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Extremal unicyclic graphs with fixed leaves via Sombor index

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Abstract

Gutman presented the Sombor index in 2021 as a topological molecular descriptor defined by graph $A = \sum_{a_1 a_2 \in E(A)} \sqrt{\beta(a_1)^2 + \beta(a_2)^2}$, where $\beta(a_1)$ is the degree of the vertex $a_1 \in A$. A connected graph is said to be unicyclic graph if it has same order and size. In this paper, we characterize the extremal graphs with respect to Sombor index in the class of unicyclic graphs having fixed leaves (nodes with degree one) associated with extremal graphs. Moreover, we compute the bounds on Sombor index in the same class of graphs.

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Keywords: *Unicyclic graph, Somber index, Topological index, Leaves.*

1. Introduction

The term topological index (TI) refers a numeric quantity for chemical graphs that remains invariant for isomorphic graphs and encodes at least one chemical or physical attribute for the underlying organic structures such as stability, solubility, boiling point, freezing point, volatility, connectedness, chirality, and melting point. TIs have been widely employed studying the quantitative structure activity and property relationships. [1] A branch of graph theory (GT), namely chemical GT, has been extensively utilized in studying the chemical structures with the help of TIs. There are vast range of applicability in the field of chemical graph theory and

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mathematical chemistry as one can see [2]-[6]. In the literature, TIs are classified into four types including polynomial related TIs, distance, degree, and spectral-based TIs. Among them, degree-based TIs have received the most attention from the researchers, as evidenced by a recent survey [7].

In 1947, TI based on the distance between nodes was initially demonstrated by Wiener [8]. After this, hundreds of TIs have been investigated by researchers in the fields of chemistry and mathematics throughout the last decades in order to anticipate certain physicochemical and biological aspects of chemical compounds. This includes the first and second Zagreb index (ZI) [9], augmented ZI [10], geometric-arithmetic index [11], Randic index [10] and atom bond connectivity index [12]. Further, Ghorbani et al. [13] initiated the fourth version of ABC index (ABC_4I). Finding sharp limits on degree-based TIs for graphs under certain given constraints is now one of the hottest research issues, which is gaining attention from researchers as one can see, [14]-[18].

Recently, a novel index is introduce by Gutman [19] named as Sombor index (SI). After the development of SI, Chen et al. [20] computed the SIs of trees with some parameters, involving diameter, branching number, matching number, segment number and pendent vertices, etc. Further, Liu [21], studied the SIs of unicyclic graph with a given diameter. Zhou et al. [22] computed Extremal SI of Unicyclic graphs and trees with given matching number. Further, Cruz and Rada [23] found the extremal values of SI in unicyclic graphs and bicyclic graphs. Moreover, some bounds of unicyclic and tricyclic graphs are calculated by Javaid et al. [24] and Akram et al. [25], respectively. More details about SIs can be taken from [26]-[31]. Motivated by [1, 8, 23, 24], we determine the bounds of SIs for unicyclic graphs with with fixed leaves.

The presence of extremal graphs with regard to SI in unicyclic graphs with fixed leaves is demonstrated in this article. In the same class of graphs, we explore the lower and upper limits of the SI. The organizations of this paper is as follows: Section 2 contains some basic results and definitions. The next Section contains the main results related to the upper bound and lower bounds of SI in the class of unicyclic graphs with fixed leaves.

2. Basic Definitions

Let $\mathcal{W} = (\mathcal{X}(\mathcal{W}), \mathcal{Y}(\mathcal{W}))$ be a graph, where $\mathcal{X}(\mathcal{W})$ is a vertex (node) set and $\mathcal{Y}(\mathcal{W})$ is an edge set. The degree of any arbitrary node x is the number of nodes which are at distance one from the node x and is denoted by $\beta(x)$. Let $e=(x,y)$, where $x,y\in\mathcal{X}(\mathcal{W})$ be an edge, then the degree of the edge is given by $d(e)=\ d(x)\ +\ d(y)\ -\ 2.$ A node with degree one is said to be pendent node (leaf node) and an edge adjacent to pendent node is termed as pendent edge. A graph is connected if there is some path between each pair of nodes. A connected graph with no cycle and with at least one cycle is said to be tree and cyclic graph, respectively. A graph is said to be unicyclic graph if it has exactly one cycle. A node is said to be a cycle node if it is on some cycle of graph. Further, a connected graph is said to be a-cyclic if $t=r-1+a$, where t and r are order and size of the graph $\mathcal{W}$ If $a=0$, $a=1$, and $a=2$ then $\mathcal{W}$ is tree, unicyclic ($\mathcal{W}$ with exactly 1 cycle) and bicyclic ($\mathcal{W}$ with exactly 2 cycles), respectively. For the further graph related terminologies, we refer [25]. Next, some definitions related to TIs have been defined which will be used in further evaluations.

Definition 1: [9] Consider a graph $\mathcal{W}=(\mathcal{X}(\mathcal{W}),\mathcal{Y}(\mathcal{W}))$, where $\mathcal{X}(\mathcal{W})$ and $\mathcal{Y}(\mathcal{W})$ be the set of nodes and edges, respectively. Then, first and second Zagreb indices based on the degree of the nodes are

1. $Z_1(\mathcal{W})=\sum_{x\in\mathcal{X}(\mathcal{W})}(\beta(x))^2=\sum_{xy\in\mathcal{Y}(\mathcal{W})}(\beta(x)+\beta(y)),$

2. $Z_2(\mathcal{W})=\sum_{xy\in\mathcal{Y}(\mathcal{W})}(\beta(x)\times\beta(y)),$

where $\beta(x)$ is the degree of the node x and $\beta(y)$ is the degree of the node y, respectively.

Definition 2: [19] Consider a graph $\mathcal{W}=(\mathcal{X}(\mathcal{W}),\mathcal{Y}(\mathcal{W}))$. Then, Sombor index is

$$S(\mathcal{W})=\sum_{xy\in\mathcal{Y}(\mathcal{W})}\sqrt{(\beta(x)^2+\beta(y)^2)}.$$

where $\beta(x)$ is the degree of the node x and $\beta(y)$ is the degree of the node y, respectively.

Now, we define some unicyclic graphs with fixed pendent nodes. Let $\mathcal{A}(t,\zeta,\alpha)$ is a unicyclic graph obtained by joining ζ leaves to any $\alpha\geq 2$ nodes of the cycle C_u, where $u=t-\zeta\alpha$. Likely, let $\mathcal{B}(t,\breve{\zeta}^*,k)$ is a unicyclic graph obtained by joining one end of path of order $k\geq 3$ with a node of cycle C_v and other end with middle node of star S_{1,ζ^*}, where path graph of order k is a graph with two leaves and $k-2$ nodes of degree 2, and star is a graph with ζ^* leaves and one middle node of degree ζ^*, and $v=t-\zeta^*-k+1$ and $3\leq k\leq t-\zeta^*-2$. For our ease, consider $\mathcal{A}(t,\zeta,\alpha)=\mathbf{A}$ and

$\mathcal{B}(t,\zeta^{*},k)=\mathbf{B}$. For $\mathbf{A}$, the division of edges and nodes on degree basis are given in Table 1 and Table 2.

Table 1

Edge-based partition of A (when all α nodes are adjacent)

$(1,\zeta+2)$	$(\zeta+2,\zeta+2)$	$(2,\zeta+2)$	$(2,2)$
$\zeta\alpha$	$\alpha-1$	2	$u-\alpha-1$

Table 2

Edge-based partition of A (when α nodes are non-adjacent)

$(1,\zeta+2)$	$(2,\zeta+2)$	$(2,2)$
$\zeta\alpha$	2α	$u-2\alpha$

For **B**, the division of edges and nodes on degree basis are given in Table 3.

Table 3

Edge-based partition of B

$(2,2)$	$(2,3)$	$(1,\zeta^{*}+1)$	$(2,\zeta^{*}+1)$
$v+k-5$	3	ζ^{*}	1

Now, we construct $\mathbf{A}_1$ from $\mathbf{A}$ by removing ζ leaves from a node of degree $\zeta+2$ from either side of the cycle and attaching these nodes with the next node of degree $\zeta+2$. Further, we obtain $\mathbf{A}_2$ from $\mathbf{A}_1$ by removing 2ζ leaves form the node of degree $2\zeta+2$ and attaching these removed nodes to the next coming node of degree $\zeta+2$. Continuing in the same manner, we obtain $\mathbf{A}_{\alpha-1}$ from $\mathbf{A}_{\alpha-2}$ by removing $(\alpha-1)\zeta$ leaves from a node of degree $(\alpha-1)\zeta+2$ and attaching these removed nodes to the last node of degree $\zeta+2$, where $2\leq\alpha\leq u$. Let $\mathbf{A}_i=\{\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \cdots \mathbf{A}_{\alpha-1}\}$ for $0\leq i\leq\alpha-1$.

Consider a class of all the unicyclic graphs denoted by $\mathcal{A}_t^{\theta}$ with total t nodes and θ leaves. Let $\tilde{\mathcal{A}}_1$ be a subclass of $\mathcal{A}_t^{\theta}$ in which all the leaf nodes are joined with cycle nodes, $\tilde{\mathcal{A}}_2$ be a subclass of $\mathcal{A}_t^{\theta}$ in which all the nodes are joined with nodes of tree and $\tilde{\mathcal{A}}_3$ be a subclass of $\mathcal{A}_t^{\theta}$ in which all the leaf nodes are joined with both. Further, let $\mathcal{A}_1^{a}, \mathcal{A}_1^{na}$ and $\mathcal{A}_1^{m}$ be further three subclasses of $\tilde{\mathcal{A}}_1$, such that all the α nodes are adjacent, non-adjacent and both of them, respectively. If $\mathcal{W} \in \mathcal{A}_1^m$, then we convert it into a graph $\mathcal{W}' \in \mathcal{A}_1^a$ (in which all the α nodes are adjacent) by removing those leaves from a cycle node x such that degree of nodes in the neighborhood of x is 2 and joining these removed nodes with a some other cycle node y such that at least one node in the neighborhood of y has degree $\zeta + 2$. We continue this process until we get a graph $\mathcal{W} \in \mathcal{A}_1^a$ with exactly two nodes of the type $(2, \zeta + 2)$. For $\mathbf{A}_i$, the partitions of the edges with respect of their degrees of the nodes are given in Table 4 and Table 5.

Table 4

Edge-based partition of $\mathbf{A}_i^a$ (when all α nodes are adjacent)

$(\beta(x), \beta(y))$	$\lvert(\beta(x), \beta(y))\rvert$
$(1, \zeta + 2)$	$\zeta\alpha - (i+1)\zeta$
$(1, (i+1)\zeta + 2)$	$(i+1)\zeta$
$(\zeta + 2, \zeta + 2)$	$\alpha - 1 - 2i$
$(\zeta + 2, (i+1)\zeta + 2)$	i
$(2, \zeta + 2)$	1
$(2, (i+1)\zeta + 2)$	1
$(2, 2)$	$u - \alpha - 1 + i$

Table 5

Edge-based partition of $\mathbf{A}_i^{na}$ (when α nodes are non-adjacent)

$(\beta(x), \beta(y))$	$\lvert(\beta(x), \beta(y))\rvert$
$(1, \zeta + 2)$	$\zeta\alpha - (i+1)\zeta$
$(1, (i+1)\zeta + 2)$	$(i+1)\zeta$
$(2, \zeta + 2)$	$2\alpha - 2i - 2$
$(2, (i+1)\zeta + 2)$	2
$(2, 2)$	$u - 2\alpha + 2i$

3. Results

This section presents the key findings of this article. Before moving towards main results, we start with some basic lemmas which help us to prove our results.

Lemma 1: *Let $\mathcal{W}$ be a graph and $\mathcal{W}^*$ be obtained by deleting the edge $uv \in \mathcal{W}$ and attaching u to another node z of $\mathcal{W}$, i.e., $\mathcal{W}^* = \mathcal{W} - uv + uz$.*

1. $S(\mathcal{W}^*) = S(\mathcal{W})$, if $\beta(z) = \beta(v) - 1$,
2. $S(\mathcal{W}^*) > S(\mathcal{W})$, if $\beta(z) > \beta(v) - 1$,
3. $S(\mathcal{W}^*) < S(\mathcal{W})$ if $\beta(z) < \beta(v) - 1$.

Proof: In a graph $\mathcal{W}, \beta(v)$ and $\beta(z)$ represent the degrees of the node v and z, respectively. Let x_i be the edges incident with v and y_i be the edges incident with z. Then, we have

$$S(\mathcal{W}^*) - S(\mathcal{W}) = \sum_i \sqrt{\beta(v)^2 + d(x_i)^2} + \sum_i \sqrt{\beta(z)^2 + d(y_i)^2} - \sum_i \sqrt{(\beta(v)-1)^2 + d(x_i)^2} - \sum_i \sqrt{(\beta(z)+1)^2 + d(y_i)^2},$$

By using $\beta(z) = \beta(v) - 1, \beta(z) > \beta(v) - 1$ and $\beta(z) < \beta(v) - 1$ in the above equation, we get $S(\mathcal{W}^*) = S(\mathcal{W})$, $S(\mathcal{W}^*) > S(\mathcal{W})$ and $S(\mathcal{W}^*) < S(\mathcal{W})$, respectively. Hence, the proof of Lemma is complete.

Lemma 2: *Let $\mathcal{W} \in \mathcal{A}_1^m$ be graph. Assume that $\mathcal{W}' \in \mathcal{A}_1^a$ is obtained form $\mathcal{W}$ by removing those leaf edges (x, y_j) from a cycle node x such that degree of nodes in the neighborhood of x is 2 and joining y_j with some other cycle node w in such a way that at least one node in the neighborhood of w has degree $\zeta + 2$. Then, we have*

$$S(\mathcal{W}') < S(\mathcal{W})$$

Proof: As $\beta(x) = \psi + 2$ in $\mathcal{W}$, after transformation edge of the type $(2, \psi + 2)$ is converted into $(2,2)$ and one edge $(2, \psi + 2)$ is converted into $(\psi + 2, \psi + 2)$. Then, we have

$$S(\mathcal{W}') - S(\mathcal{W}) = \sqrt{8} + \sqrt{(\zeta+2)^2 + (\zeta+2)^2} - \sqrt{4 + (\zeta+2)^2} - \sqrt{4 + (\zeta+2)^2} < 0$$

Lemma 3: *For $\zeta \geq 2, u, v \geq 6$, $3 \leq k \leq v - 3$ $0 \leq i \leq \alpha - 1$ and $2 \leq \alpha \leq u$, Sombor index of graphs with one cycle $\mathbf{A}_i$ and $\mathbf{B}$ are*

1. $S(\mathbf{A}_i^a) = (u - \alpha - 1 + i)\sqrt{8} + [\zeta\alpha - (i+1)\zeta]\sqrt{1 + (\zeta+2)^2} + [(i+1)\zeta]$ $\sqrt{1 + [(i+1)\zeta + 2]^2} + (\alpha - 1 - 2i)\sqrt{(\zeta+2)^2 + (\zeta+2)^2} + \sqrt{4 + (\zeta+2)^2}$ $+(i)\sqrt{(\zeta+2)^2 + [(i+1)\zeta + 2]^2} + \sqrt{4 + (\zeta+2)^2} + \sqrt{4 + [(i+1)\zeta + 2]^2},$

2. $S(\mathbf{A}_i^{na}) = (u-2\alpha+2i)\sqrt{8} + [\zeta\alpha-(i+1)\zeta]\sqrt{1+[\zeta+2]^2} + [2\alpha-2i-2]$
$\sqrt{4+(\zeta+2)^2} + 2\sqrt{4+[(i+1)\zeta+2]^2} + [(i+1)\zeta]\sqrt{1+[(i+1)\zeta+2]^2}$,

3. $S(\mathbf{B}) = (v+k-5)\sqrt{8} + 3\sqrt{13} + (\zeta)\sqrt{1+(\zeta+1)^2} + \sqrt{4+(\zeta+1)^2}$.

Proof: Lemma can be easily proved by using the definition of Sombor index, Table 5 and Table 3. Therefore, we omit.

Corollary 1 can be obtained by putting $i=0$ in above Lemma.

Corollary 1: *For* $\zeta \geq 2, u, v \geq 6,\quad 3 \leq k \leq v-3 \quad 0 \leq i \leq \alpha-1$ *and* $2 \leq \alpha \leq u$, *Sombor index of unicyclic graphs* $\mathbf{A_0} = \mathcal{A}$ *is give as*

$$S(\mathcal{A}^a) = (u-\alpha-1)\sqrt{8} + (\psi\alpha)\sqrt{1+(\psi+2)^2} + (\alpha-1)\sqrt{(\psi+2)^2+(\psi+2)^2} + 2\sqrt{4+(\psi+2)^2}, \sqrt{4+(\zeta+2)^2},$$
$$S(\mathcal{A}^{na}) = (u-2\alpha)\sqrt{8} + (2\alpha)\sqrt{4+(\zeta+2)^2} + \zeta\alpha\sqrt{1+(\zeta+2)^2}.$$

Theorem 1: For $\zeta \geq 2, u, v \geq 6,\quad 3 \leq k \leq v-3 \quad 0 \leq i \leq \alpha-1$ and $2 \leq \alpha \leq u$. Then, we have

1. $S(\mathcal{A}^a(t,\zeta,1)) = S(\mathcal{A}^{na}(t,\zeta,1))$,
2. $S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{A}^{na}(t,\zeta,\alpha))$,
3. $S(\mathcal{B}(t,\zeta,3)) < S(\mathcal{A}^{na}(t,\zeta,1))$,
4. $S(\mathcal{B}(t,\zeta,k)) = S(\mathcal{B}(t,\zeta,k+1))$
5. $S(\mathcal{B}(t,\zeta,k)) < S(\mathcal{A}^{na}(t,\zeta,1))$
6. $S(\mathbf{A}_0^a) < S(\mathbf{A}_1^a) < \cdots < S(\mathbf{A}_{\alpha-1}^a)$,
7. $S(\mathbf{A}_0^{na}) < S(\mathbf{A}_1^{na}) < \cdots < S(\mathbf{A}_{\alpha-1}^{na})$,
8. $S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{B}(t,\zeta^*,3))$,
9. $S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{B}(t,\zeta^*,k))$.

Proof:

1. By putting $\alpha = 1$ in Equation 1 and Equation 2, we get the desired result.
2. Using Equation 1 and Equation 2, we have

$$S(\mathcal{A}^{a})-S(\mathcal{A}^{na})=[(u-\alpha-1)\sqrt{8}+(\zeta\alpha)\sqrt{1+(\zeta+2)^2}+(\alpha-1)\sqrt{(\zeta+2)^2+(\zeta+2)^2}$$
$$+2\sqrt{4+(\zeta+2)^2}]-[(u-2\alpha)\sqrt{8}+(2\alpha)\sqrt{4+(\zeta+2)^2}+\zeta\alpha\sqrt{1+(\zeta+2)^2}],$$
$$=(\alpha-1)\sqrt{8}+(\alpha-1)\sqrt{(\zeta+2)^2+(\zeta+2)^2}+(2-2\alpha)\sqrt{4+(\zeta+2)^2}<0$$

Thus, $S(\mathcal{A}^{a}(t,\zeta,\alpha))<S(\mathcal{A}^{\zeta}(t,\zeta,\alpha))$.

3. Placing $k=3$ in Lemma 3(iii), we get

$$S(\mathcal{B}(t,\zeta^*,3))=(v-2)\sqrt{8}+3\sqrt{3}+(\zeta^*)\sqrt{1+(\zeta^*+1)}+\sqrt{4+(\zeta^*+1)}$$

Placing $\alpha=1$ in Equation 1 yields

$$S(\mathcal{A}^{na}(t,\zeta,1))=(u-2)\sqrt{8}+\zeta\sqrt{1+(\zeta+2)^2}+2\sqrt{4+(\zeta+2)^2}.$$

For $u=t-\zeta\alpha, v=t-\zeta^*-1$ and $\zeta^*=\zeta\alpha,$ we get

$$S(\mathcal{A}^{na}(t,\zeta,1))-S(\mathcal{B}(t,\zeta^*,3))=\zeta\sqrt{1+(\zeta+2)^2}+2\sqrt{4+(\zeta+2)^2}-(\zeta)\sqrt{1+(\zeta+1)^2}-\sqrt{4+(\zeta+1)^2}$$
$$+\sqrt{8}\sqrt{8}-3\sqrt{13}>0.$$

Thus, $S(\mathcal{B}(t,\zeta,3))<S(\mathcal{A}^{na}(t,\zeta,1))$.

4. From Lemma 3(iii), we have

$$S(\mathbf{B}(t,\zeta^*,k))=(v+k-5)\sqrt{8}+3\sqrt{13}+(\zeta^*)\sqrt{1+(\zeta^*+1)^2}+\sqrt{4+(\zeta^*+1)^2}.$$

Since, for $k=k+1$, we have $u=u-1$. Thus, we have

$$S(\mathbf{B}(t,\zeta^*,k+1))=(v+k-5)\sqrt{8}+3\sqrt{13}+(\zeta^*)\sqrt{1+(\zeta^*+1)^2}+\sqrt{4+(\zeta^*+1)^2}.$$

Thus, $S(\mathbf{B}(t,\zeta,k))=S(\mathbf{B}(t,\zeta,k+1))$.

5. Since by 3 and 4, we have

$$S(\mathcal{B}(t,\zeta,3))<S(\mathcal{A}^{na}(t,\zeta,1)) \text{ and } S(\mathcal{B}(t,\zeta,k))=S(\mathcal{B}(t,\zeta,k+1)),$$

Consequently,

$$S(\mathcal{B}(t,\zeta,3))=S(\mathcal{B}(t,\zeta,4))=\cdots=S(\mathcal{B}(t,\zeta,u-3)).$$

Thus, we have $S(\mathcal{B}(t,\zeta,k))<S(\mathcal{A}^{na}(t,\zeta,1))$, for $3\le k\le v-3$.

6. By using Lemma 3(1), we have

$$S(\mathcal{A}^{a}_{i})-S(\mathcal{A}^{a}_{i+1})=-\sqrt{8}-\zeta\sqrt{1+(\zeta+2)^2}-[(i+1)\zeta]\sqrt{1+[(i+1)\zeta+2]^2}$$
$$-[(i+2)\zeta]\sqrt{1+[(i+2)\zeta+2]^2}+2\sqrt{(\zeta+2)^2+(\zeta+2)^2}+\sqrt{4+[(i+1)\zeta+2]^2}$$
$$-\sqrt{4+[(i+2)\zeta+2]^2}+i\sqrt{(\zeta+2)^2+[(i+1)\zeta+2]^2}-(i+1)\sqrt{(\zeta+2)^2+[(i+2)\zeta+2]^2}<0$$

For $i=0,1,2\cdots,\alpha-2$, we have $S(\mathcal{A}_i^a)<S(\mathcal{A}_{i+1}^a)$.

7. By following (6), we get the desired result.

8. Using Lemma 3(iii) and Equation 1, we have

$$S(\mathcal{A}^a)=(u-\alpha-1)\sqrt{8}+(\zeta\alpha)\sqrt{1+(\zeta+2)^2}+(\alpha-1)\sqrt{(\zeta+2)^2+(\zeta+2)^2}+2\sqrt{4+(\zeta+2)^2},$$
$$S(\mathbf{B})=(v+k-5)\sqrt{8}+3\sqrt{13}+(\zeta)\sqrt{1+(\zeta^*+1)^2}+\sqrt{4+(\zeta^*+1)^2}$$

For $k=3, v=t-\zeta^*-1, u=t-\zeta\alpha$ and $\zeta^*=\zeta\alpha$, we have

$$\begin{aligned} &S(\mathcal{A}^a(t,\zeta,\alpha))-S(\mathcal{B}(t,\zeta^*,3))\\ &\quad=(-\alpha-4)\sqrt{8}+\zeta\alpha\sqrt{1+(\zeta+2)^2}+(\alpha-1)\sqrt{(\zeta+2)^2+(\zeta+2)^2}\\ &\quad+2\sqrt{4+(\zeta+2)^2}-3\sqrt{13}-(\zeta\alpha)\sqrt{1+(\zeta+1)^2}-\sqrt{4+(\zeta+1)^2}<0. \end{aligned}$$

Thus, $S(\mathcal{A}^a(t,\zeta,\alpha))<S(\mathcal{B}(t,\zeta^*,3))$.

9. Since by 8 and 4 , we have

$$S(\mathcal{A}^a(t,\zeta,\alpha))<S(\mathcal{B}(t,\zeta,3)) \text{ and } S(\mathcal{B}(t,\zeta,k))=S(\mathcal{B}(t,\zeta,k+1))$$

Consequently,

$$S(\mathcal{B}(t,\zeta,3))=S(\mathcal{B}(t,\zeta,4))=\cdots=S(\mathcal{B}(t,\zeta,u-3)).$$

Thus, $S(\mathcal{A}^a(t,\zeta,\alpha))<S(\mathcal{B}(t,\zeta,k))$.

Theorem 2: *If $\zeta\ge 2$, u, $v\ge 6$, $2\le\alpha\le u$, $3\le k\le v-3$ and $0\le i\le\alpha-1$. Then for each $\mathcal{W}\in\mathcal{A}_t^\theta$, we get*

1. $S(\mathcal{A}^a(t,\zeta,\alpha))\le S(\mathcal{W})$
2. $S(\mathcal{W})\le S(\mathcal{A}^{na}(t,\zeta,1))$,

where the equality holds for $\mathcal{W}=\mathcal{A}^a(t,\zeta,\alpha)$ and $\mathcal{W}=\mathcal{A}^{na}(t,\zeta,1)$, respectively.

Proof: 1. To prove this theorem, we have 3 cases to consider.

Case 1: Consider. Then there are further three sub-cases

Subcase 1: If $\mathcal{W}\in\mathcal{A}_1^a$, then $G\cong\mathbf{A}_i^a$ for $1\le i\le\alpha-1$. By Theorem 1(6), we have

$$S(\mathbf{A}_0^a)<S(\mathbf{A}_1^a)<\cdots<S(\mathbf{A}_{\alpha-1}^a).$$

As $\mathcal{A}^a=\mathbf{A}_0^a$, so $S(\mathcal{A}^a(t,\zeta,\alpha))\le S(\mathcal{W})\cong S(\mathbf{A}_i^a)$.

Subcase 2: If $\mathcal{W} \in \mathcal{A}_1^{na}$, then $G \cong \mathbf{A}_i^{na}$ for $1 \le i \le \alpha - 1$. By Theorem 1 (2) and (7), we have

$$S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{A}^{na}(t,\zeta,\alpha))$$

and

$$S(\mathbf{A}_0^{na}) < S(\mathbf{A}_1^{na}) < \cdots < S(\mathbf{A}_{\alpha-1}^{na}),$$

As $\mathcal{A}^{na} = \mathbf{A}_0^{na}$, so $S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{W}) \cong S(\mathbf{A}_i^{na})$.

Subcase 3: If $\mathcal{W} \in \mathcal{A}_1^{m}$, then $G \cong \mathbf{A}_i^{m}$ for $1 \le i \le \alpha - 1$. Then by transformation of deleting and adding the edges, we obtain $\mathcal{W} \in \mathcal{A}_1^{a}$. So, $S(\mathcal{A}^a(t,\zeta,\alpha))$ < $S(\mathcal{A}^m(t,\zeta,\alpha))$ using Lemma 2. So, $S(\mathcal{A}^a(t,\zeta,\alpha)) \le S(\mathcal{W})$.

Case 2: If $\mathcal{W} \in \mathcal{A}_2$, then $\mathcal{W} \cong \mathcal{B}(t,\zeta^*,k)$.. Then by Theorem 1(9), we have

$$S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{B}(t,\zeta^*,k)).$$

Thus, $S(\mathcal{A}^a(t,\zeta,\alpha)) < S(\mathcal{W})$.

Case 3: If $\mathcal{W} \in \mathcal{A}_3$, then by using some transformation of deleting and adding the edges, we get $\mathcal{W}^* \in \mathcal{A}_1$ or $\mathcal{W}^* \in \mathcal{A}_2$. Then by Lemma 1, we get $S(\mathcal{W}^*) \le S(\mathcal{W})$. Finally, by following case 1 or case 2 , we get the desired result.

2. The proof is similar to part 1.

Theorem 3: For the class of unicyclic graphs $\mathcal{A}_t^{\theta}$ with t number of nodes and θ leaves. Then

$$(t+2\theta-1)\sqrt{8}+\theta\sqrt{10}+(\theta-1)\sqrt{18}+2\sqrt{13} \le S(\mathcal{W}) \le (t-\theta-2)\sqrt{8}+2\sqrt{\theta^2+4\theta+8}+\theta\sqrt{\theta^2+4\theta+5}$$

where the equality holds if $\mathcal{W} \cong \mathcal{A}^a(t,1,\alpha)$ and $\mathcal{W} \cong \mathcal{A}^{\mathrm{na}}(t,\zeta,1)$, respectively.

Proof: From Equation 1, we get $\mathcal{A}^a(t,1,\alpha)$ = $(t+2\theta-1)$ $\sqrt{8}$ + $\theta\sqrt{10}$ + $(\theta-1)$ $\sqrt{18}$ + $2\sqrt{13}$ and $\mathcal{A}^{na}(t,\zeta,1)$ = $(t-\theta-2)$ $\sqrt{8}$ + $2\sqrt{\theta^2+4\theta+8}$ + $\theta\sqrt{\theta^2+4\theta+5}$ for $\theta = \zeta\alpha$ leaves. From Theorem 2, we obtain $S(\mathcal{A}^a(t,\zeta,\alpha)) \le S(\mathcal{W})$ implies that $S(\mathcal{A}^a(t,1,\alpha)) \le S(\mathcal{A}^a(t,\psi,\alpha)) \le S(\mathcal{W})$, and $S(\mathcal{W}) \le S(\mathcal{A}^{na}(t,\psi,1))$ for each $\mathcal{W} \in \mathcal{A}_t^{\theta}$. Consequently, we get

$$(t+2\theta-1)\sqrt{8}+\theta\sqrt{10}+(\theta-1)\sqrt{18}+2\sqrt{13}\leq S(\mathcal{W})\leq$$
$$(t-\theta-2)\sqrt{8}+2\sqrt{\theta^2+4\theta+8}+\theta\sqrt{\theta^2+4\theta+5}$$

where the equality holds if $\mathcal{W}\cong\mathcal{A}^{a}(t,1,\alpha)$ and $\mathcal{W}\cong\mathcal{A}^{na}(t,r,1)$ respectively.

4. Conclusions

In this research article, the newly introduced index namely, Sombor index, for the whole class of graphs having one cycle have been computed with fixed leaves. Furthermore, We demonstrate the extremal graphs via Sombor index in the same family of graphs having one cycle. In terms of the fixed leaves, we established a mathematical inequality consisting of the upper bound and lower bound of the same index in the same class graphs having one cycle.

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Data Availability

The data used to support the findings of this study are included within this article.

Conflict of interest

There are no conflict of interest.

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