrt{m}}\times\frac{1}{\sqrt{n}}}{\frac{1}{\sqrt{m+k}}\times\frac{1}{\sqrt{n-k}}} = \frac{\sqrt{(m+k)(n-k)}}{\sqrt{mn}}\\ &= \frac{\sqrt{mn+k(n-m-k)}}{\sqrt{mn}}.\end{aligned}$$

Now, it is easy to see that (i), (ii) and (iii) are hold. ■

Theorem 2.2. *Let G and $\widetilde{G}$ be two graphs and $V(G) = V(\widetilde{G}) = V$. Suppose that $u, v \in V(G)$, where $d_G(u) = m$, $d_G(v) = n$, $d_{\widetilde{G}}(u) = m + k$ and $d_{\widetilde{G}}(v) = n - k$, for some $k \geq 0$. If $d_G(a) = d_{\widetilde{G}}(a)$ for each $a \in V \setminus \{u, v\}$, then the following statements hold:*
(i) $k = 0$ or $k = n - m$ if and only if $NK(\widetilde{G}) = NK(G)$,
(ii) $k < n - m$ if and only if $NK(\widetilde{G}) > NK(G)$,
(iii) $k > n - m$ if and only if $NK(\widetilde{G}) < NK(G)$.

Proof. By the same way as in the proof of Theorem 2.1 and the definition of the Narumi-Katayama index, we have

$$\begin{aligned}\frac{NK(G)}{NK(\widetilde{G})} &= \frac{\prod_{a\in V(G)}d_a}{\prod_{a\in V(\widetilde{G})}d_a} = \frac{d_G(u)\times d_G(v)}{d_{\widetilde{G}}(u)\times d_{\widetilde{G}}(v)}\\ &= \frac{m\times n}{(m+k)\times(n-k)} = \frac{mn}{mn+k(n-m-k)}.\end{aligned}$$

Now, we can see that (i), (ii) and (iii) are hold. ■

A graph transformation converts the information from the primary graph into a new converted structure. Now, we present several well-known graph transformations [13, 16, 17] that will be used to attain our main results.

Transformation A: Let G be a nontrivial graph, $u, v \in V(G)$ and $d_G(v) \geq 3$. Suppose that $P_1 : uu_1u_2 \ldots u_s$ and $P_2 : vv_1v_2 \ldots v_t$ are two paths, that hang on u and v, respectively. Let $\widetilde{G}$ be the graph achieved from G by interconnecting P_1 and P_2 (see Figure 1). Therefore, the $uu_1 \ldots u_sv_1 \ldots v_t$ is a path in the new graph $\widetilde{G}$. If we use transformation A on G, then the degree of u_s increases by $k = 1$ and the degree of v decreases by $k = 1$. Also, the degrees of other vertices in G and $\widetilde{G}$ are equal. Therefore, Theorems 2.1 and 2.2 show that $TS(\widetilde{G}) < TS(G)$ and $NK(\widetilde{G}) > NK(G)$.

Transformation B: Let G be a nontrivial graph. Consider two adjacent vertices u and v in G and let $d_G(u) \geq 3$ and $P : uu_1u_2 \ldots u_s$ be a path in G. We remove the edge uv and add the new edge u_sv. We denote the new obtained graph by $\widetilde{G}$ (see Figure 2).

Let $d_G(u_s) = m$, $d_G(u) = n$ and $n \geq 3$. If we use transformation B on G, then $d_{\widetilde{G}}(u_s) = m + 1$, $d_{\widetilde{G}}(u) = n + 1$, and the degrees of other vertices in G and $\widetilde{G}$ are the same. Now by Theorems 2.1 and 2.2 , $TS(\widetilde{G}) < TS(G)$ and $NK(\widetilde{G}) > NK(G)$.

For $n \geq 4$ and $i = 3, .., n-1$, the unicyclic graph $CO_{n,i}$ consisting of the cycle C_i that is connected to a path of length $n-i$, is called a comet (Figure 3). All the comets $CO_{n,3}$,...,$CO_{n,n-1}$

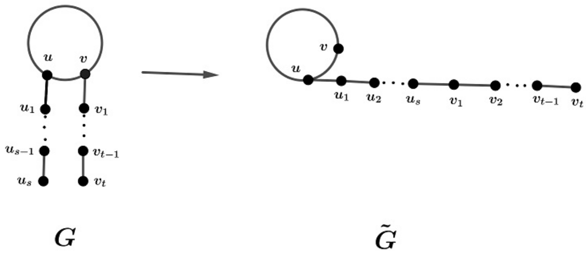

Figure 1: Transformation A.

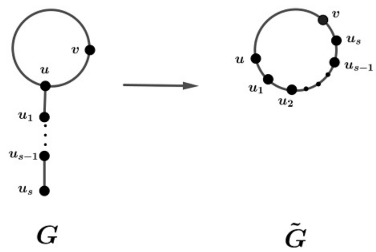

Figure 2: Transformation B.

have the same degree sequence, thus these comets have the same total structure connectivity and the Narumi-Katayama indices.

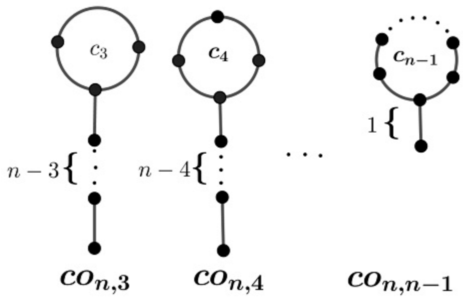

Figure 3: Comet.

Transformation C: Suppose that G is a graph, $u, v \in V(G)$ and u and v have no shared neighbor. Let $d_G(u) = m$ and $d_G(v) = n$, where $m \geq n \geq 2$. If $e = uv$, we show $(G.e) + uv$ by $\widetilde{G}$ (Figure 4).

Let u and v be two vertices of a graph G with $d_G(u) = m$ and $d_G(v) = n$. If we use transformation C on G, then $d_{\widetilde{G}}(v) = n - (n-1) = 1$ and $d_{\widetilde{G}}(u) = m + (n-1)$ and the degrees of other vertices in G and $\widetilde{G}$ are equal. By Theorems 2.1 and 2.2, if $m \geq n \geq 2$, then $TS(\widetilde{G}) > TS(G)$ and $NK(\widetilde{G}) < NK(G)$.

Remark 1. If we apply the transformation C to C_n, then we conclude that $TS(C_n) < TS(CO_{n,n-1})$ and $NK(CO_{n,n-1}) < NK(C_n)$. In addition, since all the comets $CO_{n,3}$,...,$CO_{n,n-1}$ have the

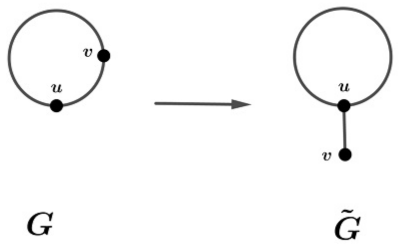

Figure 4: Transformation C.

same total structure connectivity and the Narumi-Katayama indices, so $TS(C_n) < TS(CO_{n,i})$ and $NK(CO_{n,i}) < NK(C_n)$, for each $i = 3, ..., n-1$.

Transformation D: Let G be a graph, $v \in V(G)$ and $v_1, v_2, \ldots, v_t$ be pendant vertices and neighbors of vertex v. If $u \in V(G) - \{v_1, v_2, \ldots, v_t\}$, then we show $(G - \{vv_1, vv_2, \ldots, vv_t\}) + \{uv_1, uv_2, \ldots, uv_t\}$ by $\widetilde{G}$ (Figure 5). Now, if $d_G(u) = m$ and $d_G(v) = n$, then by Theorems 2.1 and 2.2 we have

(a) if $t = n - m$, then $TS(\widetilde{G}) = TS(G)$ and $NK(\widetilde{G}) = NK(G)$,

(b) if $n - m > t$ and $t > 0$, then $TS(\widetilde{G}) < TS(G)$ and $NK(\widetilde{G}) > NK(G)$,

(c) if $t > n - m$, then $TS(\widetilde{G}) > TS(G)$ and $NK(\widetilde{G}) < NK(G)$.

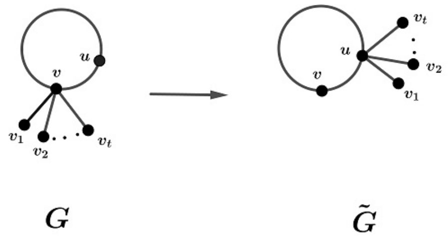

Figure 5: Transformation D.

Remark 2. For $n \geq 4$, the unicyclic graph C_n^k consists of the cycle C_k and $n - k$ pendant vertices that are attached to a vertex of C_k (Figure 6). By frequent use of the transformation C, we conclude that if $k > 3$, then $TS(C_n^k) < TS(C_n^3)$ and $NK(C_n^3) < NK(C_n^k)$.

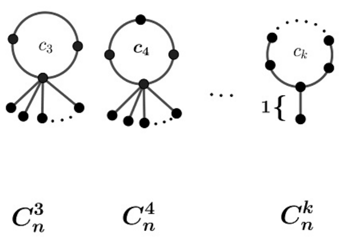

Figure 6: C_n^k.

3 Extremal unicyclic graphs with respect to the total structure connectivity and the Narumi-Katayama indices

In this section, we determine the extremal values of the total structure connectivity and the Narumi-Katayama indices on the class of all unicyclic graphs and characterize corresponding extremal unicyclic graphs.

Theorem 3.1. *Let G be a unicyclic graph of order n, where $n \geq 3$. Then $TS(C_n) \leq TS(G) \leq TS(C_n^3)$.*

Proof. If the transformation A is repeatedly applied to G, then any tree of G is transformed into a path and all paths will make a unique path, again by transformation A. In fact, the transformation A converts G into a comet. Thus, Remark 1 shows that $TS(G) \geq TS(C_n)$.

If the transformation C is repeatedly applied to G, we obtain a graph with stars connected on its cycle. Now, with sufficient use of the transformation D, we get a unicyclic graph $\widetilde{G}$ with exactly one star connected on its cycle and $TS(G) \leq TS(\widetilde{G})$. In addition, if the transformation C is repeatedly applied to $\widetilde{G}$, we achieve the unicyclic graph C_n^3. Hence $TS(\widetilde{G}) \leq TS(C_n^3)$ and by Remark 2, we conclude that $TS(G) \leq TS(C_n^3)$.

■

The following theorem is proved with a similar argument.

Theorem 3.2. *Let G be a unicyclic graph of order n, where $n \geq 3$. Then $NK(C_n^3) \leq NK(G) \leq NK(C_n)$.*

Corollary 3.3. *If G is a unicyclic graph with n vertices, where $n \geq 3$ and $G \neq C_n, C_n^3$, then*
(i) $\frac{\sqrt{2^n}}{2^n} < TS(G) < \frac{\sqrt{n-1}}{2n-2}$,
(ii) $4n - 4 < NK(G) < 2^n$.

4 Maximal and minimal values of total structure connectivity and the Narumi-Katayama indices on bicyclic graphs

In this section, we obtain maximal and minimal graphs with respect to the total structure connectivity and the Narumi-Katayama indices on the class of all bicyclic graphs, by considering the main subgraphs of the bicyclic graphs.

If G is a bicyclic graph, then G possesses two independent cycles and these cycles are denoted by C_p and C_q as in [17, 18]. Now, one of the following cases will be occurred:
(I) The subgraphs C_p and C_q in graph G possess exactly one shared vertex u.
(II) The subgraphs C_p and C_q in graph G are connected by a path of length r, where $r > 0$.
(III) The subgraphs C_{l+i} and C_{l+j} in G, posses a shared path of length l, where $0 < l \leq min\{i, j\}$.
The subgraphs $C_{p,q}$, $C_{p,r,q}$ and $\Theta_{l,i,j}$, depending on the previous three cases, are called main subgraphs of G, respectively (see Figure 7).

If G is a bicyclic graph, we transform each tree of G into a path by frequentative use of transformation A. Then, we transform all the paths with the same transformation into a unique path such as $P : w_1 w_2 \ldots w_t$. Thereupon, we acquire a bicyclic graph $\widetilde{G}$ such that the main subgraph of $\widetilde{G}$ is one of the graphs $C_{p,q}$, $C_{p,r,q}$ or $\Theta_{l,i,j}$ and it has a unique pendant path P attached at one of its vertices. According to the main subgraph of $\widetilde{G}$, we consider the following three cases:

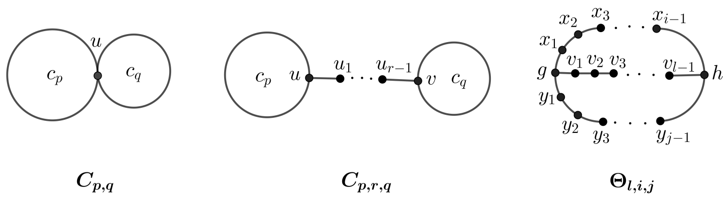

Figure 7: Main subgraphs of bicyclic graphs.

Case A: The main subgraph of $\widetilde{G}$ **is** $C_{p,q}$.

If the path P was connected to the vertex u, then we displace P and paste it to a vertex in C_p or C_q except u. Thus, we assume that P is attached to the vertex s, where $s \neq u$. Now, if the transformation B is used for s and one of its neighbors of degree 2, we obtain a graph of type I, where the length of one of its cycles is increased by the length of P as Figure 8. Also, we show that transformation B increases the Narumi-Katayama index and decreases the total structure connectivity index.

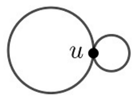

Figure 8: Bicyclic graph φ_1 of type I.

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Case B: The main subgraph of $\widetilde{G}$ **is** $C_{p,r,q}$.

If the path P was connected to the vertices $\{u, u_1, u_2, \ldots, u_{r-1}, v\}$, then we displace and paste it to a vertex s in C_p or C_q except u and v. Now, if the transformation B is used for s and one of its neighbors of degree 2, then we obtain a graph of type II, where the length of one of its cycles is increased by the length of P. In addition, the vertices $\{u_1, u_2, \ldots, u_{r-1}\}$ can be inserted into one of the cycles C_p or C_q. In this way, the degree sequence of the graph does not change, so the total structure connectivity and the Narumi-Katayama indices do not change. Eventually, we achieve a bicyclic graph, where its cycles are linked by uv as in the Figure 9.

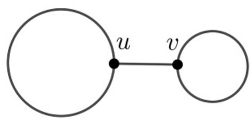


Figure 9: Bicyclic graph φ_2 of type II.

Case C: The main subgraph of $\widetilde{G}$ **is** $\Theta_{l,i,j}$

Similar to the previous cases, if the path P was connected to one of the vertices $\{g, v_1, v_2, \ldots, v_{l-1}, h\}$, then we displace and paste it to a vertex s in C_p or C_q except g and h. Now, if the transformation B is used for s and one of its neighbors of degree 2, then we obtain a graph of type III, where the length of one of its cycles is increased by the length of P. In addition, the vertices $\{v_1, v_2, \ldots, v_{l-1}\}$ can be inserted into one of the cycles C_p or C_q. In this way, the degree sequence of the graph does not change, so the total structure connectivity and the

Narumi-Katayama indices do not change. Eventually, we achieve a bicyclic graph of type III, where its cycles are shared in the edge gh as Figure 10.

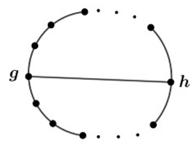


Figure 10: Bicyclic graph φ_3 of type III.

Therefore, every bicyclic graph G can be converted into one of the graphs φ_1 (Figure 8), φ_2 (Figure 9) or φ_3 (Figure 10). The degree sequences of φ_2 and φ_3 are the same. In the next lemma, we compare the total structure connectivity and the Narumi-Katayama indices of φ_1 and φ_2.

Lemma 4.1. *Let φ_1, φ_2 and φ_3 be the simple bicyclic graphs Figures 8 to 10, respectively. Then*
(*a*) $TS(\varphi_1) > TS(\varphi_2) = TS(\varphi_3)$,
(*b*) $NK(\varphi_1) < NK(\varphi_2) = NK(\varphi_3)$.

Proof. (a) We can see that the degree sequence of φ_1 is (4,2,2,. . . ,2) and φ_2 is (3,3,2,2,. . . ,2). Then by the definition we have

$$\begin{aligned}\frac{TS(\varphi_1)}{TS(\varphi_2)} &= \frac{\prod_{i=1}^{n}\frac{1}{\sqrt{\acute{d}_i}}}{\prod_{i=1}^{n}\frac{1}{\sqrt{d_i}}} = \frac{\frac{1}{\sqrt{2}}\times\ldots\times\frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{4}}}{\frac{1}{\sqrt{2}}\times\ldots\times\frac{1}{\sqrt{2}}\times\frac{1}{\sqrt{3}}\times\frac{1}{\sqrt{3}}}\\ &= \frac{\frac{1}{2\sqrt{2^{n-1}}}}{\frac{1}{3\sqrt{2^{n-2}}}} = \frac{3\sqrt{2}}{4}.\end{aligned}$$

Thus, $\frac{TS(\varphi_1)}{TS(\varphi_2)} > 1$ and $TS(\varphi_2) < TS(\varphi_1)$, for each $n \geq 5$.

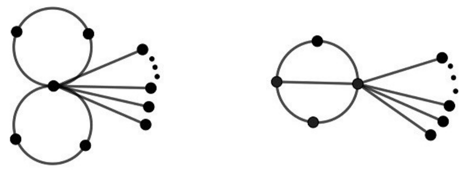
(b)With a similar argument for the Narumi-Katayama index, we have

$$\begin{aligned}\frac{NK(\varphi_1)}{NK(\varphi_2)} &= \frac{\prod_{i=1}^{n}\acute{d}_i}{\prod_{i=1}^{n}d_i} = \frac{2\times 2\times\ldots\times 2\times 4}{2\times 2\times\ldots\times 2\times 3\times 3}\\ &= \frac{8}{9}.\end{aligned}$$

Therefore, $\frac{NK(\varphi_1)}{NK(\varphi_2)} < 1$ and $NK(\varphi_1) < NK(\varphi_2)$, for each n $n \geq 5$. ∎

If G is a bicyclic graph, then by iterative use of transformation C, G can be converted to a bicyclic graph $\widetilde{G}$, where $\widetilde{G}$ consists of two triangles and some hanging stars and the Narumi-Katayama index of $\widetilde{G}$ is less than the Narumi-Katayama index of G and its total structure connectivity index is greater than the total structure connectivity index of G. Now, we repeat transformation D until G converts to ψ_1 or ψ_2 of Figure 11. Also, transformation D decreases the Narumi-Katayama index and increases the total structure connectivity index.

In the next lemma, we compare the total structure connectivity and the Narumi-Katayama indices of the graphs ψ_1 and ψ_2.



$\boldsymbol{\psi_1}$ $\boldsymbol{\psi_2}$

Figure 11: Bicyclic graphs ψ_1 and ψ_2.

Lemma 4.2. *Let ψ_1 and ψ_2 be the simple bicyclic graphs Figure 11. Then*
(*a*) $TS(\psi_1) < TS(\psi_2)$,
(*b*) $NK(\psi_1) > NK(\psi_2)$.

Proof. (a) We can see that the degree sequence of ψ_1 is (n-1,2,2,2,2,1,1,. . . ,1) and ψ_2 is (n-1,3,2,2,1,1,. . . ,1), so by the definition we have

$$\begin{aligned}\frac{TS(\psi_1)}{TS(\psi_2)} &= \frac{\prod_{i=1}^{n}\frac{1}{\sqrt{\acute{d}_i}}}{\prod_{i=1}^{n}\frac{1}{\sqrt{d_i}}} = \frac{\frac{1}{\sqrt{1}}\times\ldots\times\frac{1}{\sqrt{1}}\times\frac{1}{\sqrt{n-1}}\times\frac{1}{\sqrt{2^4}}}{\frac{1}{\sqrt{1}}\times\ldots\times\frac{1}{\sqrt{1}}\times\frac{1}{\sqrt{2^2}}\times\frac{1}{\sqrt{3}}\times\frac{1}{\sqrt{n-1}}}\\ &= \frac{\sqrt{3}}{2}.\end{aligned}$$

Thus, $\frac{TS(\psi_1)}{TS(\varphi_2)} < 1$ and $TS(\psi_1) < TS(\psi_2)$, for each $n \geq 5$.

(b)With a similar argument above for the Narumi-Katayama index, we have

$$\begin{aligned}\frac{NK(\psi_1)}{NK(\psi_2)} &= \frac{\prod_{i=1}^{n}\acute{d}_i}{\prod_{i=1}^{n}d_i} = \frac{1\times1\times\ldots\times1\times2^4\times(n-1)}{1\times1\times\ldots\times1\times2^2\times3\times(n-1)}\\ &= \frac{4}{3}.\end{aligned}$$

Therefore,$\frac{NK(\psi_1)}{NK(\psi_2)} > 1$ and $NK(\psi_2) < NK(\psi_1)$, for each $n \geq 5$. ■

Now, by the above explanations we can prove the main results of this section.

Theorem 4.3. *Let G be a bicyclic graph of order n, where $n \geq 5$. Then*
(i) $TS(\varphi_2) \leq TS(G) \leq TS(\psi_2)$,
(ii) $NK(\psi_2) \leq NK(G) \leq NK(\varphi_2)$.

Proof. (i) If G is a bicyclic graph, then we show that G can be converted into one of the graphs φ_1, φ_2 or φ_3 of Lemma 4.1, by the transformations A and B and these transformations decrease the total structure connectivity index. Therefore, Lemma 4.1 implies that $TS(\varphi_2) \leq TS(G)$. Similarly, G can be converted into one of the graphs ψ_1 or ψ_2 of Lemma 4.2 by the transformations C and D and these transformations increase the total structure connectivity index. Therefore, Lemma 4.2 shows that $TS(G) \leq TS(\psi_2)$.

Another part can be proved by a similar argument. ■

Corollary 4.4. *Let G be a bicyclic graph of order n, where $n \geq 5$ and $G \neq \varphi_2$ and ψ_2. Then*
(i) $\frac{1}{3\sqrt{2^{n-2}}} < TS(G) < \frac{1}{2\sqrt{3(n-1)}}$,
(ii) $12 \times (n-1) < NK(G) < 9 \times 2^{n-2}$.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

References

[1] G. H. Fath-Tabar, A. R. Ashrafi and D. Stevanović, Spectral properties of fullerenes, *J. Comput. Theor. Nanosci.* **9** (3) (2012) 327–329, https://doi.org/10.1166/jctn.2012.2027.

[2] O. C. Havare, QSPR analysis with curvilinear regression modeling and topological indices, *Iranian J. Math. Chem.* **10** (4) (2019) 331–341, https://doi.org/10.22052/IJMC.2019.191865.1448.

[3] H. Liu, L. You and Y. Huang, Ordering chemical graphs by Sombor indices and its applications, *MATCH Commun. Math. Comput. Chem.* **87** (1) (2022) 5–22, https://doi.org/10.46793/match.87-1.005L.

[4] F. Shafiei, Relationship between topological indices and thermodynamic properties and of the monocarboxylic acids applications in QSPR, *Iranian J. Math. Chem.* **6** (1) (2015) 15–28, https://doi.org/10.22052/IJMC.2015.8944.

[5] F. Taghvaee and G. H. Fath-Tabar, Relationship between coefficients of characteristic polynomial and matching polynomial of regular graphs and its applications, *Iranian J. Math. Chem.* **8** (1) (2017) 7–23, https://doi.org/10.22052/IJMC.2017.15093.

[6] Z. Yarahmadi and G. H. Fath-Tabar, The Wiener, Szeged, PI, vertex PI, the first and second Zagreb indices of N-branched phenylacetylenes dendrimers, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 201–208.

[7] I. Gutman and N. Trinajstić, Graph theory and molecular orbital total φ-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (4) (1972) 535–538, https://doi.org/10.1016/0009-2614(72)85099-1.

[8] G. H. Fath-Tabar, Old and new Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 79–84.

[9] M. Črepnjak and P. Ž. Pleteršek, Correlation between heat of formation and fifth geometric–arithmetic index, *Fuller. Nanotub.* **27** (7) (2019) 559–565, https://doi.org/10.1080/1536383X.2019.1617278.

[10] H. Narumi and M. Katayama, Simple topological index: A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Mem. Fac. Eng. Hokkaido Univ.* **16** (3) (1984) 209–214.

[11] M. Ghorbani, M. Songhori and I. Gutman, Modified Narumi-Katayama index, *Kragujevac J. Sci.* **34** (2012) 57–64.

[12] I. Gutman and M. Ghorbani, Some properties of the Narumi-Katayama index, *Appl. Math. Lett.* **25** (10) (2012) 1435–1438, https://doi.org/10.1016/j.aml.2011.12.018.

[13] V. Bozović, Z. K. Vukićević and G. Popivoda, Extremal values of total multiplicative sum Zagreb index and first multiplicative sum Zagreb coindex on unicyclic and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 417–430.

[14] M. A. Manian, S. Heidarian and F. khaksar Haghani, Maximum and minimum values of inverse degree and forgotten indices on the class of all unicyclic graphs, *AKCE Int. J. graphs Comb.* **20** (1) (2023) 57–60, https://doi.org/10.1080/09728600.2023.2170298.

[15] Z. You and B. Liu, On the extremal Narumi-Katayama index of graphs, *Filomat* **28** (3) (2014) 531–539.

[16] B. Wu and J. Meng, Basic properties of total transformation graphs, *J. Math. Study* **34** (2) (2001) 109–116.

[17] K. Xu and K. C. Das, Trees, unicyclic and bicyclic graphs extremal with respect to multiplicative sum Zagreb index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 257–272.

[18] K. Xu and I. Gutman, The greatest Hosoya index of bicyclic graphs with given maximum degree, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 795–824.