



*Research article***Maximal augmented sombor index in unicyclic graphs****Qinfei Tang¹ and Qinghai Liu^{2,3,4,*}**¹ Department of Mathematics Research, Fujian Institute of Education, Fuzhou 350025, China² Center for Discrete Mathematics, Fuzhou University, Fuzhou, Fujian 350108, China³ Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou, Fujian 350108, China⁴ Center for Applied Mathematics of Fujian Province, Fuzhou, Fujian 350108, China* **Correspondence:** Email: qliu@fzu.edu.cn.

Abstract: The augmented Sombor (ASO) index is a degree-based topological descriptor for connected graphs with at least three vertices, defined by

$$\text{ASO}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)^2 + d(v)^2}{d(u) + d(v) - 2}}.$$

This paper determines the sharp upper bound for the ASO index over the class of unicyclic graphs with a fixed order. Our approach is based on two local transformations, called leaf contracting and leaf transferring, together with monotonicity properties and auxiliary estimates for the edge-contribution function. We prove that these operations strictly increase the ASO index whenever the graph does not already have the required extremal structure. Consequently, every maximizing unicyclic graph of order n must consist of a triangle whose remaining $n-3$ vertices are pendant vertices adjacent to one common vertex. For every $n \geq 3$, we also derive an explicit closed formula for the resulting maximum. The argument covers the small orders directly and establishes uniqueness for all larger orders through the transformation lemmas. The result completes the upper-bound problem for the ASO index on unicyclic graphs and provides a structural benchmark for degree concentration in this graph class.

Keywords: augmented Sombor index; unicyclic graph; pendant vertex; graphical index; extremal graph; chemical graph theory

Mathematics Subject Classification: 05C09, 05C35, 05C92

1. Introduction

Throughout this paper, all graphs are finite, simple, and connected, and have at least three vertices unless stated otherwise. For a graph G , its vertex set and edge set are denoted by $V(G)$ and $E(G)$, respectively, and its order and size are $|V(G)|$ and $|E(G)|$. A unicyclic graph is a connected graph containing exactly one cycle, equivalently, a connected graph whose order and size are equal. The cycle on n vertices is denoted by C_n . When the underlying graph is clear, we write $d(v)$ instead of $d_G(v)$.

As a crucial branch of mathematical chemistry, chemical graph theory utilizes degree-based topological descriptors to model the structural features of molecules and predict their physicochemical properties. The study of degree-based descriptors was pioneered by Ivan Gutman and Trinajstić in 1972 with the introduction of the Zagreb indices [9]. Researchers have developed a wide exploration of the Zagreb indices, including its properties [11, 15] and limit values in various graph classes [1, 2, 5, 22].

Inspired by Euclidean geometry, Gutman introduced the Sombor index (SO) in 2021 [10], which sparked a new wave of global research. It is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2}.$$

Research on the Sombor index has rapidly expanded, including studies of its variants [12–14, 21] and extremal problems for chemical graphs [3], cacti [19], molecular graphs [20], two-trees [6], chemical trees with a prescribed number of pendant vertices [17], trees with a fixed segment number [16], and unicyclic graphs with fixed diameter [18]. These results show that local degree transformations are an effective tool for identifying extremal structures of degree-based topological indices.

Related constructive graph-theoretic studies include generalized decomposition algorithms for circulant-balanced complete multipartite graphs [7] and the use of mutually orthogonal graph squares to build graph-orthogonal arrays and authentication codes [8].

Building upon the success of the Sombor index, Kinkar Chandra Das, Ivan Gutman, and Akbar Ali recently introduced the augmented Sombor (ASO) index in [4]. For a connected graph G , they defined the augmented Sombor index as follows:

$$ASO(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)^2 + d(v)^2}{d(u) + d(v) - 2}}.$$

The ASO index has shown strong predictive performance in quantitative structure–property relationship studies. In particular, the numerical experiments in [4] reported Pearson correlation coefficients with absolute value greater than 0.8 for several thermodynamic properties of octane isomers, including entropy, acentric factor, and enthalpy of vaporization. These correlations motivate the study of the structural behavior of the index. They do not, however, imply that every extremal graph in an unrestricted graph class is a chemically realizable molecular graph; atomic-valence constraints must be imposed for such an interpretation.

From a mathematical perspective, understanding the structural sensitivity of such an index calls for the characterization of its extremal graphs. Das et al. [4] determined the lower bound of the ASO index for unicyclic graphs and proved that the cycle C_n uniquely minimizes the index.

Theorem 1 ([4]). *Let G be a unicyclic graph of order n . Then $\text{ASO}(G) \geq 2n$ with equality if and only if $G \cong C_n$.*

The corresponding upper-bound problem has remained open. Our purpose is to determine this bound and its equality case. The resulting extremal graph should be viewed as a mathematical benchmark describing the degree concentration favored by the ASO index. For chemically realizable structures, the result suggests a direction for subsequent investigations in degree- or valence-constrained subclasses rather than a literal prediction of a molecule with an extreme thermodynamic property.

In this paper, a vertex of degree 1 is called a *pendant* vertex, and every other vertex is *non-pendant*. The graph S_n is the star with $n - 1$ pendant vertices and one central vertex of degree $n - 1$, and $S_n + e$ is obtained by adding an edge between two pendant vertices of S_n . The graph $S_n + e$ is depicted in Figure 1.

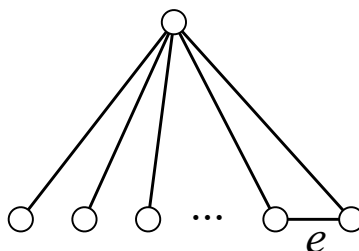


Figure 1. $S_n + e$.

We characterize the maximal augmented Sombor index in unicyclic graphs as follows.

Theorem 2. *Let G be a unicyclic graph of order $n \geq 3$. Then*

$$\text{ASO}(G) \leq (n-3) \sqrt{\frac{n^2 - 2n + 2}{n-2}} + 2 \sqrt{\frac{n^2 - 2n + 5}{n-1}} + 2$$

with equality if and only if $G \cong S_n + e$.

The form of the extremal graph has the following intuitive explanation. Edges of a cycle whose endpoints both have degree 2 contribute 2 to the ASO index, whereas concentrating many incidences at one vertex increases the contributions of the edges incident with that vertex. Subject to the unicyclic constraint, a triangle uses the fewest vertices to form the unique cycle and leaves the largest possible number of edges available as pendant edges at a common hub. The transformation lemmas below make this heuristic rigorous.

The degree of a vertex v in G is denoted by $d_G(v)$, and the maximum degree of G is denoted by $\Delta(G)$. The neighborhood of v is denoted by $N_G(v)$, and, for $S \subseteq V(G)$, we put $N_G(S) = \bigcup_{z \in S} N_G(z)$. To contract an edge uv means to delete uv and identify its endpoints. We next define two operations that will be used to increase the ASO index.

Definition 1 (leaf contracting). Let G be a graph and let $uv \in E(G)$. The leaf-contracting operation first contracts uv and then adds a new pendant vertex adjacent to the vertex produced by the contraction. The resulting graph is denoted by $G \odot uv$.

Definition 2 (leaf transferring). Let G be a graph and let $u, v \in V(G)$ be distinct, where v is not a pendant neighbor of u . The leaf-transferring operation on the ordered pair (u, v) deletes all edges joining u to its pendant neighbors and joins each of those pendant vertices to v . The resulting graph is denoted by $G \otimes (u, v)$.

Whenever these operations are applied below to a unicyclic graph, the resulting graph is again unicyclic and has the same order. For leaf transferring, only pendant edges are replaced, so the unique cycle is unchanged. For leaf contracting, the hypothesis $N_G(u) \cap N_G(v) = \emptyset$ guarantees that the contraction produces no parallel edges; the contraction decreases both the order and the size by one, and the subsequent addition of a pendant vertex and its incident edge restores both numbers. Sufficient conditions under which leaf transferring strictly increases the ASO index are stated and proved in Lemma 4. Connectivity is preserved, and the resulting graph has equal order and size, so it remains unicyclic.

For real numbers $x, y \geq 1$ satisfying $x + y > 2$, we write

$$f(x, y) = \sqrt{\frac{x^2 + y^2}{x + y - 2}}.$$

Thus,

$$\text{ASO}(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)).$$

2. Main results

We will use the following properties of the function $f(x, c)$ in our proof.

Lemma 1. For a fixed constant $c \geq 2$, the function $f(x, c) = \sqrt{\frac{x^2 + c^2}{x + c - 2}}$ is nondecreasing for $x \geq c$ and is strictly increasing for $x > c$. For integer $x \geq 2$, the function $f(x, 1) = \sqrt{\frac{x^2 + 1}{x - 1}}$ satisfies $f(2, 1) = f(3, 1) = \sqrt{5}$ and is strictly increasing for $x \geq 3$.

Proof. Let $g(x, c) = f^2(x, c) = \frac{x^2 + c^2}{x + c - 2}$, then the monotonicity of $f(x, c)$ is exactly the same as that of $g(x, c)$.

$$g'(x, c) = \frac{x^2 + (2c - 4)x - c^2}{(x + c - 2)^2}$$

The numerator $x^2 + (2c - 4)x - c^2$ is increasing for $x \geq c$ and is nonnegative for $x \geq c \geq 2$. At the boundary, $g'(2, 2) = 0$; for $x > c \geq 2$ the numerator is positive. Hence $f(x, c)$ is nondecreasing for $x \geq c$ and strictly increasing for $x > c$.

If $c = 1$, then $g(x, 1) = \frac{x^2 + 1}{x - 1}$ and $g'(x, 1) = \frac{x^2 - 2x - 1}{(x - 1)^2} > 0$ for $x \geq 3$. Together with the direct equality $f(2, 1) = f(3, 1) = \sqrt{5}$, this proves the second assertion for integer degrees. $\square$

Lemma 2. For a fixed constant c and the function $f(x, c) = \sqrt{\frac{x^2 + c^2}{x + c - 2}}$, we have $f(x, c) \leq f(x, x)$ for $x \geq c \geq 2$.

Proof. Let $\lambda = f^2(x, c) - f^2(x, x)$. Then

$$\begin{aligned}\lambda &= \frac{x^2 + c^2}{x + c - 2} - \frac{x^2}{x - 1} \\ &= -\frac{(x - c)(cx - x - c)}{(x + c - 2)(x - 1)}.\end{aligned}$$

Since $x \geq c \geq 2$, we know the denominator $(x + c - 2)(x - 1) > 0$ and $cx - x - c = (c - 1)x - c \geq (c - 2)c \geq 0$. Hence $\lambda \leq 0$, which implies $f(x, c) \leq f(x, x)$ for $x \geq c \geq 2$. $\square$

Auxiliary estimates. Put

$$p(z) = f(z, 1) = \sqrt{\frac{z^2 + 1}{z - 1}} \quad (z \geq 2).$$

For integer x in the indicated ranges, the following inequalities hold:

$$\Psi_1(x) = \sqrt{x + 4} - \sqrt{5} + (x - 1)(p(x) - p(2x - 1)) < 0 \quad (x \geq 3), \quad (2.1)$$

$$\Psi_2(x) = 2(\sqrt{x + 2} - 2) + (x - 2)(p(x) - p(2x - 1)) < 0 \quad (x \geq 4), \quad (2.2)$$

$$\Psi_3(x) = 2(\sqrt{x + 2} - 2) + (x - 2)(p(x) - p(2x - 2)) < 0 \quad (x \geq 5). \quad (2.3)$$

We provide the details because these estimates are used in the key transformation lemma. First,

$$\begin{aligned}p(2x - 1)^2 - p(x)^2 &= \frac{x(x - 2)}{x - 1}, \\ p(2x - 2)^2 - p(x)^2 &= (x - 2) \left(1 - \frac{2}{(x - 1)(2x - 3)} \right).\end{aligned}$$

Moreover, for $x \geq 3$,

$$p(x) \leq \sqrt{x + 2}, \quad p(2x - 1) < \sqrt{2x + 1}, \quad p(2x - 2) \leq \sqrt{2x}.$$

For (2.1), rationalizing the difference of the two p -terms gives

$$(x - 1)(p(2x - 1) - p(x)) = \frac{x(x - 2)}{p(x) + p(2x - 1)}.$$

If $x \geq 5$, then

$$\sqrt{x + 4} - \sqrt{5} < \frac{x - 1}{\sqrt{x}} \quad \text{and} \quad \frac{x(x - 2)}{p(x) + p(2x - 1)} > \frac{x(x - 2)}{2\sqrt{3x}}.$$

The first inequality follows by adding $\sqrt{5}$ to both sides and squaring the resulting positive quantities. After cancellation and division by $x - 1 > 0$, the resulting inequality is equivalent to $1 < 2\sqrt{5x}$. The second inequality follows from the preceding bounds because $p(x) < \sqrt{3x}$ and $p(2x - 1) < \sqrt{3x}$. Since

$$\frac{x(x - 2)}{x - 1} = x - 1 - \frac{1}{x - 1} \geq \frac{15}{4} > 2\sqrt{3}.$$

Consequently,

$$(x - 1)(p(2x - 1) - p(x)) > \frac{x(x - 2)}{2\sqrt{3x}} > \frac{x - 1}{\sqrt{x}} > \sqrt{x + 4} - \sqrt{5},$$

and hence $\Psi_1(x) < 0$. The two remaining values are transparent from

$$\begin{aligned}\Psi_1(3) &= \sqrt{7} + \sqrt{5} - 2\sqrt{\frac{13}{2}} < 0, \\ \Psi_1(4) &= \sqrt{8} - \sqrt{5} + 3\left(\sqrt{\frac{17}{3}} - \frac{5}{\sqrt{3}}\right) < 0;\end{aligned}$$

each sign follows after moving the positive radical term to the other side and squaring twice.

For (2.2), rationalization yields

$$(x-2)(p(2x-1) - p(x)) = \frac{x(x-2)^2}{(x-1)(p(x) + p(2x-1))}.$$

For $x \geq 7$, we compare the magnitude of the negative term in Ψ_2 with its positive term. The preceding bounds, $\sqrt{2x+1} < \sqrt{2}\sqrt{x+2}$, and rationalization of the radical give, respectively,

$$\begin{aligned}p(x) + p(2x-1) &< (1 + \sqrt{2})\sqrt{x+2}, \\ 2(\sqrt{x+2} - 2) &= \frac{2(x-2)}{\sqrt{x+2} + 2} < \frac{2(x-2)}{\sqrt{x+2}}.\end{aligned}$$

Since $\frac{x(x-2)}{x-1} \geq \frac{35}{6} > 2(1 + \sqrt{2})$, the resulting lower bound for the negative term is larger than the upper bound for the positive term. Thus,

$$\begin{aligned}(x-2)(p(2x-1) - p(x)) &> \frac{x(x-2)^2}{(1 + \sqrt{2})(x-1)\sqrt{x+2}} \\ &> \frac{2(x-2)}{\sqrt{x+2}} > 2(\sqrt{x+2} - 2),\end{aligned}$$

and hence $\Psi_2(x) < 0$ for $x \geq 7$. The remaining values follow by the same direct comparison:

$$\begin{aligned}\Psi_2(4) &= 2(\sqrt{6} - 2) + 2\left(\sqrt{\frac{17}{3}} - \frac{5}{\sqrt{3}}\right) < 0, \\ \Psi_2(5) &= 2(\sqrt{7} - 2) + 3\left(\sqrt{\frac{13}{2}} - \frac{\sqrt{41}}{2}\right) < 0, \\ \Psi_2(6) &= 2(\sqrt{8} - 2) + 4\left(\sqrt{\frac{37}{5}} - \sqrt{\frac{61}{5}}\right) < 0.\end{aligned}$$

Finally, let

$$\eta_x = 1 - \frac{2}{(x-1)(2x-3)}.$$

For (2.3), using the preceding difference-of-squares identity and rationalizing the two p -terms, we obtain

$$(x-2)(p(2x-2) - p(x)) = \frac{(x-2)^2\eta_x}{p(x) + p(2x-2)}.$$

For $x \geq 8$, $\eta_x \geq 13/14$ and

$$\frac{(x-2)^2\eta_x}{p(x)+p(2x-2)} > \frac{(x-2)^2\eta_x}{(1+\sqrt{2})\sqrt{x+2}},$$

$$2(\sqrt{x+2}-2) < \frac{2(x-2)}{\sqrt{x+2}}.$$

Because $(x-2)\eta_x \geq 39/7 > 2(1+\sqrt{2})$, this proves (2.3) for $x \geq 8$. Finally,

$$\Psi_3(5) = 2(\sqrt{7}-2) + 3\left(\sqrt{\frac{13}{2}} - \sqrt{\frac{65}{7}}\right) < 0,$$

$$\Psi_3(6) = 2(\sqrt{8}-2) + 4\left(\sqrt{\frac{37}{5}} - \frac{\sqrt{101}}{3}\right) < 0,$$

$$\Psi_3(7) = 2 + 5\left(\frac{5}{\sqrt{3}} - \sqrt{\frac{145}{11}}\right) < 0.$$

Each of these finite inequalities follows exactly by successive squaring of positive quantities.

Lemma 3. Let G be a connected graph and uv an edge of G such that $N_G(u) \cap N_G(v) = \emptyset$. Suppose $d_G(u), d_G(v) \geq 2$, and $d_G(w) \leq d_G(u) + d_G(v) - 1$ for any $w \in N_G(\{u, v\})$. Then $\text{ASO}(G \odot uv) > \text{ASO}(G)$.

Proof. Denote $d_G(u) = x$ and $d_G(v) = y$. Then, by hypothesis, $x, y \geq 2$. Let the degrees of the neighbors of u other than v be $a_1, \dots, a_{x-1}$ and let the degrees of the neighbors of v other than u be $b_1, \dots, b_{y-1}$. Then, for each $i = 1, \dots, x-1$ and each $j = 1, \dots, y-1$, $a_i, b_j \leq x+y-1$.

Let $G' = G \odot uv$ and let u_0 be the new vertex obtained from the contracting. Then $d_{G'}(u_0) = x+y-1$, and our goal is to show that

$$\text{ASO}(G) - \text{ASO}(G') = E_1 + E_2 + E_3 < 0, \quad (2.4)$$

where

$$E_1 = \sum_{i=1}^{x-1} (f(x, a_i) - f(x+y-1, a_i)),$$

$$E_2 = \sum_{i=1}^{y-1} (f(y, b_i) - f(x+y-1, b_i)),$$

$$E_3 = f(x, y) - f(x+y-1, 1).$$

For each a_i , if $x \geq a_i$, then Lemma 1 gives $f(x, a_i) \leq f(x+y-1, a_i)$. If $x < a_i$, symmetry of f and Lemma 2 give $f(x, a_i) = f(a_i, x) \leq f(a_i, a_i)$. Since $a_i \leq x+y-1$, Lemma 1 further gives $f(a_i, a_i) \leq f(x+y-1, a_i)$. Hence $f(x, a_i) \leq f(x+y-1, a_i)$ for every a_i , and therefore $E_1 \leq 0$. The same argument gives $E_2 \leq 0$.

On the other hand, noting that $f^2(x, y) - f^2(x+y-1, 1) = -\frac{2(x-1)(y-1)}{x+y-2} < 0$. Hence, we have $E_3 < 0$ and thus $\text{ASO}(G') > \text{ASO}(G)$. The proof is complete. $\square$

Lemma 4. Let G be a connected graph, and let $u, v \in V(G)$ be distinct vertices. Suppose that u has $t \geq 1$ pendant neighbors, that $d_G(v) \geq d_G(w)$ for every $w \in N_G(v)$, and that $d_G(v) \geq d_G(u)$. If $t = d_G(u) - 1$ or $t = d_G(u) - 2$, then

$$\text{ASO}(G \otimes (u, v)) > \text{ASO}(G).$$

Proof. Put $x = d_G(u)$, $y = d_G(v)$, and $r = x - t \in \{1, 2\}$. Let L be the set of the t pendant neighbors of u , let

$$\mu = \begin{cases} 1, & uv \in E(G), \\ 0, & uv \notin E(G), \end{cases}$$

and define

$$A = N_G(u) \setminus (L \cup \{v\}), \quad B = N_G(v) \setminus \{u\}.$$

Thus $|A| = r - \mu$ and $|B| = y - \mu$. Write $a_z = d_G(z)$ for $z \in A$ and $b_z = d_G(z)$ for $z \in B$. Since the vertices in A are non-pendant, $a_z \geq 2$, while the hypothesis at v gives $b_z \leq y$.

Let $G' = G \otimes (u, v)$ (see Figure 2). Then $d_{G'}(u) = r$, $d_{G'}(v) = y + t$, and

$$\text{ASO}(G) - \text{ASO}(G') = E_1 + E_2 + E_3 + E_4, \quad (2.5)$$

where

$$\begin{aligned} E_1 &= \sum_{z \in A} (f(x, a_z) - f(r, a_z)), \\ E_2 &= t(f(x, 1) - f(y + t, 1)), \\ E_3 &= \sum_{z \in B} (f(y, b_z) - f(y + t, b_z)), \\ E_4 &= \mu(f(x, y) - f(r, y + t)). \end{aligned}$$

The sets used in this decomposition also cover the adjacent case $\mu = 1$: The edge uv is then represented only by E_4 .

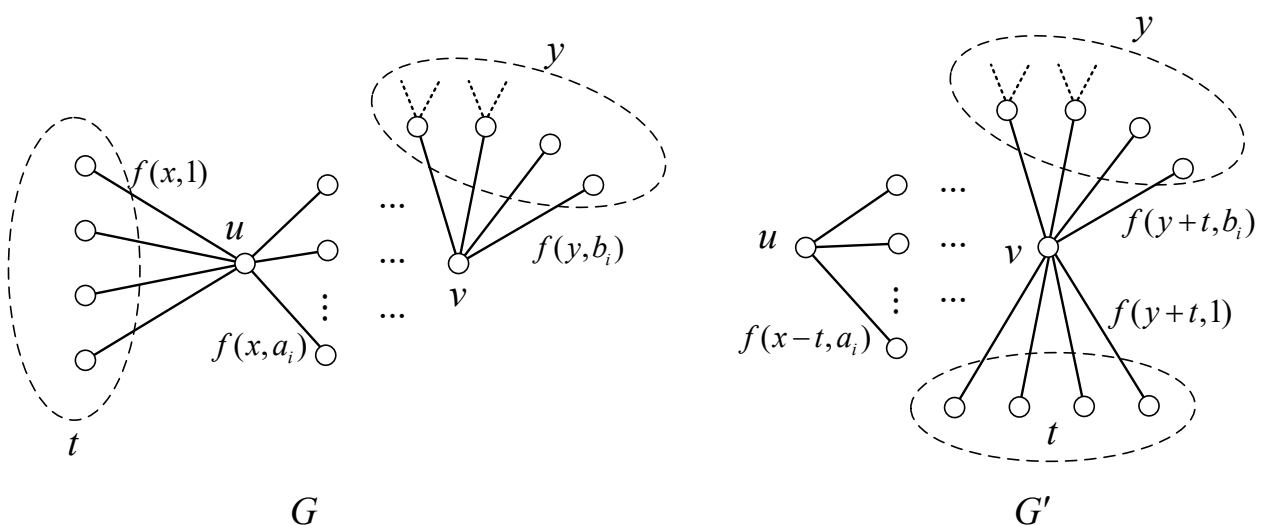


Figure 2. A schematic illustration of the graphs G and G' in Lemma 4.

We first estimate E_1 . For every $z \in A$,

$$f^2(x, a_z) - f^2(r, a_z) = t \left[1 - \frac{2(a_z^2 - 2a_z + 2)}{(x + a_z - 2)(r + a_z - 2)} \right] < t.$$

Consequently,

$$f(x, a_z) - f(r, a_z) < \sqrt{f^2(r, a_z) + t} - f(r, a_z).$$

For fixed $t > 0$, the function $H_t(q) = \sqrt{q+t} - \sqrt{q}$ is strictly decreasing in $q > 0$. If $r = 1$, then, because a_z is an integer at least 2,

$$f^2(1, a_z) = a_z + 1 + \frac{2}{a_z - 1} \geq 5.$$

If $r = 2$, then

$$f^2(2, a_z) = a_z + \frac{4}{a_z} \geq 4,$$

with equality exactly when $a_z = 2$. Hence,

$$E_1 \leq (1 - \mu)(\sqrt{t+5} - \sqrt{5}) \quad \text{if } r = 1, \quad (2.6)$$

$$E_1 < (2 - \mu)(\sqrt{t+4} - 2) \quad \text{if } r = 2. \quad (2.7)$$

In (2.6), the inequality is strict when $\mu = 0$. When $\mu = 1$, the set A is empty and both sides of (2.6) are zero.

Next, Lemma 1 and $b_z \leq y$ imply $E_3 \leq 0$. Moreover,

$$\begin{aligned} f^2(x, y) - f^2(r, y+t) &= \frac{x^2 + y^2 - r^2 - (y+t)^2}{x+y-2} \\ &= \frac{2t(x-y-t)}{x+y-2} \leq 0, \end{aligned}$$

so $E_4 \leq 0$.

It remains to control $E_1 + E_2$. Suppose first that $r = 1$, so $t = x - 1$. If $x = 2$ and $\mu = 0$, then A has one vertex of degree $a \geq 2$, and

$$f^2(2, a) - f^2(1, a) = \frac{-a^2 + 3a - 4}{a(a-1)} < 0.$$

Thus $E_1 < 0$ and $E_2, E_3 \leq 0$. If $x = 2$ and $\mu = 1$, then $E_1 = 0$ and $E_4 < 0$. In either case, (2.5) is negative. If $x \geq 3$, then $y+t \geq 2x-1$. When $\mu = 0$, the bound in (2.6) is strict. When $\mu = 1$, we have $E_1 = 0 < \sqrt{x+4} - \sqrt{5}$. Hence, in both cases,

$$\begin{aligned} E_1 + E_2 &< \sqrt{x+4} - \sqrt{5} + (x-1)(p(x) - p(2x-1)) \\ &= \Psi_1(x) < 0 \end{aligned}$$

where Ψ_1 is the auxiliary function defined in (2.1); hence $E_1 + E_2 < 0$.

Now suppose that $r = 2$, so $t = x - 2$ and $x \geq 3$. If $x \geq 4$ and $y \geq x + 1$, then (2.7) gives

$$E_1 + E_2 < 2(\sqrt{x+2} - 2) + (x-2)(p(x) - p(2x-1)) = \Psi_2(x) < 0.$$

If $y = x \geq 5$, then similarly

$$E_1 + E_2 < 2(\sqrt{x+2} - 2) + (x-2)(p(x) - p(2x-2)) = \Psi_3(x) < 0.$$

It remains to consider $y = x = 4$ and $x = 3$. For every integer $a \geq 2$, direct calculation gives

$$f(4, a) - f(2, a) \leq f(4, 2) - f(2, 2) = \sqrt{5} - 2.$$

Indeed, $f^2(4, a) - f^2(2, a) = -2(a^2 - 6a + 4)/(a(a+2))$ is nonpositive for $a \geq 6$, and the four values $a = 2, 3, 4, 5$ are checked directly. Therefore, when $x = y = 4$,

$$E_1 + E_2 \leq 2(\sqrt{5} - 2) + 2\left(\sqrt{\frac{17}{3}} - \sqrt{\frac{37}{5}}\right) < 0.$$

Finally, let $x = 3$, so $t = 1$ and $y \geq 3$. Define $\delta(a) = f(3, a) - f(2, a)$. Since

$$f^2(3, a) - f^2(2, a) = -\frac{(a-1)(a-4)}{a(a+1)},$$

the difference is nonpositive for $a \geq 4$, while direct comparison gives $\delta(3) < \delta(2)$. Therefore,

$$\begin{aligned}\delta(a) &\leq \delta(2) = \sqrt{\frac{13}{3}} - 2 & (a \geq 2), \\ \delta(a) &\leq \delta(3) = \sqrt{\frac{9}{2}} - \sqrt{\frac{13}{3}} & (a \geq 3).\end{aligned}$$

If $\mu = 1$, then

$$E_1 + E_2 \leq \delta(2) + p(3) - p(4) < 0.$$

If $\mu = 0$ and $y \geq 4$, then

$$E_1 + E_2 \leq 2\delta(2) + p(3) - p(5) < 0.$$

We are left with $\mu = 0$ and $y = 3$. If at least one of the two degrees a_z is at least 3, then

$$E_1 + E_2 \leq \delta(2) + \delta(3) + p(3) - p(4) < 0.$$

If both degrees are 2, then every b_z belongs to $\{1, 2, 3\}$. Direct comparison for these three values gives

$$f(3, b_z) - f(4, b_z) \leq f(3, 3) - f(4, 3),$$

and hence

$$\text{ASO}(G) - \text{ASO}(G') \leq 2\left(\sqrt{\frac{13}{3}} - 2\right) + \left(\sqrt{5} - \sqrt{\frac{17}{3}}\right) + 3\left(\sqrt{\frac{9}{2}} - \sqrt{5}\right) < 0.$$

All cases give $\text{ASO}(G) - \text{ASO}(G') < 0$, and the proof is complete. $\square$

Lemma 4 is deliberately restricted to vertices with at most two non-pendant neighbors. This is sufficient for the main theorem because a non-leaf vertex farthest from the unique cycle in an attached tree has one non-pendant neighbor, whereas a cycle vertex carrying only pendant attachments has two.

Proof of Theorem 2. For $n = 3$, the only unicyclic graph is $C_3 = S_3 + e$, and $\text{ASO}(C_3) = 6$, which is the value in the stated formula. For $n = 4$, there are two unicyclic graphs up to isomorphism, namely C_4 and $S_4 + e$. Directly,

$$\text{ASO}(C_4) = 8 < \sqrt{5} + 2\sqrt{\frac{13}{3}} + 2 = \text{ASO}(S_4 + e).$$

Thus the assertion holds for $n = 3, 4$.

Assume henceforth that $n \geq 5$, and choose, among all unicyclic graphs of order n , a graph G with maximum ASO index. Let v be a vertex of maximum degree $\Delta(G)$.

We first show that every non-pendant neighbor u of v has a common neighbor with v . Indeed, $d_G(u) \geq 2$, and for every $z \in N_G(\{u, v\})$,

$$d_G(z) \leq d_G(v) \leq d_G(u) + d_G(v) - 1.$$

If $N_G(u) \cap N_G(v) = \emptyset$, Lemma 3 applies to uv and gives

$$\text{ASO}(G \odot uv) > \text{ASO}(G).$$

The graph $G \odot uv$ is again unicyclic of order n , contradicting the choice of G . Therefore,

$$d_G(u) \geq 2 \implies N_G(u) \cap N_G(v) \neq \emptyset \quad (u \in N_G(v)). \quad (2.8)$$

At least one neighbor of v is non-pendant. Indeed, if every neighbor of v were pendant, the connectivity of G would force G to be a star, contradicting the assumption that G is unicyclic. Choose such a non-pendant neighbor u of v . By (2.8), there exists a vertex $w \in N_G(u) \cap N_G(v)$. Thus u, v, w form a triangle, which is the unique cycle of G .

We next prove that every vertex of $N_G(v) \setminus \{u, w\}$ is pendant. If some z in this set were non-pendant, (2.8) would provide a vertex $q \in N_G(z) \cap N_G(v)$. Then v, z, q would form a cycle distinct from the triangle u, v, w , contradicting unicyclicity. Hence all neighbors of v outside $\{u, w\}$ are pendant.

It remains to exclude vertices attached to u or w outside the triangle. Suppose that such a vertex exists. If all off-cycle neighbors of u and w are pendant, choose as z one of u, w having at least one such neighbor. Then z has exactly $d_G(z) - 2$ pendant neighbors. Otherwise, root every tree attached to the triangle at its cycle vertex and choose a non-leaf vertex z of maximum distance from the triangle. Every child of z is then pendant, so z has exactly $d_G(z) - 1$ pendant neighbors. In both cases $z \neq v$, z has at least one pendant neighbor, and

$$d_G(v) = \Delta(G) \geq d_G(z), \quad d_G(v) \geq d_G(s) \quad \text{for every } s \in N_G(v).$$

Lemma 4 therefore yields

$$\text{ASO}(G \otimes (z, v)) > \text{ASO}(G).$$

Leaf transferring leaves the unique cycle unchanged, so $G \otimes (z, v)$ is another unicyclic graph of order n , again a contradiction. Consequently, no vertex is attached to u or w outside the triangle. Thus $d_G(u) = d_G(w) = 2$, every other vertex is a pendant neighbor of v , and

$$G \cong S_n + e.$$

Finally, in $S_n + e$, $n - 3$ edges join vertices of degrees $n - 1$ and 1, two edges join vertices of degrees $n - 1$ and 2, and one edge joins two vertices of degree 2. Hence

$$\begin{aligned}\text{ASO}(S_n + e) &= (n - 3)f(n - 1, 1) + 2f(n - 1, 2) + f(2, 2) \\ &= (n - 3)\sqrt{\frac{n^2 - 2n + 2}{n - 2}} + 2\sqrt{\frac{n^2 - 2n + 5}{n - 1}} + 2.\end{aligned}$$

This proves the upper bound and its unique equality case.

3. Conclusions

We have determined the maximum ASO index over unicyclic graphs of order $n \geq 3$ and shown that $S_n + e$ is the unique extremal graph. The proof shows that the index favors degree concentration at a common hub and a triangle as the unique cycle. This graph is a benchmark for the unrestricted class, while chemical interpretations require degree or valence constraints. Beyond the present setting, the two transformations may facilitate ASO extremal studies in bicyclic, tricyclic, and degree- or valence-constrained graph classes. In particular, they can help simplify attached-tree structures and concentrate pendant branches at high-degree vertices.

Author contributions

Qinfei Tang: Conceptualization, methodology, formal analysis, investigation, writing – original draft; Qinghai Liu: Conceptualization, supervision, validation, writing – review & editing. All authors have read and approved the final version of the manuscript.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflict of interest.

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