MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **96** (2026) 545–585
ISSN: 0340–6253
doi: 10.46793/match.96-2.28525

On the Hyperbolic Sombor Index of Graphs

Sourav Mondal[a], **Zahid Raza**[b,*]

[a] *Research Institute of Sciences and Engineering (RISE), Research Group MASEP, University of Sharjah, Sharjah, 27272, United Arab Emirates*

[b] *Department of Mathematics, College of Sciences, University of Sharjah, United Arab Emirates*

souravmath94@gmail.com, zraza@sharjah.ac.ae

(Received October 29, 2025)

Abstract

The hyperbolic Sombor index (HSO) is a recently introduced vertex-degree–based topological index that originates from the geometric properties of a hyperbola. In this work, we explore several mathematical properties of the HSO index, as well as revisit and refine some previously reported results. We first provide a counterexample to the claim that $HSO(G)$ always increases with the addition of an edge and establish a sufficient condition under which this monotonicity holds. We then present refined versions of some existing results and proofs. Furthermore, we establish sharp upper and lower bounds for the HSO index across various classes of graphs, including trees, unicyclic graphs, and bicyclic graphs, and characterize the corresponding extremal graphs that attain these bounds. Finally, we identify the first eight minimal trees, as well as seven minimal unicyclic and bicyclic graphs with respect to HSO.

1 Introduction

Let G be a simple connected graph of order n and size m with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The degree of a vertex v_i

*Corresponding author.

is denoted by $d_G(v_i)$. By Δ, we mean the maximum degree in G. The path, cycle and star graphs of order n are represented by P_n, C_n, and S_n respectively. By $T(n)$, $U(n)$, and $B(n)$, we mean the collection of all trees, unicyclic graphs, and bicyclic graphs of order n, respectively. We consider n_i to represent the number of vertices having degree i. A pendent edge is an edge incident with a vertex of degree one, whereas a path $v_1v_2\dots v_t$ is said to be a pendent path of length $t-1$ attached to v_1 if $d_G(v_1)\geq 3$, $d_G(v_i)=2$ for $i=2,\dots,t-1$, and $d_G(v_t)=1$. Throughout this work, we consider ℓ and ℓ_1 to represent the number of pendent paths and the number of pendent paths of length 1, respectively.
The interplay between graph theory and chemistry, known as chemical graph theory, provides a powerful framework for modeling and understanding the properties of molecules [12]. In this paradigm, a molecular structure is represented by a graph where vertices correspond to atoms and edges to chemical bonds. A central tool in this field is the topological index, a numerical descriptor derived from the graph that encodes its structural information. These indices have proven invaluable in establishing quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR), allowing researchers to predict physicochemical properties and biological activities of chemical compounds without costly and time-consuming laboratory experiments.

Among the plethora of topological indices proposed over the years, degree-based indices are some of the most studied due to their intuitive definition and strong correlative power [7]. These indices are formulated as a sum over the edges of a graph of a function $f(d_G(v_i), d_G(v_j))$, where $d_G(v_i)$ and $d_G(v_j)$ are the degrees of the adjacent vertices v_i and v_j. Seminal examples include the first Zagreb index [10], the Atom-Bond Connectivity (ABC) index [4], and the Geometric-Arithmetic (GA) index [13].

A recent and fruitful trend in the field involves the geometric interpretation of topological indices. This approach was pioneered by Gutman [6] with the introduction of the Sombor index (SO), defined as $SO(G)=\sum_{v_iv_j\in E(G)}\sqrt{d_G(v_i)^2+d_G(v_j)^2}$. This index was conceived by viewing the degree pair $(d_G(v_i), d_G(v_j))$ as coordinates of a point in the Cartesian plane, with the index value being the Euclidean distance from the origin.

The success and mathematical richness of the Sombor index [3,5,9,11,14] inspired a family of related geometric indices. Following this paradigm, the elliptic Sombor index [8] and the hyperbolic Sombor index (HSO) [1,2] were subsequently developed.

The Hyperbolic Sombor index, which is the focus of this work, draws its inspiration from the eccentricity of a hyperbola. For a hyperbola defined by $\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1$, the eccentricity is given by $e = \frac{\sqrt{a^2+b^2}}{a}$. By associating the degrees $d_G(v_i)$ and $d_G(v_j)$ of adjacent vertices with the semi-axes a and b (with $a \leq b$), this formula leads to the definition of the HSO index for a graph G:

$$HSO(G) = \sum_{v_iv_j \in E(G)} \frac{\sqrt{d_G(v_i)^2 + d_G(v_j)^2}}{\min\{d_G(v_i), d_G(v_j)\}} .$$

The aforesaid formulation can also be represented as

$$HSO(G) = \sum_{\substack{v_iv_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} \sqrt{1 + \left(\frac{d_G(v_i)}{d_G(v_j)}\right)^2} . \tag{1}$$

Initial studies of the HSO index have demonstrated its significant potential. Barman and Das [1] established fundamental mathematical properties and provided bounds for the index, while a subsequent work [2] showcased its strong predictive power for properties such as π-electron energy and polarizability in benzenoid hydrocarbons through QSPR analysis.

However, as the mathematical theory of this new index continues to develop, some initial claims require re-examination. For instance, it was stated in [1] that $HSO(G) > HSO(G - e)$ for any edge e, implying universal monotonicity with respect to edge addition. We demonstrate that this property does not hold in general by providing a counterexample. Furthermore, the characterization of the equality case for the lower bound $HSO(G) \geq \sqrt{2}m$ was incompletely stated to be achieved only by complete graphs, whereas it is, in fact, achieved by all regular graphs.

This manuscript aims to provide a rigorous and systematic mathematical analysis of the Hyperbolic Sombor index, addressing existing inaccuracies and establishing a more complete theoretical foundation. Our main contributions are as follows. We refute the general monotonicity claim regarding edge addition and establish a sufficient condition under which $HSO(G) > HSO(G-e)$ holds. We prove the lower bound $HSO(G) \geq \sqrt{2}m$, precisely characterizing the extremal graphs as all regular graphs. We also present refined proofs of existing results. Moreover, we derive sharp upper and lower bounds for HSO in unicyclic and bicyclic graphs, characterizing the extremal graphs when the order n is fixed. Finally, we extend this analysis by identifying the first eight trees and seven unicyclic and bicyclic graphs with minimal HSO values, thereby providing a finer ordering of these graph families with respect to this index.

2 Main results

Consider a function $f : [1, \infty) \to \mathbb{R}$ with

$$f(x) = \sqrt{1+x^2}.$$

Clearly

$$f'(x) = \frac{x}{\sqrt{x^2+1}} > 0,$$

which implies that f is a strictly increasing function and $f(x) \geq \sqrt{2}$ with equality iff $x = 1$. Thus, we can state the following remark, which will be used frequently throughout this work. Let G and G' be two graphs. Consider $v_iv_j \in E(G)$ and $v'_iv'_j \in E(G')$ with $1 \leq \frac{d_G(v_i)}{d_G(v_j)} \leq \frac{d_{G'}(v'_i)}{d_{G'}(v'_j)}$, then we have

$$f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\left(\frac{d_{G'}(v'_i)}{d_{G'}(v'_j)}\right), \tag{2}$$

with equality iff $\frac{d_G(v_i)}{d_G(v_j)} = \frac{d_{G'}(v'_i)}{d_{G'}(v'_j)}$. Employing the function f, we can represent the formulation (1) of HSO for graph G as follows.

$$HSO(G) = \sum_{\substack{v_iv_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right). \tag{3}$$

Also for any edge $v_iv_j \in E(G)$, we have $f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) = \sqrt{2}$ iff $d_G(v_i) = d_G(v_j)$.

In [1], it was claimed that the HSO value always increases when an edge is added to a graph, i.e.,

$$HSO(G) > HSO(G - e), \tag{4}$$

where $e = v_iv_j$ is an edge of G. However, we provide a counterexample to this claim. As shown in Figure 1, we have

$$HSO(G) - HSO(G - e) < -0.14 < 0,$$

which implies that

$$HSO(G) < HSO(G - e).$$

Therefore, the general claim in [1] does not hold. In the following, we establish a sufficient condition under which the HSO value indeed increases after adding an edge.

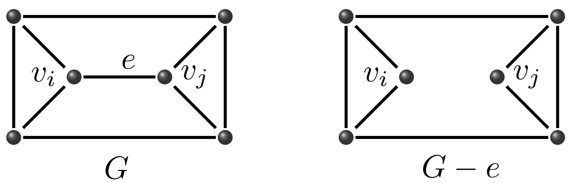

Figure 1. The graphs G and $G - e$.

Theorem 1. *Let $v_iv_j \in E(G)$ with $d_G(v_i) \geq d_G(v_j)$. Define*

$$d_i^* = \max\{d_G(v_p) : v_p \in N_G(v_i) \setminus \{v_j\}\},\ d_j^* = \max\{d_G(v_q) : v_q \in N_G(v_j) \setminus \{v_i\}\}.$$

If $d_G(v_j) > \max\{d_i^*, d_j^*\}$, then

$$HSO(G) > HSO(G - v_iv_j).$$

Proof. Let $d_G(v_j) > \max\{d_i^*, d_j^*\}$. Then, it is clear that $d_G(v_i) > d_G(v_p)$ for all $v_p \in N_G(v_i) \setminus \{v_j\}$ and $d_G(v_j) > d_G(v_q)$ for all $v_q \in N_G(v_j) \setminus \{v_i\}$.

Now, we have

$$
\begin{aligned}
& HSO(G) - HSO(G - v_i v_j) \\
= \;& f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) + \sum_{v_p \in N_G(v_i)\setminus\{v_j\}} \left[f\left(\frac{d_G(v_i)}{d_G(v_p)}\right) - f\left(\frac{d_G(v_i)-1}{d_G(v_p)}\right)\right] \\
& + \sum_{v_q \in N_G(v_j)\setminus\{v_i\}} \left[f\left(\frac{d_G(v_j)}{d_G(v_q)}\right) - f\left(\frac{d_G(v_j)-1}{d_G(v_q)}\right)\right] \qquad (5)
\end{aligned}
$$

It is cleat that $\frac{d_G(v_i)}{d_G(v_p)} > \frac{d_G(v_i)-1}{d_G(v_p)}$ for all $v_p \in N_G(v_i) \setminus \{v_j\}$ and $\frac{d_G(v_j)}{d_G(v_q)} > \frac{d_G(v_j)-1}{d_G(v_q)}$ for all $v_q \in N_G(v_j) \setminus \{v_i\}$, which implies by (2) that

$$f\left(\frac{d_G(v_i)}{d_G(v_p)}\right) > f\left(\frac{d_G(v_i)-1}{d_G(v_p)}\right) \quad \forall v_p \in N_G(v_i) \setminus \{v_j\},$$

and

$$f\left(\frac{d_G(v_j)}{d_G(v_q)}\right) > f\left(\frac{d_G(v_j)-1}{d_G(v_q)}\right) \quad \forall v_q \in N_G(v_j) \setminus \{v_i\}.$$

Employing these facts in (5), we obtain $HSO(G) > HSO(G - v_i v_j)$. Hence the proof is completed. ■

In Theorem 1 of [1], it is stated that $HSO(G) \geq \sqrt{2}\, m$, where equality appears iff G is complete. However, in Figure 2, we present three non-complete graphs G_1, G_2, and G_3 that also satisfy $HSO(G) = \sqrt{2}\, m$. Based on this observation, we now propose a modification of Theorem 1 [1].

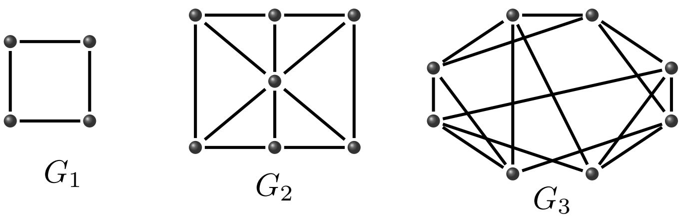

Figure 2. The graphs G_1, G_2 and G_3.

Theorem 2. *Let G be a simple connected graph with m edges. Then*

$$HSO(G) \geq \sqrt{2}m,$$

where equality appear if and only if G is regular.

Proof. We know that $f(x)$ is strictly increasing for $x \in [1, \infty)$, and that $f(x) \geq \sqrt{2}$, with equality if and only if $x = 1$. Therefore, from (3) we immediately obtain

$$HSO(G) = \sum_{\substack{v_i v_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \geq \sqrt{2}m, \tag{6}$$

where equality holds if and only if $d_G(v_i) = d_G(v_j)$ for all $v_i v_j \in E(G)$. Since G is connected, the equality holds if and only if G is regular. ■

To prove the minimal case of Theorem 5 in [1], the relation (4) was assumed to be obvious; however, it has been shown here that this assumption does not hold in general. Therefore, we present a different proof as follows.

Theorem 3. *For a tree T of order $n\,(\geq 3)$, we have*

$$HSO(T) \geq \sqrt{2}(n-3) + 2\sqrt{5},$$

where the equality occurs iff $T \cong P_n$.

Proof. Let $T \cong P_n$. Then $HSO(T) = \sqrt{2}(n-3) + 2\sqrt{5}$, and therefore equality is attained. Now consider the case $T \ncong P_n$. In this case, T contains at least three pendent edges. For any pendent edge $v_i v_j \in E(T)$ with $d_T(v_i) \geq d_T(v_j) = 1$, we have $f\left(\frac{d_T(v_i)}{d_T(v_j)}\right) \geq f(2)$. Moreover, for any edge $v_i v_j \in E(T)$ with $d_T(v_i) \geq d_T(v_j)$, it holds that $f\left(\frac{d_T(v_i)}{d_T(v_j)}\right) \geq f(1)$. Therefore,

$$\begin{aligned} HSO(T) &\geq 3f(2) + (n-4)f(1) = 3\sqrt{5} + (n-4)\sqrt{2} \\ &> \sqrt{2}(n-3) + 2\sqrt{5} = HSO(P_n). \end{aligned}$$

■

To prove the minimal case of Theorem 4 in [1], the following reasoning was provided: the only graph in which all vertices have degree 2 is C_n. Here, we present a logical proof of this result.

Theorem 4. *For a simple connected graph G of order $n\,(\geq 3)$, we have*

$$HSO(G) \geq \sqrt{2}\,n,$$

where the equality occurs iff $G \cong C_n$.

Proof. Let G be a tree. Then G has at least two pendent edges and $|E(G)| = n-1$. Thus, we obtain

$$\begin{aligned} HSO(G) &\geq 2f(2) + (n-3)f(1) = 2\sqrt{5} + (n-3)\sqrt{2} \\ &> 2\sqrt{5} - 3\sqrt{2} + \sqrt{2}n > HSO(C_n). \end{aligned}$$

Next, suppose that G is not a tree. Then $|E(G)| = m \geq n$. Therefore, by Theorem 2, we have

$$HSO(G) \geq \sqrt{2}m \geq \sqrt{2}n,$$

where equality holds if and only if G is regular and $m = n$, i.e., if and only if $G \cong C_n$. Hence, the lower bound and the extremal graph are established. ∎

Now, we are going to characterize the maximal unicyclic graph for HSO, when n is given. Let us construct a unicyclic graph S'_n by connecting two pendent vertices of S_n by an edge. It is clear that

$$\begin{aligned} HSO(S'_n) &= (n-3)f(n-1) + 2f\left(\frac{n-1}{2}\right) + f(1) \\ &= (n-3)\sqrt{(n-1)^2+1} + \sqrt{(n-1)^2+4} + \sqrt{2}. \end{aligned}$$

Theorem 5. *Let G be a unicyclic graph of order $n\,(\geq 3)$. Then*

$$\sqrt{2}n \leq HSO(G) \leq (n-3)\sqrt{(n-1)^2+1} + \sqrt{(n-1)^2+4} + \sqrt{2},$$

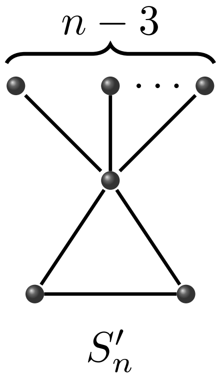

Figure 3. The unicyclic graph S'_n.

where the left equality occurs iff $G \cong C_n$ and the right equality occurs iff $G \cong S'_n$.

Proof. The lower bound and the minimal graph follow directly from Theorem 4. Next, we will establish the upper bound. Let G be a unicyclic graph of order $n\,(\geq 3)$. If $\Delta = n-1$, then $G \cong S'_n$. In this case, $HSO(G) = (n-3)\sqrt{(n-1)^2+1} + \sqrt{(n-1)^2+4} + \sqrt{2}$, and hence the equality holds. Now, we consider $\Delta \leq n-2$. Let q be the number of non-pendent edges in G. It is clear that $q \geq 3$. Each non-pendent edge v_iv_j follows $f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\left(\frac{n-2}{2}\right)$. Again, for any edge $v_iv_j \in E(G)$, we have $f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\,(n-2)$. Employing these facts on (3), we derive

$$HSO(G) = \sum_{\substack{v_iv_j \in E(G)\\ d_G(v_i) \geq d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq (n-q)f(n-2) + qf\left(\frac{n-2}{2}\right)$$

$$= nf(n-2) - q\left[f(n-2) - f\left(\frac{n-2}{2}\right)\right]$$

$$\leq nf(n-2) - 3\left[f(n-2) - f\left(\frac{n-2}{2}\right)\right]$$

$$= (n-3)\sqrt{(n-2)^2+1} + \frac{3\sqrt{(n-2)^2+4}}{2} = f_1(n)(say).$$

We aim to prove that $f_1(n) < HSO(S'_n)$. Note that

$$\begin{aligned} f_1(n) - HSO(S'_n) &= -\sqrt{2} + \tfrac{3}{2}\sqrt{4+(n-2)^2} - \sqrt{4+(n-1)^2} \\ &\quad +(n-3)\sqrt{1+(n-2)^2} - (n-3)\sqrt{1+(n-1)^2}. \end{aligned}$$

One can easily check with Mathematica software that $f_1(n) - HSO(S'_n) < 0$ for $3 \le n \le 6$. Now, we take $n \ge 7$. We consider $A = \sqrt{1+\frac{1}{4}(n-2)^2}$, $B = \sqrt{1+\frac{1}{4}(n-1)^2}, C = \sqrt{1+(n-2)^2}, D = \sqrt{1+(n-1)^2}$. Then

$$f_1(n) - HSO(S'_n) = -\sqrt{2} + 3A - 2B + (n-3)(C-D).$$

We have $B^2 - A^2 = \dfrac{(n-1)^2-(n-2)^2}{4} = \dfrac{2n-3}{4} > 0$, which implies $B > A$ and hence $3A - 2B < A$. Thus, we obtain

$$f_1(n) - HSO(S'_n) < -\sqrt{2} + A + (n-3)(C-D).$$

Now, we have $D^2 - C^2 = (n-1)^2 - (n-2)^2 = 2n-3 > 0$, that yields $D > C$ and $C - D = -\dfrac{2n-3}{C+D}$. It follows that

$$(n-3)(C-D) < -\frac{(n-3)(2n-3)}{2D}.$$

As $D = \sqrt{1+(n-1)^2} < n$, this implies

$$(n-3)(C-D) < -\frac{(n-3)(2n-3)}{2n}.$$

Again note that $A < \frac{n}{2} + 1$. Therefore, finally we derive

$$f_1(n) - HSO(S'_n) < 1 - \sqrt{2} + \frac{n}{2} - \frac{(n-3)(2n-3)}{2n} = \frac{11}{2} - \sqrt{2} - \frac{1}{2}\left(n + \frac{9}{n}\right).$$

Let us construct $f(x) = x + \frac{9}{x}$ for $x \ge 7$. Then $f'(x) = 1 - \frac{9}{x^2} > 0$ for

$x \geq 7$. So, $f(x)$ is increasing and $f(x) \geq f(7) = \frac{58}{7}$. Hence, we obtain

$$f_1(n) - HSO(S'_n) < \frac{11}{2} - \sqrt{2} - \frac{29}{7} < 0 \ . \qquad \blacksquare$$

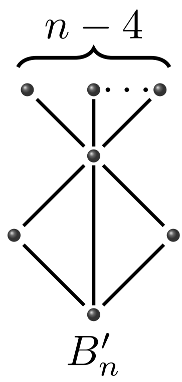

Figure 4. The bicyclic graph B'_n.

Now we characterize the maximal bicyclic graph for HSO when the graph order n is provided. Let us construct a bicyclic graph B'_n (see Figure 4) by attaching $n-4$ pendent vertices to a vertex of degree 3 of $K_4 - e$. It is clear that

$$\begin{aligned} HSO(B'_n) &= (n-4)f(n-1) + 2f\left(\frac{n-1}{2}\right) + f\left(\frac{n-1}{3}\right) + 2f\left(\frac{3}{2}\right) \\ &= (n-4)\sqrt{(n-1)^2+1} + \sqrt{(n-1)^2+4} + \frac{\sqrt{(n-1)^2+9}}{3} \\ &\quad +\sqrt{13}. \end{aligned}$$

Lemma 1. *For every positive integer n,*

$$F(n) = -\sqrt{13} + 2\sqrt{4+(n-2)^2} + \tfrac{1}{3}\sqrt{9+(n-2)^2} - \sqrt{4+(n-1)^2}$$

$$-\tfrac{1}{3}\sqrt{9+(n-1)^2} + (n-4)\sqrt{1+(n-2)^2} - (n-4)\sqrt{1+(n-1)^2}$$

is strictly negative, i.e. $F(n) < 0$.

Proof. One can easily check by the Mathematica software that $F(n) < 0$ for $1 \le n \le 3$. Next we take $n \ge 4$. Let us construct a function for $x \ge 4$ as

$$F(x) = -\sqrt{13} + 2\sqrt{4+(x-2)^2} + \tfrac{1}{3}\sqrt{9+(x-2)^2} - \sqrt{4+(x-1)^2}$$

$$-\tfrac{1}{3}\sqrt{9+(x-1)^2} + (x-4)\sqrt{1+(x-2)^2} - (x-4)\sqrt{1+(x-1)^2}.$$

Now we have

$$\begin{aligned} F'(x) &= \sqrt{1+(x-2)^2} - \sqrt{1+(x-1)^2} + (x-4)\Big(\frac{x-2}{\sqrt{1+(x-2)^2}} \\ &\quad - \frac{x-1}{\sqrt{1+(x-1)^2}}\Big) + \frac{2(x-2)}{\sqrt{4+(x-2)^2}} + \frac{x-2}{3\sqrt{9+(x-2)^2}} \\ &\quad - \frac{x-1}{\sqrt{4+(x-1)^2}} - \frac{x-1}{3\sqrt{9+(x-1)^2}} \\ &= \big(\phi(x-2) - \phi(x-1)\big) + (x-4)\big(g_1(x-2) - g_1(x-1)\big) + g_4(x-2) \\ &\quad + \tfrac{1}{3}\left(g_9(x-2) - g_9(x-1)\right) + g_4(x-2) - g_4(x-1), \qquad (7) \end{aligned}$$

where for any real $c \ge 0$,

$$g_c(x) = \frac{x}{\sqrt{c+x^2}}, \quad \phi(x) = \sqrt{1+x^2}.$$

Note that

$$g'_c(x) = \frac{c}{\left(c+x^2\right)^{3/2}} \ge 0,$$

which implies that $g_c(x)$ is increasing in x. Consequently, from (7) we obtain

$$F'(x) \le \phi(x-2) - \phi(x-1) + g_4(x-2).$$

By the Mean Value Theorem, we can write

$$\phi(x-1)-\phi(x-2)=\frac{\xi}{\sqrt{1+\xi^2}}=g_1(\xi),$$

for some $\xi \in (x-2,\, x-1)$. Thus $\phi(x-2)-\phi(x-1) \leq -g_1(x-2)$. Thus

$$\begin{aligned} F'(x) &\leq g_4(x-2)-g_1(x-2) \\ &= (x-2)\left(\frac{1}{\sqrt{4+(x-2)^2}}-\frac{1}{\sqrt{1+(x-2)^2}}\right) < 0. \end{aligned}$$

So, $F(x)$ is strictly decreasing. It is evident that $F(n) \leq F(4) < -1.7 < 0$ for $n \geq 4$. Hence, the proof is completed. ■

Theorem 6. *Let G be a bicyclic graph of order $n\,(\geq 4)$. Then*

$$HSO(G) \leq (n-4)\sqrt{(n-1)^2+1}+\sqrt{(n-1)^2+4}+\frac{\sqrt{(n-1)^2+9}}{3}+\sqrt{13},$$

where the equality occurs iff $G \cong B'_n$.

Proof. Let G be a bicyclic graph of order $n\,(\geq 4)$. We take q as the number of non-pendent edges in G. Then $q \geq 5$. Now we consider the following cases.

Case 1. $q = 5$. In this case, G is of the form as shown in Figure 5, where the non-pendent vertices v_1, v_2, v_3 and v_4 are adjacent with k_1, k_2, k_3, and k_4 number of pendent vertices, respectively. Without loss of generality, we assume that $k_1 \geq max\{k_2,\, k_3,\, k_4\}$. Now we consider the following two cases.

Case 1.1. $d_G(v_1) = n-1$. In this case, $k_2 = k_3 = k_4 = 0$ and $k_1 = n-4$. Consequently, $G \cong B'_n$ and

$$HSO(G) = (n-4)\sqrt{(n-1)^2+1}+\sqrt{(n-1)^2+4}+\frac{\sqrt{(n-1)^2+9}}{3}+\sqrt{13},$$

which implies that the equality holds.

Case 1.2. $d_G(v_1) \leq n-2$. For each pendent edge $v_iv_j \in E(G)$, we can

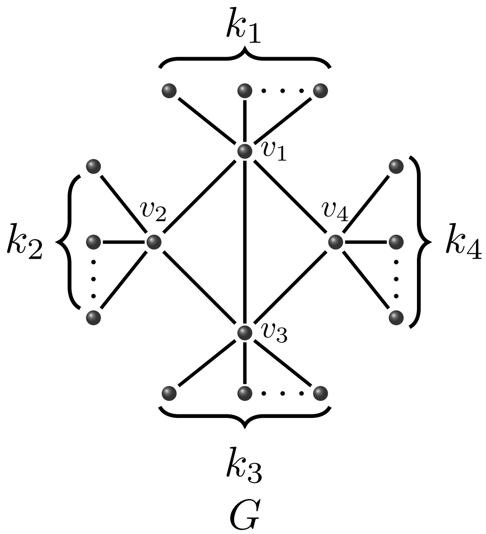

Figure 5. The bicyclic graph G for $q = 5$.

write

$$f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\,(n-2).$$

Also from Figure 5, it is evident that there is at least one non-pendent edge $v_iv_j \in E(G)$ such that

$$f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\left(\frac{n-2}{3}\right).$$

Again, we know that for any non-pendent edge $v_iv_j \in E(G)$

$$f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \leq f\left(\frac{n-2}{2}\right).$$

Employing these facts on (3), we derive

$$HSO(G) = \sum_{\substack{v_iv_j \in E(G)\\ d_G(v_i) \geq d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right)$$

$$\leq (n-4)f(n-2) + 4f\left(\frac{n-2}{2}\right) + f\left(\frac{n-2}{3}\right)$$

$$= (n-4)\sqrt{(n-2)^2+1} + 2\sqrt{(n-2)^2+4} + \frac{\sqrt{(n-2)^2+9}}{3}$$

$$= f_2(n)(say).$$

We have

$$f_2(n) - HSO(B'_n)$$

$$= \quad -\sqrt{13} + 2\sqrt{4+(n-2)^2} + \tfrac{1}{3}\sqrt{9+(n-2)^2} - \sqrt{4+(n-1)^2}$$

$$- \quad \tfrac{1}{3}\sqrt{9+(n-1)^2} + (n-4)\sqrt{1+(n-2)^2} - (n-4)\sqrt{1+(n-1)^2}.$$

Now, by Lemma 1, it is evident that $f_2(n) < HSO(B'_n)$. Therefore, $HSO(G) < HSO(B'_n)$. Thus, this case is done.

Case 2. $q = 6$. It is clear that $n \geq 5$. We construct this case in two subcases.

Case. 2.1 $\Delta = n-1$. In this case, G is of the form as shown in Figure 6.

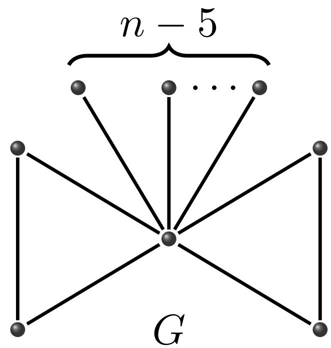

Figure 6. The bicyclic graph G for $q = 6$ and $\Delta = n-1$.

Therefore, we have

$$HSO(G) \quad = \quad (n-5)f(n-1) + 4f\left(\frac{n-1}{2}\right) + 2f(1)$$

$$= \quad (n-5)\sqrt{(n-1)^2+1}+2\sqrt{(n-1)^2+4}+2\sqrt{2}.$$

One can easily find that

$$HSO(G) - HSO(B'_n) = 2\sqrt{2} - \sqrt{13} + f_3(n),$$

where $f_3(n) = -\sqrt{n^2-2n+2} + \sqrt{n^2-2n+5} - \frac{1}{3}\sqrt{n^2-2n+10}$. Let us construct a function for $x > 0$ as

$$\psi(x) = -\sqrt{x^2+1} + \sqrt{x^2+4} - \frac{1}{3}\sqrt{x^2+9}.$$

Then, we have

$$\psi'(x) = x\left(-\frac{1}{\sqrt{x^2+1}} + \frac{1}{\sqrt{x^2+4}} - \frac{1}{3\sqrt{x^2+9}}\right) < 0,$$

which implies that $\psi(x)$ is strictly decreasing. Note that $f_3(n) = \psi(n-1) \le \psi(4) < -1.3 < 0$, which implies that $f_3(n) < 0$ for $n \ge 5$. Consequently, we have

$$HSO(G) - HSO(B'_n) < 2\sqrt{2} - \sqrt{13} < 0.$$

Hence, this case is completed.

Case. **2.2** $\Delta \le n-2$. For any edge $v_iv_j \in E(G)$, we can write $f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \le f\,(n-2)$. For any non-pendent edge $v_iv_j \in E(G)$, we have $f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \le f\left(\frac{n-2}{2}\right)$. Employing these facts on (3), we derive

$$HSO(G) = \sum_{\substack{v_iv_j \in E(G)\\ d_G(v_i) \ge d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \le (n-5)f(n-2) + 6f\left(\frac{n-2}{2}\right)$$

$$= (n-5)\sqrt{(n-2)^2+1} + 3\sqrt{(n-2)^2+4} = f_4(n)(say).$$

Now we have

$$
\begin{aligned}
&f_4(n) - HSO(B'_n) \\
&= -\sqrt{13} + 6\sqrt{1+\tfrac{1}{4}(n-2)^2} - \sqrt{1+\tfrac{1}{9}(n-1)^2} - 2\sqrt{1+\tfrac{1}{4}(n-1)^2} \\
&\quad + (n-5)\sqrt{1+(n-2)^2} - (n-4)\sqrt{1+(n-1)^2}.
\end{aligned}
$$

Claim 1. *For every integer $n \geq 5$ the function*

$$
\begin{aligned}
F(n) = &-\sqrt{13} + 6\sqrt{1+\tfrac{1}{4}(n-2)^2} - \sqrt{1+\tfrac{1}{9}(n-1)^2} - 2\sqrt{1+\tfrac{1}{4}(n-1)^2} \\
&+ (n-5)\sqrt{1+(n-2)^2} - (n-4)\sqrt{1+(n-1)^2}
\end{aligned}
$$

satisfies $F(n) < 0$.

Proof. One can easily check with Mathematica software that $F(n) < 0$ for $5 \leq n \leq 7$. Next, we consider $n \geq 8$. For $x > 0$, we use the following standard inequalities.

$$
\sqrt{1+x^2} < x + \frac{1}{2x}, \quad \sqrt{1+x^2} > x, \quad \sqrt{1+\frac{x^2}{4}} < \frac{x}{2} + \frac{1}{x}.
$$

Thus, we have

$$
\left.
\begin{aligned}
(n-5)\sqrt{1+(n-2)^2} &< (n-5)\Big(n-2+\frac{1}{2(n-2)}\Big), \\
(n-4)\sqrt{1+(n-1)^2} &> (n-4)(n-1), \\
6\sqrt{1+\frac{(n-2)^2}{4}} &< 6\Big(\frac{n-2}{2}+\frac{1}{n-2}\Big), \\
2\sqrt{1+\frac{(n-1)^2}{4}} &> (n-1), \\
\sqrt{1+\frac{(n-1)^2}{9}} &> \frac{n-1}{3}.
\end{aligned}
\right\} \tag{8}
$$

Thus, employing (8) on the expression of $F(n)$, we derive

$$
F(n) \quad < \quad 6\Big(\frac{n-2}{2}+\frac{1}{n-2}\Big) - \frac{n-1}{3} - (n-1) + (n-5)\Big(n-2
$$

$$+\frac{1}{2(n-2)}\Bigg) - (n-4)(n-1) = \frac{5+15n-2n^2}{6(n-2)} < 0 \ \text{ for } \ n \geq 8.$$

This completes the proof of claim 1.

Consequently, by claim 1, we can write $f_4(n) < HSO(B_n')$, which immediately implies $HSO(G) < HSO(B_n')$. Hence, this case is done.

Case 3. $q \geq 7$. Suppose that $\Delta(G) = n-1$, and let $v \in V(G)$ be a vertex of degree $n-1$. Then $|V(G) \setminus \{v\}| = n-1$. Let $E'(G)$ be the collection of edges incident on v. So, we have $|E'(G)| = n-1$. Since G is bicyclic, it has $|E(G)| = n+1$ edges, and hence $|E(G) \setminus E'(G)| = 2$. Let k denote the number of vertices incident to the two edges in $E(G) \setminus E'(G)$. Clearly, $k \leq 4$, since each edge has two endpoints. Each of these k vertices is adjacent to v and thus contributes to non-pendent edges. Therefore, the total number of non-pendent edges is $q = k+2$. Since $q \geq 7$, we must have $k \geq 5$, which contradicts the fact that $k \leq 4$. Hence, no vertex can have degree $n-1$, and it follows that $\Delta(G) \leq n-2$. Consequently, we can write

$$\begin{aligned}
HSO(G) &= \sum_{\substack{v_iv_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} f\left(\frac{d_G(v_i)}{d_G(v_j)}\right) \\
&\leq (n-q+1)f(n-2) + qf\left(\frac{n-2}{2}\right) \\
&= (n+1)f(n-2) - q\left[f(n-2) - f\left(\frac{n-2}{2}\right)\right] \\
&\leq (n+1)f(n-2) - 7\left[f(n-2) - f\left(\frac{n-2}{2}\right)\right] \\
&= (n-6)f(n-2) + 7f\left(\frac{n-2}{2}\right) \\
&< (n-5)f(n-2) + 6f\left(\frac{n-2}{2}\right) = f_4(n).
\end{aligned}$$

In view of claim 1, we can write $HSO(G) < HSO(B_n')$. Hence, the proof is completed. ■

Lemma 2. *Let ℓ be the number of pendent paths of G. Then*

$$HSO(G) \geq \sqrt{2}\,|E(G)| + \ell\Big(f(2) + f(\tfrac{3}{2}) - 2\sqrt{2}\Big).$$

Proof. Since $f(x) \geq f(1) = \sqrt{2}$ for all $x \geq 1$, summing $\sqrt{2}$ over the $|E(G)|$ edges gives the baseline $\sqrt{2}\,|E(G)|$. Now, fix a pendent path $P = v_1v_2\ldots v_t$ with $t \geq 3$. The terminal edge $v_{t-1}v_t$ contributes $f(2)$, while the edge v_1v_2 (with $d(v_2) = 2$) contributes at least $f(3/2)$. Hence, these two distinguished edges together contribute at least $f(2)+f(3/2)$, whereas their baseline contribution is $2\sqrt{2}$. Thus, each pendent path of length at least 2 yields a surplus of at least $f(2)+f(3/2)-2\sqrt{2}$ above the baseline. If G contains a pendent path $P = v_1v_2$ of length 1, then this edge contributes at least $f(3)$, so its surplus over baseline is at least $f(3) - \sqrt{2}$, which is strictly greater than $f(2) + f(3/2) - 2\sqrt{2}$. Therefore every pendent path contributes a surplus of at least $f(2) + f(3/2) - 2\sqrt{2}$. Adding the baseline $\sqrt{2}\,|E(G)|$ and the ℓ surpluses completes the proof. ■

Now we are going to characterize first eight minimum trees for HSO when the tree order n is provided. For that, we construct some families of trees as follows. Let $\mathcal{T}(n)$ be the family of trees of order n such that $\Delta = 3$. Now, we construct two families $\mathcal{T}^1(n)$ and $\mathcal{T}^2(n)$ as $\mathcal{T}^1(n) = \{T \in \mathcal{T}(n) : n_3 = 1\}$ and $\mathcal{T}^2(n) = \{T \in \mathcal{T}(n) : n_3 = 2\}$. Then we construct the following families. For $n \geq 7$, $\mathcal{T}_1(n) = \{T \in \mathcal{T}^1(n) : \ell_1 = 0\}$ (see Figure 7(i)); for $n \geq 6$, $\mathcal{T}_2(n) = \{T \in \mathcal{T}^1(n) : \ell_1 = 1\}$ (see Figure 7(ii)); For $n \geq 5$, $\mathcal{T}_3(n) = \{T \in \mathcal{T}^1(n) : \ell_1 = 2\}$ (see Figure 7(iii)).

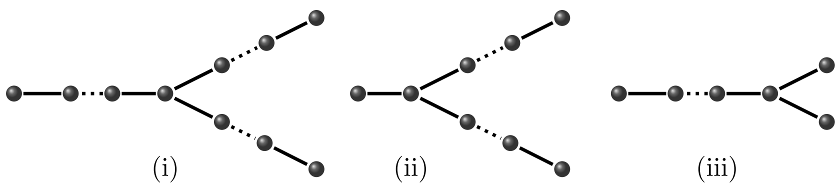

Figure 7. The example of trees belonging to (i) $\mathcal{T}_1(n)$, (ii) $\mathcal{T}_2(n)$ and (iii) $\mathcal{T}_3(n)$.

Let $\mathcal{T}^{2*}(n) \subseteq \mathcal{T}^2(n)$ be the collection of trees such that the two vertices of degree 3 are adjacent. Then we construct the following families. For

$n \geq 10$, $\mathcal{T}_4(n) = \{T \in \mathcal{T}^{2*}(n) : \ell_1 = 0\}$ (see Figure 8(i)); for $n \geq 9$, $\mathcal{T}_5(n) = \{T \in \mathcal{T}^{2*}(n) : \ell_1 = 1\}$ (see Figure 8(ii)); For $n \geq 11$, $\mathcal{T}_6(n) = \{T \in \mathcal{T}^2(n) \backslash \mathcal{T}^{2*}(n) : \ell_1 = 0\}$ (see Figure 9); For $n \geq 8$, $\mathcal{T}_7(n) = \{T \in \mathcal{T}^{2*}(n) : \ell_1 = 2\}$ (see Figure 10).

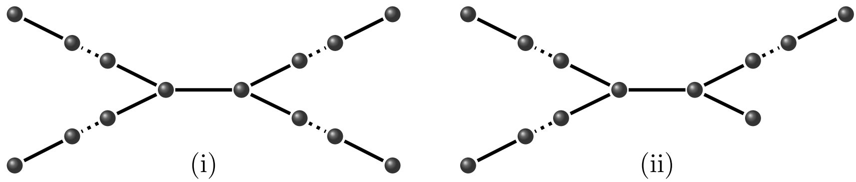

Figure 8. The example of trees belonging to (i) $\mathcal{T}_4(n)$ and (ii) $\mathcal{T}_5(n)$.

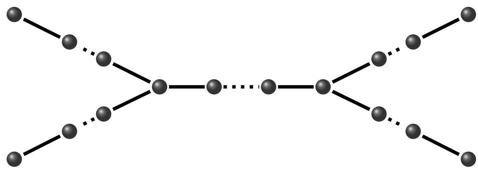

Figure 9. The example of tree belongs to $\mathcal{T}_6(n)$.

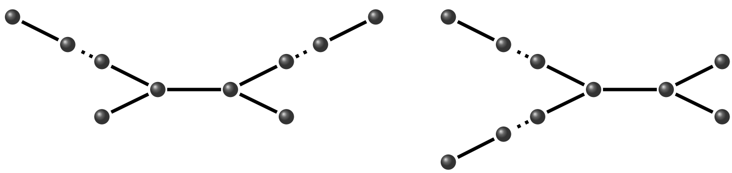

Figure 10. The example of trees belonging to $\mathcal{T}_7(n)$.

Theorem 7. *Among all n-vertex trees, the following results hold for the HSO index:*

1. *For $n \geq 7$, the HSO index attains its second minimum value*

$$HSO(T) = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + (n-7)\sqrt{2}$$

if and only if $T \in \mathcal{T}_1(n)$.

2. *For* $n \geq 7$, *the HSO index attains its third minimum value*

$$HSO(T) = \sqrt{13} + 2\sqrt{5} + \sqrt{10} + (n-6)\sqrt{2}$$

if and only if $T \in \mathcal{T}_2(n)$.

3. *For* $n \geq 7$, *the HSO index attains its fourth minimum value*

$$HSO(T) = \frac{\sqrt{13}}{2} + \sqrt{5} + 2\sqrt{10} + (n-5)\sqrt{2}$$

if and only if $T \in \mathcal{T}_3(n)$.

4. *For* $n \geq 10$, *the HSO index attains its fifth minimum value*

$$HSO(T) = 2\sqrt{13} + 4\sqrt{5} + (n-9)\sqrt{2}$$

if and only if $T \in \mathcal{T}_4(n)$.

5. *For* $n \geq 10$, *the HSO index attains its sixth minimum value*

$$HSO(T) = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + \sqrt{10} + (n-8)\sqrt{2}$$

if and only if $T \in \mathcal{T}_5(n)$.

6. *For* $n \geq 11$, *the HSO index attains its seventh minimum value*

$$HSO(T) = 3\sqrt{13} + 4\sqrt{5} + (n-11)\sqrt{2}$$

if and only if $T \in \mathcal{T}_6(n)$.

7. *For* $n \geq 11$, *the HSO index attains its eighth minimum value*

$$HSO(T) = \sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-7)\sqrt{2}$$

if and only if $T \in \mathcal{T}_7(n)$.

Proof. Let T be a tree of order n. We know from Theorem 3 that P_n is the minimal tree for HSO. So in this proof, we consider $T \not\cong P_n$. One can easily verify the results by Sage software for $7 \leq n \leq 10$. Next, we consider $n \geq 11$. If $T \in \mathcal{T}_i(n)$ $(1 \leq i \leq 7)$, then we denote the value of $HSO(T)$ as A_i. Thus, we have

$$A_i = \begin{cases} 3f\left(\frac{3}{2}\right) + 3f(2) + (n-7)\sqrt{2} = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + (n-7)\sqrt{2} & \text{for } i = 1, \\ 2f\left(\frac{3}{2}\right) + 2f(2) + f(3) + (n-6)\sqrt{2} = \sqrt{13} + 2\sqrt{5} + \sqrt{10} + (n-6)\sqrt{2} & \text{for } i = 2, \\ f\left(\frac{3}{2}\right) + f(2) + 2f(3) + (n-5)\sqrt{2} = \frac{\sqrt{13}}{2} + \sqrt{5} + 2\sqrt{10} + (n-5)\sqrt{2} & \text{for } i = 3, \\ 4f\left(\frac{3}{2}\right) + 4f(2) + (n-9)\sqrt{2} = 2\sqrt{13} + 4\sqrt{5} + (n-9)\sqrt{2} & \text{for } i = 4. \\ 3f\left(\frac{3}{2}\right) + 3f(2) + f(3) + (n-8)\sqrt{2} = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + \sqrt{10} + (n-8)\sqrt{2} & \text{for } i = 5, \\ 6f\left(\frac{3}{2}\right) + 4f(2) + (n-11)\sqrt{2} = 3\sqrt{13} + 4\sqrt{5} + (n-11)\sqrt{2} & \text{for } i = 6, \\ 2f\left(\frac{3}{2}\right) + 2f(2) + 2f(3) + (n-7)\sqrt{2} = \sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-7)\sqrt{2} & \text{for } i = 7. \end{cases}$$

One can easily check that $A_7 > A_6 > A_5 > A_4 > A_3 > A_2 > A_1$. Let $\mathcal{A}(n) = \bigcup_{i=1}^{7} \mathcal{T}_i(n)$. Now, it is sufficient to prove that $HSO(T) > A_7$ for all $T \in T(n) \backslash \mathcal{A}(n)$. Let $T \in T(n) \backslash \mathcal{A}(n)$. Since $T \not\cong P_n$, we must have $\ell \geq 3$. If $\ell = 3$, then since $n \geq 11$, we must have $T \in \mathcal{T}_1(n) \cup \mathcal{T}_2(n) \cup \mathcal{T}_3(n) \subseteq \mathcal{A}(n)$, which is a contradiction. So we consider $\ell \geq 4$. Now, we construct the proof in the following two cases.

Case 1. $\ell = 4$. In this case $3 \leq \Delta \leq 4$. So, we construct this case into following sub-cases.

Case. 1.1. $\Delta = 3$. In this case, T contains exactly two vertices of degree 3. Let $u, v \in V(T)$ such that $d_T(u) = d_T(v) = 3$. Now, we consider the following two sub-cases.

Case. 1.1.1. $uv \in E(T)$. Then $0 \leq \ell_1 \leq 3$, as $n \geq 11$. If $0 \leq \ell_1 \leq 2$, then we must have $T \in \mathcal{T}_4(n) \cup \mathcal{T}_5(n) \cup \mathcal{T}_7(n) \subseteq \mathcal{A}(n)$, a contradiction. Hence we consider $\ell_1 = 3$, in which case

$$\begin{aligned} HSO(T) &= f\left(\frac{3}{2}\right) + f(2) + 3f(3) + (n-6)\sqrt{2} \\ &= \frac{\sqrt{13}}{2} + \sqrt{5} + 3\sqrt{10} + (n-6)\sqrt{2} > A_7. \end{aligned}$$

Case. 1.1.2. $uv \notin E(T)$. Then $0 \leq \ell_1 \leq 4$. For $\ell_1 = 0$, we must have $T \in \mathcal{T}_6(n) \subseteq \mathcal{A}(n)$. So we consider $1 \leq \ell_1 \leq 4$. If we represent the value of $HSO(T)$ at $\ell_1 = i$ by B_i, then we have

$$B_i = \begin{cases} 5f\left(\frac{3}{2}\right) + 3f(2) + f(3) + (n-10)\sqrt{2} = \frac{5\sqrt{13}}{2} + 3\sqrt{5} + \sqrt{10} + (n-10)\sqrt{2} & \text{for } i = 1, \\ 4f\left(\frac{3}{2}\right) + 2f(2) + 2f(3) + (n-9)\sqrt{2} = 2\sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-9)\sqrt{2} & \text{for } i = 2, \\ 3f\left(\frac{3}{2}\right) + f(2) + 3f(3) + (n-8)\sqrt{2} = \frac{3\sqrt{13}}{2} + \sqrt{5} + 3\sqrt{10} + (n-8)\sqrt{2} & \text{for } i = 3. \\ 2f\left(\frac{3}{2}\right) + 4f(3) + (n-7)\sqrt{2} = \sqrt{13} + 4\sqrt{10} + (n-7)\sqrt{2} & \text{for } i = 4. \end{cases}$$

One can easily check that

$$B_4 > B_3 > B_2 > B_1 > \sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-7)\sqrt{2} = A_7.$$

Case. 1.2. $\Delta = 4$. Note that T contains exactly one vertex of degree 4. Let $u \in V(T)$ such that $d_T(u) = 4$. As, $n \geq 11$, we have $0 \leq \ell_1 \leq 3$. If we represent the value of $HSO(T)$ at $\ell_1 = i$ by C_i, then we have

$$C_i = \begin{cases} 4f\left(\frac{4}{2}\right) + 4f(2) + (n-9)\sqrt{2} = 8\sqrt{5} + (n-9)\sqrt{2} & \text{for } i = 0, \\ 3f\left(\frac{4}{2}\right) + 3f(2) + f(4) + (n-8)\sqrt{2} = 6\sqrt{5} + \sqrt{17} + (n-8)\sqrt{2} & \text{for } i = 1, \\ 2f\left(\frac{4}{2}\right) + 2f(2) + 2f(4) + (n-7)\sqrt{2} = 4\sqrt{5} + 2\sqrt{17} + (n-7)\sqrt{2} & \text{for } i = 2, \\ f\left(\frac{4}{2}\right) + f(2) + 3f(4) + (n-6)\sqrt{2} = 2\sqrt{5} + 3\sqrt{17} + (n-6)\sqrt{2} & \text{for } i = 3. \end{cases}$$

One can easily check that

$$C_3 > C_2 > C_1 > C_0 > \sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-7)\sqrt{2} = A_7.$$

Case 2. $\ell \geq 5$. By Lemma 2, it is evident that

$$\begin{aligned} HSO(T) &\geq \sqrt{2}\,(n-1) + 5\Big(f(2) + f\left(\tfrac{3}{2}\right) - 2\sqrt{2}\Big) \\ &= (n-11)\sqrt{2} + 5\sqrt{5} + \frac{5\sqrt{13}}{2} \\ &> \sqrt{13} + 2\sqrt{5} + 2\sqrt{10} + (n-7)\sqrt{2} = A_7. \end{aligned}$$

■

Table 1. Ordering of minimal trees with respect to the HSO index for small values of n.

	Second	Third	Fourth	Fifth	Sixth	Seventh	Eighth
$n = 4$	T_1	–	–	–	–	–	–
$n = 5$	T_2	T_3	–	–	–	–	–
$n = 6$	T_4	T_5	T_6	T_7	T_8	–	–
$n = 7$	–	–	–	T_9	T_{10}	T_{11}	T_{12}
$n = 8$	–	–	–	T_{13}, T_{14}	T_{15}	T_{16}	T_{17}
$n = 9$	–	–	–	T_{18}	T_{19}, T_{20}	T_{21}	T_{22}
$n = 10$	–	–	–	–	–	T_i $(23 \leq i \leq 26)$	T_{27}

Remark 1. *Theorem 7 does not completely determine the ordering of trees with minimal HSO for small values of n. The remaining cases are summarized in Table 1. The structures of T_i for $1 \leq i \leq 27$ in Table 1 are depicted in Figure 11.*

Next, we identify the first seven minimal unicyclic graphs with respect to the HSO index for a given order n. Accordingly, six families of unicyclic graphs are constructed as follows.

1. $\mathcal{U}_1(n)$ is the collection of graphs generated by attaching a pendent path of length $n - k \geq 2$ to a vertex of C_k (see Figure 12 (i)).
2. $\mathcal{U}_2(n)$ is the collection of graphs generated by attaching a pendent path of length one to a vertex of C_{n-1} (see Figure 12 (ii)).
3. $\mathcal{U}_3(n)$ denotes the collection of graphs having exactly two adjacent vertices of maximum degree 3, each of which is adjacent to two vertices of degree 2. (see Figure 13).
4. $\mathcal{U}_4(n)$ is the collection of graphs generated by attaching a pendent path of length at least 2 to each vertex of C_3 (see Figure 14).
5. $\mathcal{U}_5(n)$ denotes the collection of graphs having exactly two adjacent vertices of maximum degree 3, where one of them is adjacent to two vertices of degree 2, and the other is adjacent to one pendent vertex and one vertex of degree 2 (see Figure 15).
6. $\mathcal{U}_6(n)$ denotes the collection of graphs having exactly two non-adjacent vertices of maximum degree 3, each of which is adjacent to three vertices of degree 2. (see Figure 16).

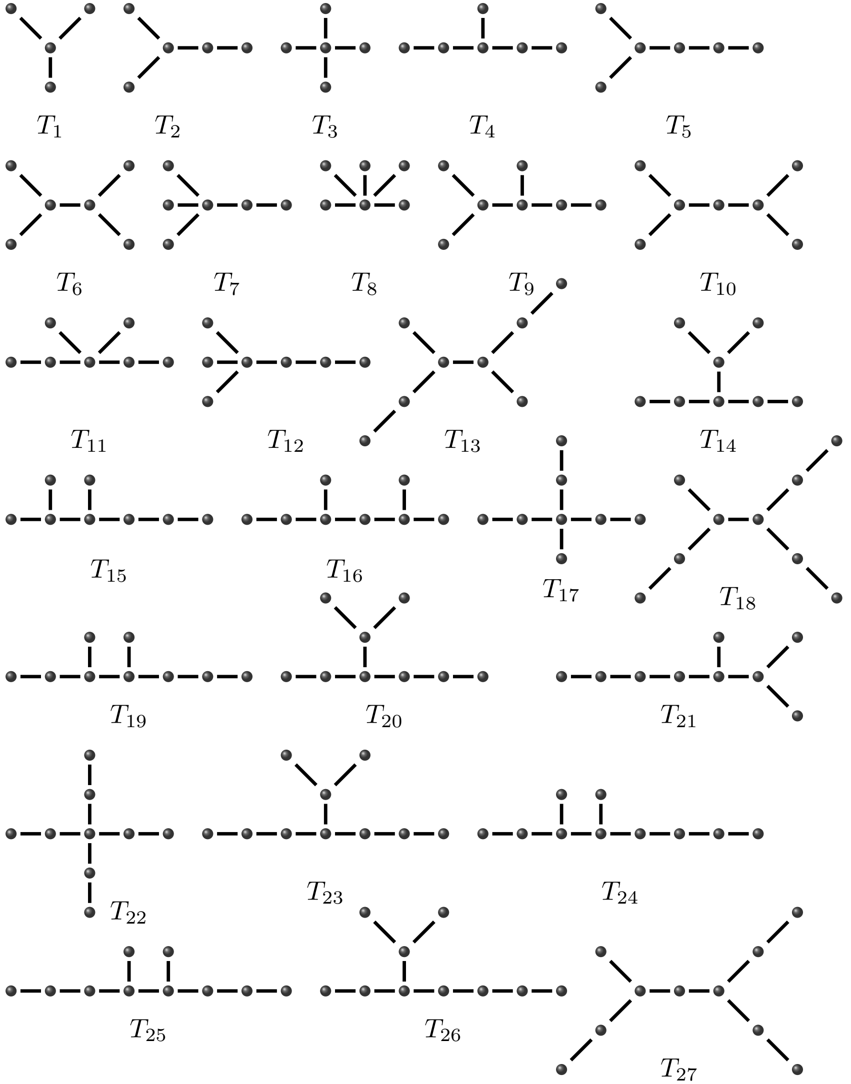

Figure 11. The trees T_i, $1 \leq i \leq 27$.

It is clear that the classes $\mathcal{U}_1(n), \mathcal{U}_2(n), \mathcal{U}_3(n), \mathcal{U}_4(n), \mathcal{U}_5(n)$, and $\mathcal{U}_6(n)$ are defined for $n \geq 5, 4, 8, 9, 7, 8$, respectively.

Theorem 8. *Among all n-vertex unicyclic graphs, the following results hold for the HSO index:*

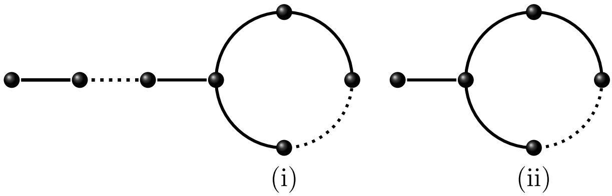

Figure 12. The example of unicyclic graphs belonging to (i) $\mathcal{U}_1(n)$ and (ii) $\mathcal{U}_2(n)$.

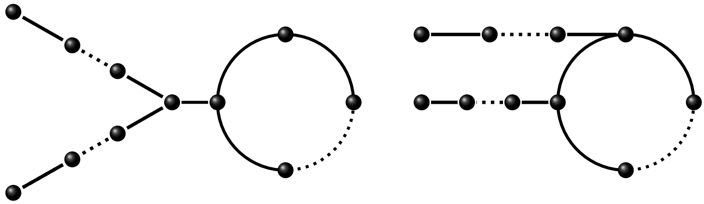

Figure 13. The example of unicyclic graphs belonging to $\mathcal{U}_3(n)$.

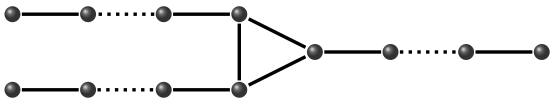

Figure 14. The example of unicyclic graph belonging to $\mathcal{U}_4(n)$.

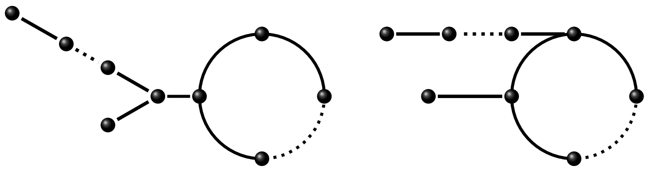

Figure 15. The example of unicyclic graphs belonging to $\mathcal{U}_5(n)$.

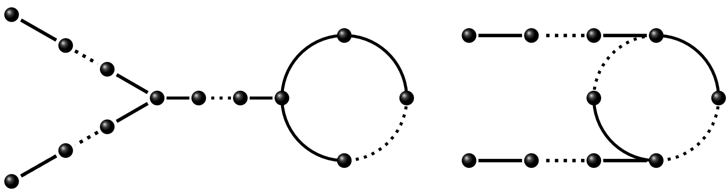

Figure 16. The example of unicyclic graphs belonging to $\mathcal{U}_6(n)$.

1. *For $n \geq 5$, the HSO index attains its second minimum value*

$$HSO(U) = 3f\left(\tfrac{3}{2}\right) + f(2) + (n-4)\sqrt{2} = \frac{3\sqrt{13}}{2} + \sqrt{5} + (n-4)\sqrt{2}$$

if and only if $U \in \mathcal{U}_1(n)$.

2. *For $n \geq 5$, the HSO index attains its third minimum value*

$$HSO(U) = 2f\left(\tfrac{3}{2}\right) + f(3) + (n-3)\sqrt{2} = \sqrt{13} + \sqrt{10} + (n-3)\sqrt{2}$$

if and only if $U \in \mathcal{U}_2(n)$.

3. *For $n \geq 7$, the HSO index attains its fourth minimum value*

$$HSO(U) = 4f\left(\tfrac{3}{2}\right) + 2f(2) + (n-6)\sqrt{2} = 2\sqrt{13} + 2\sqrt{5} + (n-6)\sqrt{2}$$

if and only if $U \in \mathcal{U}_3(n)$.

4. *For $n \geq 9$, the HSO index attains its fifth minimum value*

$$HSO(U) = 3f\left(\tfrac{3}{2}\right) + 3f(2) + (n-6)\sqrt{2} = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + (n-6)\sqrt{2}$$

if and only if $U \in \mathcal{U}_4(n)$.

5. *For $n \geq 9$, the HSO index attains its sixth minimum value*

$$HSO(U) = \frac{3\sqrt{13}}{2} + \sqrt{5} + \sqrt{10} + (n-5)\sqrt{2}$$

if and only if $U \in \mathcal{U}_5(n)$.

6. *For $n \geq 9$, the HSO index attains its seventh minimum value*

$$HSO(U) = 6f\left(\tfrac{3}{2}\right) + 2f(2) + (n-8)\sqrt{2} = 3\sqrt{13} + 2\sqrt{5} + (n-8)\sqrt{2}$$

if and only if $U \in \mathcal{U}_6(n)$.

Proof. Let U be a unicyclic graph of order n. We know from Theorem 4 that C_n is the minimal unicyclic graph for HSO. So in this proof, we consider $U \ncong C_n$. One can easily verify the results by Sage for $5 \leq n \leq 8$.

Next, we consider $n \geq 9$. If $U \in \mathcal{U}_i(n)$ $(1 \leq i \leq 6)$, then we denote the value of $HSO(U)$ as D_i. Thus, we have

$$D_i = \begin{cases} 3f\left(\frac{3}{2}\right) + f(2) + (n-4)\sqrt{2} = \frac{3\sqrt{13}}{2} + \sqrt{5} + (n-4)\sqrt{2} & \text{for } i = 1, \\ 2f\left(\frac{3}{2}\right) + f(3) + (n-3)\sqrt{2} = \sqrt{13} + \sqrt{10} + (n-3)\sqrt{2} & \text{for } i = 2, \\ 4f\left(\frac{3}{2}\right) + 2f(2) + (n-6)\sqrt{2} = 2\sqrt{13} + 2\sqrt{5} + (n-6)\sqrt{2} & \text{for } i = 3, \\ 3f\left(\frac{3}{2}\right) + 3f(2) + (n-6)\sqrt{2} = \frac{3\sqrt{13}}{2} + 3\sqrt{5} + (n-6)\sqrt{2} & \text{for } i = 4. \\ 3f\left(\frac{3}{2}\right) + f(2) + f(3) + (n-5)\sqrt{2} = \frac{3\sqrt{13}}{2} + \sqrt{5} + \sqrt{10} + (n-5)\sqrt{2} & \text{for } i = 5. \\ 6f\left(\frac{3}{2}\right) + 2f(2) + (n-8)\sqrt{2} = 3\sqrt{13} + 2\sqrt{5} + (n-8)\sqrt{2} & \text{for } i = 6. \end{cases}$$

One can easily check that $D_6 > D_5 > D_4 > D_3 > D_2 > D_1$. Let $\mathcal{A}(n) = \bigcup_{i=1}^{6} \mathcal{U}_i(n)$. Now, it is sufficient to prove that $HSO(U) > D_6$ for all $U \in U(n) \backslash \mathcal{A}(n)$. Let $U \in U(n) \backslash \mathcal{A}(n)$. As, $U \ncong C_n$, we must have $\ell \geq 1$. If $\ell = 1$, then we must have $U \in \mathcal{U}_1(n) \cup \mathcal{U}_2(n) \subseteq \mathcal{A}(n)$, a contradiction. So we consider $\ell \geq 2$. Now, we construct the proof in the following two cases.

Case 1. $\ell = 2$. In this case $3 \leq \Delta \leq 4$. So, we construct this case into following sub-cases.

Case. 1.1. $\Delta = 3$. In this case, U contains exactly two vertices of degree 3. Let u, $v \in V(U)$ such that $d_U(u) = d_U(v) = 3$. Now, we consider the following two sub-cases.

Case. 1.1.1. $uv \in E(U)$. In this case, the only possibility is that each pendent path of U is of length 1. Otherwise, $U \in \mathcal{U}_3(n) \cup \mathcal{U}_5(n) \subseteq \mathcal{A}(n)$, a contradiction. Consequently, we obtain

$$HSO(U) = 2f\left(\frac{3}{2}\right) + 2f(3) + (n-4)\sqrt{2} = \sqrt{13} + 2\sqrt{10} + (n-4)\sqrt{2} > D_6.$$

Case. 1.1.2. $uv \notin E(U)$. Note that $0 \leq \ell_1 \leq 2$. If $\ell_1 = 0$, then $U \in \mathcal{U}_6(n) \subseteq \mathcal{A}(n)$, a contradiction. Thus, we consider $\ell_1 \neq 0$. Then we get at least two pendent edges $v_p v_q$ and $v_r v_s$ with $d_U(v_q) = d_U(v_s) = 1$ such that $\frac{d_U(v_p)}{d_U(v_q)} = 3$ and $\frac{d_U(v_r)}{d_U(v_s)} \geq 2$. Also, it is clear that there are at least four edges $v_i v_j$ with $d_U(v_i) \geq d_U(v_j)$ such that $\frac{d_U(v_i)}{d_U(v_j)} = \frac{3}{2}$. Therefore, we can write

$$\begin{aligned} HSO(U) &\geq 4f\Big(\tfrac{3}{2}\Big) + f(3) + f(2) + (n-6)\sqrt{2} \\ &= 2\sqrt{13} + \sqrt{10} + \sqrt{5} + (n-6)\sqrt{2} > D_6. \end{aligned}$$

Case. 1.2. $\Delta = 4$. We know that $0 \leq \ell_1 \leq 2$. First we consider $\ell_1 \neq 0$. Then we get at least two pendent edges v_pv_q and v_rv_s with $d_U(v_q) = d_U(v_s) = 1$ such that $\frac{d_U(v_p)}{d_U(v_q)} = 4$ and $\frac{d_U(v_r)}{d_U(v_s)} \geq 2$. Also, it is clear that there are at least two edges v_iv_j with $d_U(v_i) \geq d_U(v_j)$ such that $\frac{d_U(v_i)}{d_U(v_j)} = \frac{4}{2}$. Therefore, we can write

$$HSO(U) \geq f(4) + 3f(2) + (n-4)\sqrt{2} = \sqrt{17} + 3\sqrt{5} + (n-4)\sqrt{2} > D_6.$$

Next we take $\ell_1 = 0$. In this case

$$HSO(U) = 6f(2) + (n-6)\sqrt{2} = 6\sqrt{5} + (n-6)\sqrt{2} > D_6.$$

Case 2. $\ell = 3$. In this case $0 \leq \ell_1 \leq 3$. First we consider $\ell_1 \geq 1$. Then we get at least one pendent edge v_iv_j with $d_U(v_j) = 1$ such that $\frac{d_U(v_i)}{d_U(v_j)} \geq 3$. It is clear that there are at least two pairs of edges v_pv_q and v_rv_s other than v_iv_j with $d_U(v_p) \geq d_U(v_q)$ and $d_U(v_r) \geq d_U(v_s)$ such that $f\left(\frac{d_U(v_p)}{d_U(v_q)}\right) + f\left(\frac{d_U(v_r)}{d_U(v_s)}\right) \geq f\left(\frac{3}{2}\right) + f(2)$. Therefor, we can write

$$\begin{aligned} HSO(U) &\geq f(3) + 2f(2) + 2f\left(\frac{3}{2}\right) + (n-5)\sqrt{2} \\ &= \sqrt{13} + 2\sqrt{5} + \sqrt{10} + (n-5)\sqrt{2} > D_6. \end{aligned}$$

Now, we consider $\ell_1 = 0$. It is clear that $3 \leq \Delta \leq 5$. Next, we construct this case in the following sub-cases.

Case 2.1. $\Delta = 3$. In this case U contains three vertices of degree 3. Consider three vertices u, v, w such that $d_U(u) = d_U(v) = d_U(w) = 3$. If u, v, w are pairwise adjacent, then $U \in \mathcal{U}_4(n) \subseteq \mathcal{A}(n)$, a contradiction. Thus, we consider that at most two pairs of u, v, w are adjacent. It is easy to check that U contains three pendent edges v_pv_q, with $d_U(v_q) = 1$ such that $\frac{d_U(v_p)}{d_U(v_q)} = 2$. Again, since $n \geq 9$, it is clear that there are at least five edges v_iv_j, with $d_U(v_i) \geq d_U(v_j)$ such that $\frac{d_U(v_i)}{d_U(v_j)} = \frac{3}{2}$. Consequently, we have

$$HSO(U) \geq 3f(2)+5f\left(\frac{3}{2}\right)+(n-8)\sqrt{2} = \frac{5\sqrt{13}}{2}+3\sqrt{5}+(n-8)\sqrt{2} > D_6.$$

Case 2.2. $4 \leq \Delta \leq 5$. In this case, one can easily obtain likewise previous cases that

$$HSO(U) \geq 4f(2)+2f\left(\frac{3}{2}\right)+(n-6)\sqrt{2} = \sqrt{13}+4\sqrt{5}+(n-6)\sqrt{2} > D_6.$$

Case 3. $\ell \geq 4$. By Lemma 2, it is evident that

$$\begin{aligned} HSO(U) &\geq \sqrt{2}n + 4\Big(f(2)+f(\tfrac{3}{2}) - 2\sqrt{2}\Big) \\ &= (n-8)\sqrt{2}+4\sqrt{5}+2\sqrt{13} \\ &> 3\sqrt{13}+2\sqrt{5}+(n-8)\sqrt{2} = D_6. \end{aligned}$$

■

Remark 2. *Theorem 8 does not completely determine the ordering of unicyclic graphs with minimal HSO for small values of n. The remaining cases are summarized in Table 2.*

Table 2. Ordering of minimal unicyclic graphs with respect to the HSO index for small values of n.

	Third	Fourth	Fifth	Sixth	Seventh
$n=5$	U_1	U_2	U_3	–	–
$n=6$	–	U_4	U_5, U_6	U_7	U_8
$n=7$	–	–	U_9,U_{10}, U_{11}	U_{12}, U_{13}	U_{14}
$n=8$	–	–	U_i $(15 \leq i \leq 19)$	U_{20}	U_{21}

The structures of U_i for $1 \leq i \leq 21$ are depicted in Figure 17.

Now we characterize the first seven minimal bicyclic graphs with re-

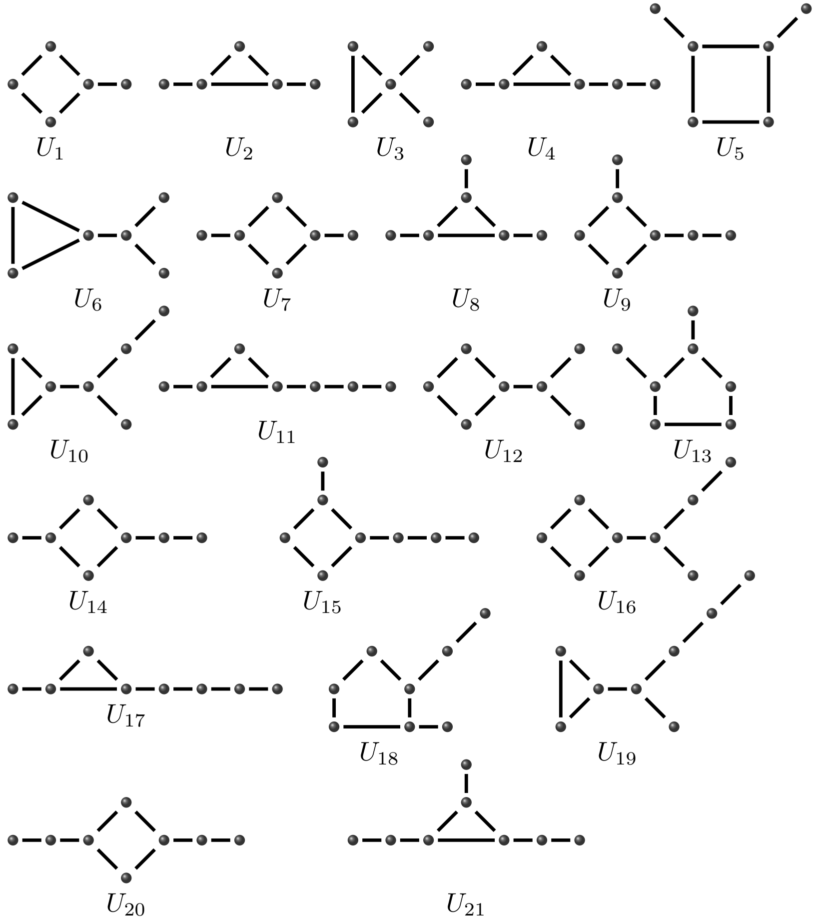

Figure 17. The unicyclic graphs U_i, $1 \leq i \leq 21$.

spect to the HSO index for a given graph order n. To this end, we construct numerous families of bicyclic graphs. First, we define three families of bicyclic graphs that contain no pendent vertices. Let $\mathcal{B}_0^1(n) \subseteq B(n)$ denote the collection of bicyclic graphs obtained by joining two nonadjacent vertices of a cycle C_t $(4 \leq t \leq n)$ by a path of length $n-t+1$ (see Figure 18(iii)). Next, let $\mathcal{B}_0^2(n) \subseteq B(n)$ denote the collection of bicyclic graphs obtained by joining two disjoint cycles C_s and C_t $(s+t \leq n)$ by a path of length $n-s-t+1$ (see Figure 18(ii)). Finally, let $\mathcal{B}_0^3(n) \subseteq B(n)$

denote the collection of bicyclic graphs formed by two cycles C_s and C_t sharing exactly one common vertex, where $s+t-1=n$ (see Figure 18(i)).

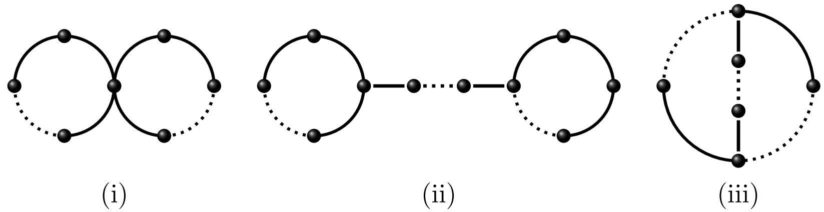

Figure 18. The example of bicyclic graphs belonging to (i) $\mathcal{B}_0^3(n)$, (ii) $\mathcal{B}_0^2(n)$ and (iii) $\mathcal{B}_0^1(n)$.

Now we construct four classes of bicyclic graphs from the aforesaid families as follows (see Figures 19 (i), (ii)):

$$\mathcal{B}_1(n) = \{B \in \mathcal{B}_0^1(n) : t = n\}, \quad \mathcal{B}_2(n) = \{B \in \mathcal{B}_0^2(n) : s + t = n\},$$

$$\mathcal{B}_3(n) = \{B \in \mathcal{B}_0^1(n) : t < n\}, \quad \mathcal{B}_4(n) = \{B \in \mathcal{B}_0^2(n) : s + t < n\}.$$

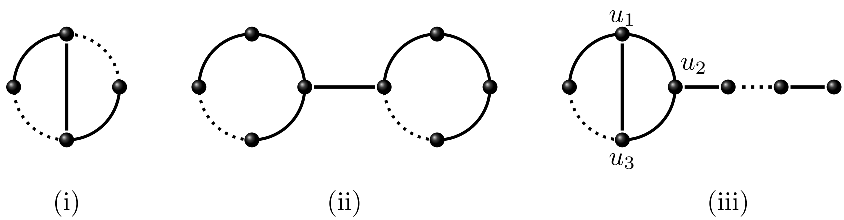

Figure 19. The example of bicyclic graphs belonging to (i) $\mathcal{B}_1(n)$, (ii) $\mathcal{B}_2(n)$ and (iii) $\mathcal{B}_5(n)$.

Next, we construct six families of bicyclic graphs of order n having at least one pendent vertices as follows:
(1) $\mathcal{B}_5(n)$ is the collection of graphs generated from $C_t : u_1u_2\cdots u_t$ with $4 \le t \le n-2$ by joining u_1 and u_3 by an edge, and attaching a pendent path of length $n-t$ to u_2 (see Figure 19 (iii)).
(2) $\mathcal{B}_6(n)$ is the collection of graphs $B \subseteq B(n)$ generated from the unique member of $\mathcal{B}_1(4)$ by attaching a pendent path of length at least 2 on two vertices u, v with $d_B(u) = d_B(v) = 3$ (see Figure 20 (i)).

(3) $\mathcal{B}_7(n)$ is the collection of graphs generated from $C_{n-1} : u_1u_2\cdots u_{n-1}$ by joining u_1 and u_3 by an edge, and attaching a pendent path of length 1 to u_2 (see Figure 20 (ii)).

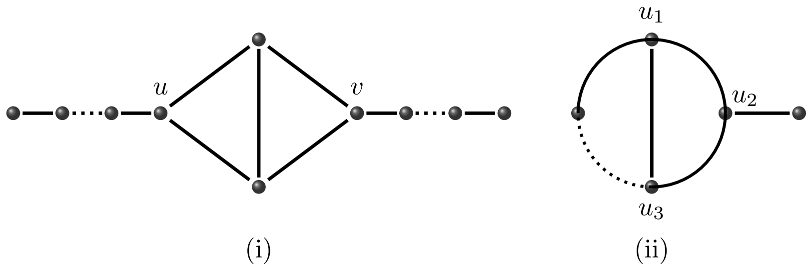

Figure 20. The example of bicyclic graphs belonging to (i) $\mathcal{B}_6(n)$ and (ii) $\mathcal{B}_7(n)$.

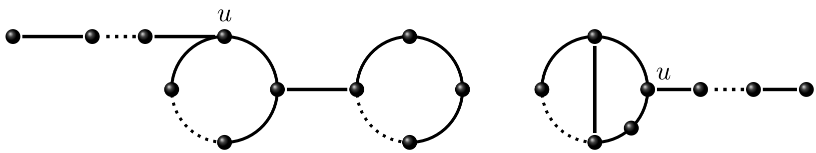

Figure 21. The example of bicyclic graphs belonging to $\mathcal{B}_8(n)$.

(4) $\mathcal{B}_8(n)$ is the collection of graphs B generated from a member of $\mathcal{B}_1(k)$ ($k \geq 5$) or $\mathcal{B}_2(k)$ ($k \geq 6$) by attaching a pendent path of length $n - k \geq 2$ to a vertex u with $d_B(u) = 3$, where u is adjacent to a vertex of degree 3 and two vertices of degree 2 (see Figure 21).

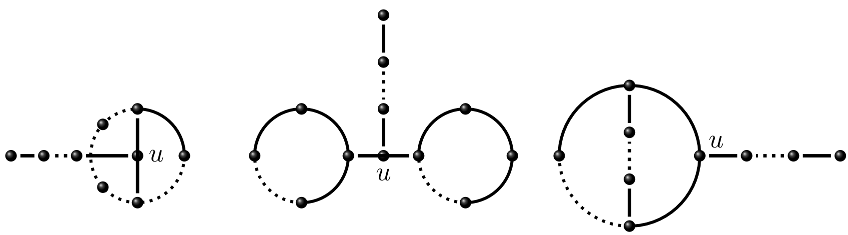

Figure 22. The example of bicyclic graphs belonging to $\mathcal{B}_9(n)$.

(5) $\mathcal{B}_9(n)$ is the collection of graphs B generated from a member of $\mathcal{B}_3(k)$ ($k \geq 5$) or $\mathcal{B}_4(k)$ ($k \geq 7$) by attaching a pendent path of length

$n-k \geq 2$ to a vertex u with $d_B(u) = 3$, where u is adjacent to a vertex of degree 2 and two vertices of degree 3 (see Figure 22).

(6) $\mathcal{B}_{10}(n)$ is the collection of graphs B generated from the unique member of $\mathcal{B}_1(4)$ by attaching a pendent path on two vertices u, v with $d_B(u) = d_B(v) = 3$, where one pendent path has length 1, another has length greater than 1.

It is clear that the classes $\mathcal{B}_1(n)$, $\mathcal{B}_2(n)$, $\mathcal{B}_3(n)$, $\mathcal{B}_4(n)$, $\mathcal{B}_5(n)$, $\mathcal{B}_6(n)$, $\mathcal{B}_7(n)$, $\mathcal{B}_8(n)$, $\mathcal{B}_9(n)$ and $\mathcal{B}_{10}(n)$ are defined for $n \geq 4, 6, 5, 7, 6, 8, 5, 7, 7, 7$, respectively.

Theorem 9. *Among all n-vertex bicyclic graphs, the following results hold for the HSO index:*

1. *For $n \geq 4$, the HSO index attains its minimum value*

$$HSO(B) = 2\sqrt{13} + (n-3)\sqrt{2}$$

if and only if $B \in \mathcal{B}_1(n) \cup \mathcal{B}_2(n)$.

2. *For $n \geq 6$, the HSO index attains its second minimum value*

$$HSO(B) = \frac{3\sqrt{13}}{2} + \sqrt{5} + (n-3)\sqrt{2}$$

if and only if $B \in \mathcal{B}_5(n)$.

3. *For $n \geq 6$, the HSO index attains its third minimum value*

$$HSO(B) = 3\sqrt{13} + (n-5)\sqrt{2}$$

if and only if $B \in \mathcal{B}_3(n) \cup \mathcal{B}_4(n)$.

4. *For $n \geq 8$, the HSO index attains its fourth minimum value*

$$HSO(B) = \sqrt{13} + 2\sqrt{5} + (n-3)\sqrt{2}$$

if and only if $B \in \mathcal{B}_6(n)$.

5. *For $n \geq 8$, the HSO index attains its fifth minimum value*

$$HSO(B) = \sqrt{13} + \sqrt{10} + (n-2)\sqrt{2}$$

if and only if $B \in \mathcal{B}_7(n)$.

6. *For $n \geq 8$, the HSO index attains its sixth minimum value*

$$HSO(B) = \frac{5\sqrt{13}}{2} + \sqrt{5} + (n-5)\sqrt{2}$$

if and only if $B \in \mathcal{B}_8(n) \cup \mathcal{B}_9(n)$.

7. *For $n \geq 8$, the HSO index attains its seventh minimum value*

$$HSO(B) = \frac{\sqrt{13}}{2} + \sqrt{10} + \sqrt{5} + (n-2)\sqrt{2}$$

if and only if $B \in \mathcal{B}_{10}(n)$.

Proof. Let B be a unicyclic graph of order n. One can easily verify the results by Sage for $4 \leq n \leq 7$. Next, we consider $n \geq 8$. If $B \in \mathcal{B}_i(n)$ $(1 \leq i \leq 10)$, then we denote the value of $HSO(B)$ as L_i. Thus, we have

$$L_i = \begin{cases} 4f\left(\frac{3}{2}\right) + (n-3)\sqrt{2} = 2\sqrt{13} + (n-3)\sqrt{2} & \text{for } i = 1, 2, \\ 3f\left(\frac{3}{2}\right) + f(2) + (n-3)\sqrt{2} = \frac{3\sqrt{13}}{2} + \sqrt{5} + (n-3)\sqrt{2} & \text{for } i = 5, \\ 6f\left(\frac{3}{2}\right) + (n-5)\sqrt{2} = 3\sqrt{13} + (n-5)\sqrt{2} & \text{for } i = 3, 4, \\ 2f\left(\frac{3}{2}\right) + 2f(2) + (n-3)\sqrt{2} = \sqrt{13} + 2\sqrt{5} + (n-3)\sqrt{2} & \text{for } i = 6, \\ 2f\left(\frac{3}{2}\right) + f(3) + (n-2)\sqrt{2} = \sqrt{13} + \sqrt{10} + (n-2)\sqrt{2} & \text{for } i = 7, \\ 5f\left(\frac{3}{2}\right) + f(2) + (n-5)\sqrt{2} = \frac{5\sqrt{13}}{2} + \sqrt{5} + (n-5)\sqrt{2} & \text{for } i = 8, 9, \\ f\left(\frac{3}{2}\right) + f(3) + f(2) + (n-2)\sqrt{2} = \frac{\sqrt{13}}{2} + \sqrt{10} + \sqrt{5} + (n-2)\sqrt{2} & \text{for } i = 10. \end{cases}$$

One can easily check that

$$L_{10} > L_8 = L_9 > L_7 > L_6 > L_3 = L_4 > L_5 > L_1 = L_2.$$

Let $\mathcal{A}(n) = \bigcup_{i=1}^{10} \mathcal{B}_i(n)$. Now, it is sufficient to prove that $HSO(B) > L_{10}$

for all $B \in B(n)\backslash\mathcal{A}(n)$. Let $B \in B(n)\backslash\mathcal{A}(n)$. If $\ell = 0$, then $B \in \mathcal{B}_0^3(n)$. Evidently, $HSO(B) = 4f(2) + (n-3)\sqrt{2} = 4\sqrt{5} + (n-3)\sqrt{2} > L_{10}$. Next, we consider $\ell \geq 1$. Now, we construct the proof in the following three cases.

Case 1. $\ell = 1$. It is clear that $3 \leq \Delta \leq 5$ and $0 \leq \ell_1 \leq 1$. Now we divide this case into the following sub-cases.

Case 1.1. $\Delta = 3$. In this case, B contains three vertices of degree 3. Let $u, v, w \in V(B)$ such that $d_B(u) = d_B(v) = d_B(w) = 3$. Note that u, v, w are not pairwise adjacent, otherwise, $B \in \mathcal{B}_5(n) \cup \mathcal{B}_7(n) \subseteq \mathcal{A}(n)$, a contradiction. Thus, at most two pairs of three vertices of degree 3 are adjacent. Next we consider the following two cases.

Case 1.1.1. $\ell_1 = 0$. If two pairs of u, v, w are adjacent, then $B \in \mathcal{B}_8(n) \cup \mathcal{B}_9(n) \subseteq \mathcal{A}(n)$, a contradiction. Thus, we consider that at most one pair of three vertices of degree 3 are adjacent. Then, B contains at least seven edges connecting vertices of degree 2 and 3. Consequently, we have

$$HSO(B) \geq 7f\left(\frac{3}{2}\right) + f(2) + (n-7)\sqrt{2} = \frac{7\sqrt{13}}{2} + \sqrt{5} + (n-7)\sqrt{2} > L_{10}.$$

Case 1.1.2. $\ell_1 = 1$. In this case, the graph B necessarily contains at least four edges incident with a vertex of degree 2 and a vertex of degree 3. Therefore, we can write

$$HSO(B) \geq 4f\left(\frac{3}{2}\right) + f(3) + (n-4)\sqrt{2} = 2\sqrt{13} + \sqrt{10} + (n-4)\sqrt{2} > L_{10}.$$

Case 1.2. $4 \leq \Delta \leq 5$. We prove this case in following two sub-cases.

Case 1.2.1. $\ell_1 = 0$. In this case, B must contain at least three edges joining vertices of degree 2 with a vertex of degree Δ. In addition, G has one pendent edge. Consequently, we obtain

$$\begin{aligned} HSO(G) &\geq 3f\left(\frac{\Delta}{2}\right) + f(2) + (n-3)\sqrt{2} \\ &\geq 4f(2) + (n-3)\sqrt{2} = 4\sqrt{5} + (n-3)\sqrt{2} > L_{10}. \end{aligned}$$

Case 1.2.2. $\ell_1 = 1$. In this case B must contain at least two edges joining vertices of degree 2 and Δ. In addition, B has exactly one pendent edge. Consequently, we obtain

$$\begin{aligned} HSO(B) &\geq 2f\left(\frac{\Delta}{2}\right) + f(3) + (n-2)\sqrt{2} \\ &\geq 2f(2) + f(3) + (n-2)\sqrt{2} = 2\sqrt{5} + \sqrt{10} + (n-2)\sqrt{2} > L_{10}. \end{aligned}$$

Case 2. $\ell = 2$. It is clear that $3 \leq \Delta \leq 6$ and $0 \leq \ell_1 \leq 2$. Now we construct the following two cases.

Case 2.1. $\Delta = 3$. In this case, B contains four vertices of degree 3. Let $u, v, w, x \in V(B)$ such that $d_B(u) = d_B(v) = d_B(w) = d_B(x) = 3$. Note that, at most five pairs of vertices u, v, w, x are adjacent, as B is bicyclic. If five pairs of them are adjacent, then $n \geq 8$ implies $B \in \mathcal{B}_6(n) \cup \mathcal{B}_{10}(n) \subseteq \mathcal{A}(n)$, a contradiction. Thus, we consider that at most four pairs of them are adjacent. It is evident that there exists at least two edges $v_iv_j \in E(B)$ that do not belong to any pendent path with $d_B(v_i) \geq d_B(v_j)$ such that $\dfrac{d_B(v_i)}{d_B(v_j)} = \dfrac{3}{2}$. Again, we know that $f(3) + f(1) > f\left(\frac{3}{2}\right) + f(2)$. Thus, we obtain

$$HSO(B) \geq 4f\left(\frac{3}{2}\right) + 2f(2) + (n-5)\sqrt{2} = 2\sqrt{13} + 2\sqrt{5} + (n-5)\sqrt{2} > L_{10}.$$

Case 2.2. $4 \leq \Delta \leq 6$. We consider the following three sub-cases.

Case 2.2.1. $\ell_1 = 0$. In this case, we definitely get two pendent edges connecting the pendent vertex with a vertex of degree 2. Again, it is clear that there exist at least two non-pendent edges $v_iv_j \in E(B)$ with $d_B(v_i) \geq d_B(v_j)$ such that $\dfrac{d_B(v_i)}{d_B(v_j)} \geq \dfrac{4}{2}$. Consequently, we obtain

$$HSO(B) \geq 2f\left(\frac{4}{2}\right) + 2f(2) + (n-3)\sqrt{2} = 4\sqrt{5} + (n-3)\sqrt{2} > L_{10}.$$

Case 2.2.2. $\ell_1 = 1$. Then B contains at least three non-pendent edges v_iv_j with $d_B(v_i) \geq d_B(v_j)$ such that $\dfrac{d_B(v_i)}{d_B(v_j)} \geq \dfrac{3}{2}$. Again, there are two pendent edges u_pu_q, u_ru_s in B with $d_B(u_q) = d_B(u_s) = 1$ such that

$\dfrac{d_B(u_p)}{d_B(u_q)} \geq 3$ and $\dfrac{d_B(u_r)}{d_B(u_s)} = 2$. Thus, we derive

$$\begin{aligned} HSO(B) &\geq 3f\left(\frac{3}{2}\right) + f(2) + f(3) + (n-4)\sqrt{2} \\ &= \frac{3\sqrt{13}}{2} + \sqrt{5} + \sqrt{10} + (n-4)\sqrt{2} > L_{10}. \end{aligned}$$

Case 2.2.3. $\ell_1 = 2$. It is evident that there exist two pendent edges $v_iv_j \in E(B)$ with $d_B(v_j) = 1$ such that $\dfrac{d_B(v_i)}{d_B(v_j)} \geq 3$. Therefore, we have

$$HSO(B) \geq 2f(3) + (n-1)\sqrt{2} = 2\sqrt{10} + (n-1)\sqrt{2} > L_{10}.$$

Case 3. $\ell \geq 3$. By Lemma 2, it is evident that

$$\begin{aligned} HSO(T) &\geq \sqrt{2}\,(n+1) + 3\Big(f(2) + f(\tfrac{3}{2}) - 2\sqrt{2}\Big) \\ &= (n-5)\sqrt{2} + 3\sqrt{5} + \frac{3\sqrt{13}}{2} > L_{10}. \end{aligned}$$ ■

Remark 3. *Theorem 9 does not completely determine the ordering of bicyclic graphs with minimal HSO for small values of n. The remaining cases are summarized in Table 3.*

Table 3. Ordering of minimal bicyclic graphs with respect to the HSO index for small values of n.

	Second	Third	Fourth	Fifth	Sixth	Seventh
$n = 5$	B_1	B_2	B_3	B_4	–	–
$n = 6$	–	–	B_5	B_6	B_7, B_8	B_9
$n = 7$	–	–	B_{10}	B_{11}, B_{12}	B_{13}	B_{14}, B_{15}

The structures of B_i for $1 \leq i \leq 15$ are depicted in Figure 23.

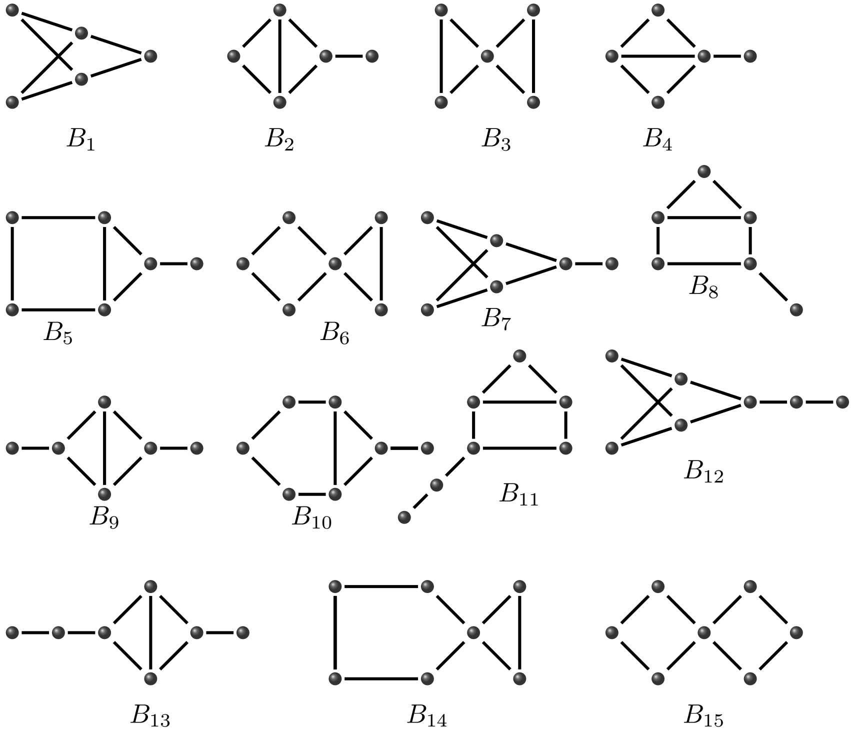

Figure 23. The bicyclic graphs B_i, $1 \leq i \leq 15$.

3 Concluding remarks

In this work, we revisited and refined some existing results concerning the Hyperbolic Sombor index. We disproved the general monotonicity claim under edge addition and established a sufficient condition for its validity. Sharp bounds were also obtained for trees, unicyclic, and bicyclic graphs, with the corresponding extremal structures characterized. Finally, we identified the first eight minimal trees and seven unicyclic and bicyclic graphs with respect to HSO, providing a finer structural ordering and a more complete theoretical foundation for this index.

To prove the maximal case of Theorem 4 in [1], the relation (4) was assumed to be obvious, which is not true in general. Although the result itself is correct, the proof remains incomplete. In [1], this result was established for trees. From Theorems 5 and 6, one can readily verify that the same holds for unicyclic and bicyclic graphs as well. Therefore, proving the result for the remaining graph classes can be considered as future work. This study identifies the maximal graphs for the HSO index up to the bicyclic family. Generalizing these findings to c-cyclic graphs may serve as an interesting direction for future research. Furthermore, the characterization of extremal graphs with respect to the HSO index for fixed parameters–such as the number of pendent vertices, chromatic number, domination number, and vertex or edge connectivity–also presents promising avenues for further investigation.

***Acknowledgment*:** We are extremely grateful to the referee for the insightful comments to improve the quality of the manuscript. Z. R. is supported by the University of Sharjah Research Grant No. 23021440148. Z. R. and S. M. are supported by the MASEP Research Group.

References

[1] J. Barman, S. Das, Geometric approach to degree-based topological index: hyperbolic Sombor index, *MATCH Commun. Math. Comput. Chem.* **95** (2026) 63–94.

[2] J. Barman, S. Das, Chemical applicability of the hyperbolic Sombor index, *Chem. Phys. Lett.* **878** (2025) #142340.

[3] R. Cruz, I. Gutman, J. Rada, Sombor index of chemical graphs, *Appl. Math. Comput.* **399** (2021) #126018.

[4] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[5] I. Gutman, Sombor index of thorny graphs, *Vojnotehnički glasnik* **73** (2025) 413–422.

[6] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[7] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[8] I. Gutman, B. Furtula, M. S. Oz, Geometric approach to vertex-degree-based topological indices – Elliptic Sombor index, theory and application, *Int. J. Quantum Chem.* **124** (2024) e27346.

[9] I. Gutman, I. Redžepović, B. Furtula, On the product of Sombor and modified Sombor indices, *Open J. Discr. Appl. Math.* **6** (2023) 1–6.

[10] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[11] S. Hayat, M. Arshad, I. Gutman, Proofs to some open problems on the maximum Sombor index of graphs, *Comp. Appl. Math.* **42** (2023) #279.

[12] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[13] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[14] Z. Wang, Y. Mao, Y. Li, B. Furtula, On relations between Sombor and other degree-based indices, *J. Appl. Math. Comput.* **68** (2022) 1–17.