AIMS Mathematics

https://www.aimspress.com/journal/Math

AIMS Mathematics, 10(10): 24500–24513.
DOI: 10.3934/math.20251086
Received: 25 June 2025
Revised: 20 September 2025
Accepted: 13 October 2025
Published: 27 October 2025

Research article

On degree-based graph invariants of fixed-order unicyclic graphs with prescribed maximum degree

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Abstract: Consider a graph G having edge set E, and denote by d_x the degree of a vertex x in G. A unicyclic graph is defined as a connected graph containing exactly one cycle. This work focuses on unicyclic graphs of a fixed order and examines the graph invariants of such graphs of the form $BID_\phi(G) = \sum_{yz\in E} \phi(d_y, d_z)$, where ϕ is a symmetric and real-valued function. Such graph invariants are known as BID (bond incident degree) indices. The main objective is to determine the graphs that either minimize or maximize the quantity BID_ϕ among fixed-order unicyclic graphs with prescribed maximum degree, under specific assumptions on the function ϕ. These assumptions are satisfied by several classical and modern degree-based graph invariants. Generally, the results obtained are applicable to a wide range of such invariants. In particular, one of the obtained results covers the harmonic and sum-connectivity indices, while another applies to the recently proposed Sombor and Euler–Sombor indices as well as their reduced versions.

Keywords: bond incident degree indices; unicyclic graph; extremal problem; maximum degree
Mathematics Subject Classification: 05C07, 05C09, 05C35

1. Introduction

This work is concerned solely with simple, finite, and connected graphs. For fundamental graph-theoretic and chemical graph-theoretic terminology, the reader is referred to standard texts such as [9, 11, 16] for general graph theory and [32, 35] for chemical graph theory.

In chemical graph theory, real-valued graph invariants are often referred to as topological indices [12]. The first Zagreb index, appeared in 1970s (see [10, 20, 21]) within the study of certain energy, is one of the most-studied topological indices. Given a graph G, this index can be defined [5, 10] as

$$\mathcal{Z}_1(G) = \sum_{xy\in E(G)} (d_x + d_y),$$

where d_y denotes the degree of vertex y and $E(G)$ is the set of edges in G. When comparing multiple graphs, we denote the degree of y in G by $d_y(G)$. Numerous known properties of $\mathcal{Z}_1$ can be found in the surveys [5, 10].

The harmonic index [8, 13] and the sum-connectivity index [38] can be considered as variants of $\mathcal{Z}_1$, which are defined, respectively, as

$$\mathcal{H}(G) = \sum_{xy\in E(G)} \frac{2}{d_x + d_y} \quad \text{and} \quad \mathcal{SC}(G) = \sum_{xy\in E(G)} \frac{1}{\sqrt{d_x + d_y}}.$$

The readers interested in the existing properties of these two indices are referred to the survey [8].

A geometry-based approach was introduced by Gutman [18] to develop certain degree-based topological indices, which led to the formation of the Sombor and reduced Sombor indices. The Sombor index ($\mathcal{SO}$) and its reduced version are, respectively, defined as

$$\mathcal{SO}(G) = \sum_{xy\in E(G)} \sqrt{d_x^2 + d_y^2} \quad \text{and} \quad \mathcal{RSO}(G) = \sum_{xy\in E(G)} \sqrt{(d_x-1)^2 + (d_y-1)^2}.$$

We refer the reader to [17, 25–27] for applications and various known properties of the $\mathcal{SO}$.

The Euler-Sombor (EU) index [19, 30] and its reduced version [2] (namely, the reduced Euler-Sombor (REU) index) are, respectively, defined as

$$\mathcal{EU}(G) = \sum_{xy\in E(G)} \sqrt{d_x d_y + d_x^2 + d_y^2}$$

and

$$\mathcal{REU}(G) = \sum_{xy\in E(G)} \sqrt{(d_x-1)(d_y-1) + (d_x-1)^2 + (d_y-1)^2}.$$

Several mathematical characteristics of the EU index can be found in [23, 29].

Each of the indices above fits into a broader class of degree-based topological indices expressible [22, 34] as

$$\mathfrak{BID}_\phi(G) = \sum_{xy\in E(G)} \phi(d_x, d_y), \tag{1.1}$$

where ϕ is a symmetric real-valued function defined on the set of all distinct vertex degrees of G. These indices are commonly referred to as bond incident degree (BID) indices [7, 36, 37], a term introduced in [33]. Recent developments related to BID indices can be found, for instance, in [4, 14, 28, 31] (see also the survey [3]).

A unicyclic graph is a connected graph containing exactly one cycle. The primary aim of the present study is to identify the graphs that either minimize or maximize $\mathfrak{BID}_\phi$ among all unicyclic graphs of a given order and prescribed maximum degree, under specific conditions on the function ϕ. These conditions on ϕ are met by several classical and contemporary degree-based indices. Generally, the obtained findings are broadly applicable. Notably, one of the results obtained is applicable to the harmonic and sum-connectivity indices, while another one covers the recently introduced Sombor and Euler–Sombor indices, along with their reduced versions.

2. Results

Before stating and proving the results of this paper, some definitions and notions are recalled first.

We denote the vertex set in a graph G by $V(G)$. A graph with a predetermined number of vertices is referred to as a fixed-order graph. Specifically, if a graph has n vertices, we call it an n-order graph. Given a vertex $x \in V(G)$, the set of all vertices adjacent to it is denoted by $N_G(x)$. Any vertex $y \in N_G(x)$ is referred to as a neighbor of x. A vertex of degree one is known as a pendent vertex. A nontrivial path $P : s_1 s_2 \dots s_r$ in G is termed a pendent path if $\min\{d_{s_1}(G), d_{s_r}(G)\} = 1$, $\max\{d_{s_1}(G), d_{s_r}(G)\} \geq 3$, and $d_{s_i}(G) = 2$ when $2 \leq i \leq r-1$. Adjacent pendent paths in a graph are the ones sharing a common vertex. The complement of a graph G is represented as $\overline{G}$. If A and B are two nonempty sets such that $A \subseteq E(G)$ and $B \subseteq E(\overline{G})$, then the graph constructed from G by dropping all the members of A and inserting all the members of B is denoted by $G - A + B$. If either A or B is a singleton, we replace it in the notation $G - A + B$ by its element; for instance, if $A = \{xy\}$, then we write $G - xy + B$ instead of $G - A + B$. The set of all real numbers is denoted by $\mathbb{R}$.

Now, we are in a position to prove our first result.

Lemma 1. *Let ϕ be a real-valued symmetric function defined on the set*

$$\{(r_1, r_2) \in \mathbb{R}^2 : r_1 \geq 1 \text{ and } r_2 \geq 1\}$$

such that ϕ meets the following constraints:

(i) The function Ψ defined as $\Psi(\eta) = \phi(\eta, \xi_1) - \phi(\eta, \xi_2)$, with $\eta \geq 1$, is decreasing (that is, if $1 \leq \eta_1 < \eta_2$ then $\Psi(\eta_1) \geq \Psi(\eta_2)$), where ξ_1 and ξ_2 are fixed integers satisfying $\xi_1 > \xi_2 \geq 1$.

(ii) The inequality

$$\phi(i,3) - \phi(i,2) + \min\{\phi(3,3) - \phi(2,3) + \phi(1,3) - \phi(2,2), \phi(3,3) + \phi(1,2) - 2\phi(2,2)\} > 0$$

holds for every integer $i \geq 3$.

Let G be a given graph such that it contains a pendent path $P : s_1 s_2 \dots s_r$, where $d_{s_1}(G) = 3$. Let s_1', s_2', and s_2 be the neighbors of s_1. Define $G' := G - s_1' s_1 + s_1' s_r$. If $d_{s_1'}(G) \leq 3$, then $\mathfrak{BID}_\phi(G') < \mathfrak{BID}_\phi(G)$.

Proof. Let $\Delta := \max\{d_x(G) : x \in V(G)\}$. Then, $\Delta \geq 3$. We note that $d_x(G) = d_x(G')$ for every $x \in V(G) \setminus \{s_1, s_r\}$, whereas $d_{s_1}(G) - 1 = d_{s_1}(G') = 2$ and $d_{s_r}(G) + 1 = d_{s_r}(G') = 2$.

First, we consider the case where $r = 2$. Then, we obtain

$$\mathfrak{BID}_\phi(G) - \mathfrak{BID}_\phi(G') = \sum_{i=1}^{2} \left[\phi(d_{s_i'}(G), 3) - \phi(d_{s_i'}(G), 2)\right] + \phi(1,3) - \phi(2,2).$$

By conditions (i) and (ii), it holds that

$$\mathfrak{BID}_\phi(G) - \mathfrak{BID}_\phi(G') \geq [\phi(\Delta,3) - \phi(\Delta,2)] + \phi(3,3) - \phi(2,3) + \phi(1,3) - \phi(2,2) > 0.$$

Now, we consider the case where $r \geq 3$. Then, again because of conditions (i) and (ii), we obtain

$$\mathfrak{BID}_\phi(G) - \mathfrak{BID}_\phi(G') = \sum_{i=1}^{2} \left[\phi(d_{s_i'}(G), 3) - \phi(d_{s_i'}(G), 2)\right]$$

$$+\phi(2,3)+\phi(1,2)-2\phi(2,2)$$
$$\geq [\phi(\Delta,3)-\phi(\Delta,2)]+\phi(3,3)-\phi(2,3)$$
$$+\phi(2,3)+\phi(1,2)-2\phi(2,2)>0.$$

□

The following lemma's proof is obtained by similar steps as in Lemma 1, and is omitted for brevity.

Lemma 2. *Let ϕ be a real-valued symmetric function defined on the set*

$$\{(r_1,r_2)\in\mathbb{R}^2 : r_1\geq 1 \text{ and } r_2\geq 1\}$$

such that ϕ meets the following constraints:

(i) The function Ψ defined as $\Psi(\eta)=\phi(\eta,\xi_1)-\phi(\eta,\xi_2)$, with $\eta\geq 1$, is increasing (that is, if $1\leq\eta_1<\eta_2$, then $\Psi(\eta_1)\leq\Psi(\eta_2)$), where ξ_1 and ξ_2 are fixed integers satisfying $\xi_1>\xi_2\geq 1$.

(ii) The inequality

$$\phi(i,3)-\phi(i,2)+\max\{\phi(3,3)-\phi(2,3)+\phi(1,3)-\phi(2,2),\phi(3,3)+\phi(1,2)-2\phi(2,2)\}<0$$

holds for every integer $i\geq 3$.

Let G be a given graph such that it contains a pendent path $P: s_1s_2\ldots s_r$, where $d_{s_1}(G)=3$. Let s_1', s_2', and s_2 be the neighbors of s_1. Define $G':=G-s_1's_1+s_1's_r$. If $d_{s_1'}(G)\leq 3$, then $\mathfrak{BID}_\phi(G')>\mathfrak{BID}_\phi(G)$.

Lemma 3. *Let ϕ be the function defined in Lemma 1, satisfying condition (i) stated therein. Also, assume that the inequality*

$$2[\phi(i,4)-\phi(i,3)]+\phi(3,4)-2\phi(2,3)+\min\{\phi(1,4),\phi(2,4)+\phi(1,2)-\phi(2,2)\}>0 \tag{2.1}$$

holds for every integer $i\geq 4$.

Let G be a given graph such that it contains a pendent path $P: s_1s_2\ldots s_r$, where $d_{s_1}(G)=4$. Let s_1', s_2', s_3', and s_2 be the neighbors of s_1. Define $G':=G-s_1's_1+s_1's_r$. If $d_{s_1'}(G)\leq 3$, then $\mathfrak{BID}_\phi(G')<\mathfrak{BID}_\phi(G)$.

Proof. Let $\Delta:=\max\{d_x(G): x\in V(G)\}$. Then, $\Delta\geq 4$.

First, we assume that $r=2$. Then, by condition (i) of Lemma 1 and inequality (2.1), we have

$$\mathfrak{BID}_\phi(G)-\mathfrak{BID}_\phi(G')=\sum_{i=2}^{3}\left[\phi(d_{s_i'}(G),4)-\phi(d_{s_i'}(G),3)\right]+\phi(d_{s_1'}(G),4)-\phi(d_{s_1'}(G),2)$$
$$+\phi(1,4)-\phi(2,3)$$
$$\geq 2[\phi(\Delta,4)-\phi(\Delta,3)]+\phi(3,4)-\phi(2,3)+\phi(1,4)-\phi(2,3)>0.$$

Now, we assume that $r\geq 3$. Then, again by condition (i) of Lemma 1 and inequality (2.1), we have

$$\mathfrak{BID}_\phi(G)-\mathfrak{BID}_\phi(G')=\sum_{i=2}^{3}\left[\phi(d_{s_i'}(G),4)-\phi(d_{s_i'}(G),3)\right]+\phi(d_{s_1'}(G),4)-\phi(d_{s_1'}(G),2)$$

$$
\begin{aligned}
&+\phi(2,4)-\phi(2,3)+\phi(1,2)-\phi(2,2) \\
\geq\ & 2\left[\phi(\Delta,4)-\phi(\Delta,3)\right]+\phi(3,4)-\phi(2,3) \\
&+\phi(2,4)-\phi(2,3)+\phi(1,2)-\phi(2,2)>0.
\end{aligned}
$$

□

The next lemma's proof is obtained by similar steps as in Lemma 3, and is omitted for brevity.

Lemma 4. *Let ϕ be the function defined in Lemma 2, satisfying condition (i) stated therein. Also, assume that the inequality*

$$2\left[\phi(i,4)-\phi(i,3)\right]+\phi(3,4)-2\phi(2,3)+\max\{\phi(1,4),\phi(2,4)+\phi(1,2)-\phi(2,2)\}<0$$

holds for every integer $i \geq 4$.

Let G be a given graph such that it contains a pendent path $P : s_1 s_2 \dots s_r$, where $d_{s_1}(G) = 4$. Let s'_1, s'_2, s'_3, and s_2 be the neighbors of s_1. Define $G' := G - s'_1 s_1 + s'_1 s_r$. If $d_{s'_1}(G) \leq 3$, then $\mathfrak{BID}_\phi(G') > \mathfrak{BID}_\phi(G)$.

Lemma 5. *Let ϕ be the function defined in Lemma 1, satisfying condition (i) stated therein. Also, assume that the inequalities*

$$(b-2)\left[\phi(a,b)-\phi(a,b-1)\right]-\phi(b-1,2)+2\phi(b,1)-\phi(1,2)>0, \tag{2.2}$$

$$(b-2)\left[\phi(a,b)-\phi(a,b-1)\right]-\phi(b-1,2)+\phi(b,1)+\phi(b,2)-\phi(2,2)>0, \tag{2.3}$$

$$(b-2)\left[\phi(a,b)-\phi(a,b-1)\right]-\phi(b-1,2)+2\phi(b,2)+\phi(1,2)-2\phi(2,2)>0 \tag{2.4}$$

hold for all integers a and b satisfying $a \geq b \geq 3$. Let $Q : q_1 q_2 \dots q_r$ and $Q' : q'_1 q'_2 \dots q'_s$ be pendent paths in a connected graph G such that $q_1 = q'_1 := w$. Define $G' := G - q'_1 q'_2 + q_r q'_2$. Then, it holds that $\mathfrak{BID}_\phi(G) > \mathfrak{BID}_\phi(G')$.

Proof. We note that $d_w(G) \geq 3$. Let $\Delta := \max\{d_x(G) : x \in V(G)\}$. Then, $\Delta \geq 3$.

Case 1. Both r and s are equal to 1.
Here, by condition (i) of Lemma 1 and inequality (2.2), we have

$$
\begin{aligned}
\mathfrak{BID}_\phi(G)-\mathfrak{BID}_\phi(G') &= \sum_{w'\in N_G(w)\setminus\{q_2,q'_2\}} \left[\phi(d_{w'}(G),d_w(G))-\phi(d_{w'}(G),d_w(G)-1)\right] \\
&\quad +2\phi(d_w(G),1)-\phi(d_w(G)-1,2)-\phi(1,2) \\
&\geq (d_w(G)-2)\left[\phi(\Delta,d_w(G))-\phi(\Delta,d_w(G)-1)\right] \\
&\quad +2\phi(d_w(G),1)-\phi(d_w(G)-1,2)-\phi(1,2)>0.
\end{aligned}
$$

Case 2. One of r and s is equal to 1, and the other is greater than 1.
In this case, by condition (i) of Lemma 1 and inequality (2.3), we have

$$\mathfrak{BID}_\phi(G)-\mathfrak{BID}_\phi(G') = \sum_{w'\in N_G(w)\setminus\{q_2,q'_2\}} \left[\phi(d_{w'}(G),d_w(G))-\phi(d_{w'}(G),d_w(G)-1)\right]$$

$$+ \phi(d_w(G), 2) - \phi(d_w(G) - 1, 2) + \phi(d_w(G), 1) - \phi(2, 2)$$
$$\geq (d_w(G) - 2) [\phi(\Delta, d_w(G)) - \phi(\Delta, d_w(G) - 1)]$$
$$+ \phi(d_w(G), 2) - \phi(d_w(G) - 1, 2) + \phi(d_w(G), 1) - \phi(2, 2) > 0.$$

Case 3. Both r and s are greater than 1.
Here, by condition (i) of Lemma 1 and inequality (2.4), we have

$$\begin{aligned}\mathfrak{BID}_\phi(G) - \mathfrak{BID}_\phi(G') &= \sum_{w' \in N_G(w) \setminus \{q_2, q_2'\}} [\phi(d_{w'}(G), d_w(G)) - \phi(d_{w'}(G), d_w(G) - 1)] \\ &\quad + 2\phi(d_w(G), 2) - \phi(d_w(G) - 1, 2) + \phi(1, 2) - 2\phi(2, 2) \\ &\geq (d_w(G) - 2) [\phi(\Delta, d_w(G)) - \phi(\Delta, d_w(G) - 1)] \\ &\quad + 2\phi(d_w(G), 2) - \phi(d_w(G) - 1, 2) + \phi(1, 2) - 2\phi(2, 2) > 0.\end{aligned}$$

□

The next lemma's proof is completely analogous to that of Lemma 5, and is omitted for brevity.

Lemma 6. *Let ϕ be the function defined in Lemma 2, satisfying condition (i) stated therein. Also, assume that the inequalities*

$$(b - 2) [\phi(a, b) - \phi(a, b - 1)] - \phi(b - 1, 2) + 2\phi(b, 1) - \phi(1, 2) < 0,$$
$$(b - 2) [\phi(a, b) - \phi(a, b - 1)] - \phi(b - 1, 2) + \phi(b, 1) + \phi(b, 2) - \phi(2, 2) < 0,$$
$$(b - 2) [\phi(a, b) - \phi(a, b - 1)] - \phi(b - 1, 2) + 2\phi(b, 2) + \phi(1, 2) - 2\phi(2, 2) < 0$$

hold for all integers a and b satisfying $a \geq b \geq 3$. Let $Q : q_1q_2 \dots q_r$ and $Q' : q_1'q_2' \dots q_s'$ be pendent paths in a connected graph G such that $q_1 = q_1' := w$. Define $G' := G - q_1'q_2' + q_rq_2'$. Then, it holds that $\mathfrak{BID}_\phi(G) < \mathfrak{BID}_\phi(G')$.

The following result immediately follows from Lemmas 5 and 6.

Corollary 1. *Let ϕ be the function defined in Lemma 1 (respectively, in Lemma 2), satisfying condition (i) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemma 5 (respectively, in Lemma 6) hold. Then, the path graph P_n uniquely minimizes (respectively, maximizes) $\mathfrak{BID}_\phi$ in the class of n-order trees for every $n \geq 4$.*

The next lemma follows from Lemmas 1, 2, 5, and 6.

Corollary 2. *Let ϕ be the function defined in Lemma 1 (respectively, in Lemma 2), satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemma 5 (respectively, in Lemma 6) hold. Then, only the cycle graph C_n attains the minimum (respectively, maximum) value of $\mathfrak{BID}_\phi$ among n-order unicyclic graphs for every $n \geq 4$.*

Lemma 7. *Let ϕ be the function defined in Lemma 1, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemma 5 hold. If U is a unicyclic graph of maximum degree $\Delta \geq 3$ and order n such that it yields the minimum value of $\mathfrak{BID}_\phi$ among all such graphs, then U contains a single vertex having the maximum degree.*

Proof. Assume, for the sake of contradiction, that U has $\ell \geq 2$ vertices with the maximum degree.

If the unique cycle of U does not contain all vertices of maximum degree, then U necessarily possesses adjacent pendent paths outside the cycle. So, Lemma 5 confirms the existence of a unicyclic graph U' of order n and maximum degree Δ such that

$$\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U) > \mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U'),$$

which contradicts the definition of U.

On the other hand, if the unique cycle of U contains every vertex of maximum degree and if $\Delta \geq 4$, then we can apply Lemma 5 at least $\ell - 1$ times without affecting the maximum degree of U. This leads to the construction of another n-order unicyclic graph U'' of maximum degree Δ with a strictly smaller $\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}$ value than that of U, again resulting in a contradiction.

The final case to consider is when $\Delta = 3$, and multiple vertices with degree 3 are located on the cycle of U. In this scenario, Lemma 1 guarantees the existence of a graph U''' in the class of the considered graphs with the maximum degree 3 satisfying

$$\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U) > \mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U'''),$$

yielding yet another contradiction. □

The following result's proof is fully analogous to that of Lemma 7, and is omitted for brevity.

Lemma 8. *Let ϕ be the function defined in Lemma 2, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemma 6 hold. If U is a unicyclic graph of maximum degree $\Delta \geq 3$ and order n such that it yields the maximum value of $\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}$ among all such graphs, then U has a single vertex with the maximum degree.*

Lemma 9. *Let ϕ be the function defined in Lemma 1, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 3 and 5 hold. If U is a unicyclic graph of maximum degree $\Delta \geq 3$ and order n such that it yields the minimum value of $\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}$ among all such graphs, then any vertex of U with degree Δ must necessarily be located on the cycle.*

Proof. Let $x \in V(U)$ such that $d_x(U) = \Delta$. Then, Lemma 7 confirms that x is the unique vertex having degree Δ.

Let C denote the unique cycle in the graph U, and let $V(C)$ be the set of vertices that belong to this cycle. Assume, for contradiction, that the vertex x lies outside C. Select $x' \in V(C)$ such that the distance between x and x' is the least.

Then, according to Lemmas 1, 3, and 5, U has exactly two vertices with degrees exceeding 2: the vertex x, with $d_x(U) = \Delta$, and the vertex x', for which $d_{x'}(U) = 3$. Let the set of all neighbors of x be $\{x_1, x_2, \ldots, x_\Delta\}$; here, x_1 is assumed to lie on the path connecting x to x'. Also, here we remark that the vertices x_1 and x' may or may not be the same. Given that x is the only vertex having degree Δ and that $d_{x'}(U) = 3$, it follows that $\Delta \geq 4$. Define a new graph $U' := U - \{x_4x, x_5x, \ldots, x_\Delta x\} + \{x_4x', x_5x', \ldots, x_\Delta x'\}$. Then, we have $d_{x'}(U') = \Delta$ and $d_x(U') = 3$. Whether $x_1 = x'$ or $x_1 \neq x'$, in either of the two cases, by using condition (i) of Lemma 1 we obtain

$$\mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U) - \mathfrak{B}\mathfrak{I}\mathfrak{D}_{\phi}(U') = \sum_{i=2}^{3} [\phi(d_{x_i}(U), \Delta) - \phi(d_{x_i}(U), 3)] + 2[\phi(2, 3) - \phi(2, \Delta)]$$

$$\geq 2\left[\phi(2,\Delta) - \phi(2,3)\right] + 2[\phi(2,3) - \phi(2,\Delta)] = 0. \tag{2.5}$$

Observe that, in U', there exist pendent paths that share vertex x and $d_x(U') < \Delta$. By using the graph transformation described in Lemma 5 to the mentioned paths, we find a new graph U'' in the considered class of graphs, such that $\mathfrak{BID}_\phi(U') > \mathfrak{BID}_\phi(U'')$. Combining this inequality with (2.5), yields $\mathfrak{BID}_\phi(U) > \mathfrak{BID}_\phi(U'')$, which contradicts the assumption that U minimizes $\mathfrak{BID}_\phi$ in the considered class of graphs. □

The next lemma's proof is totally analogous to that of Lemma 9, and is therefore omitted.

Lemma 10. *Let ϕ be the function defined in Lemma 2, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 4 and 6 hold. If U is a unicyclic graph of maximum degree $\Delta \geq 3$ and order n such that it yields the maximum value of $\mathfrak{BID}_\phi$ among all such graphs, then any vertex of U with degree Δ must necessarily be located on the cycle.*

Now, we are ready to prove the first main result of this paper.

Theorem 1. *Let ϕ be the function defined in Lemma 1, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 3 and 5 hold. If U is a unicyclic graph with the order n and maximum degree Δ such that it yields the minimum value of $\mathfrak{BID}_\phi$ among all such graphs, then U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle, where $3 \leq \Delta \leq n-2$.*

Proof. According to Lemma 7, the graph U possesses a single vertex with degree Δ. Also, Lemma 9 ensures that this unique maximum-degree vertex lies on U's cycle. Let C denote this cycle, and let $x \in V(U)$ be the vertex for which $d_x(U) = \Delta$. Then, by Lemma 5, each of the vertices not belonging to C, has a degree no greater than 2. Applying Lemma 5 once more, it follows that every vertex on the cycle, except x, has a degree not more than 3. Then, applying Lemma 1, we conclude that every vertex on the cycle, except x, must actually have degree exactly 2. □

Remark 1. *Theorem 1 covers all of the following indices, as their associated functions meet the required assumptions: $\mathcal{Z}_1$, $\mathcal{F}$, $\mathcal{RSC}$, $\mathcal{SO}$, $\mathcal{RSO}$, $\mathcal{EU}$, and $\mathcal{REU}$; where $\mathfrak{BID}_\phi$ corresponds to the forgotten index $\mathcal{F}$ (see [5, 15]) or the reciprocal sum-connectivity index $\mathcal{RSC}$ (see [6]) when $\phi(\xi_1,\xi_2) = \xi_1^2 + \xi_2^2$ or $\phi(\xi_1,\xi_2) = \sqrt{\xi_1+\xi_2}$, respectively, whereas all the remaining indices are defined in the introduction section.*

The next theorem's proof is completely analogous to that of Theorem 1, and is therefore omitted.

Theorem 2. *Let ϕ be the function defined in Lemma 2, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 4 and 6 hold. If U is a unicyclic graph with the order n and maximum degree Δ such that it yields the maximum value of $\mathfrak{BID}_\phi$ among all such graphs, then U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle, where $3 \leq \Delta \leq n-2$.*

Remark 2. *Theorem 2 is applicable to the indices $\mathcal{SC}$, $\mathcal{H}$, and ${}^m\mathcal{SO}$, as their associated functions meet the required assumptions, where $\mathfrak{BID}_\phi$ corresponds to the modified Sombor index ${}^m\mathcal{SO}$ (introduced in [24]) when $\phi(\xi_1,\xi_2) = \frac{1}{\sqrt{\xi_1^2+\xi_2^2}}$, whereas the definitions of the other two indices are given in the introduction section.*

When $\mathfrak{BID}_\phi$ depends solely on the degree sequence of a graph, without requiring information about vertex adjacencies, all extremal graphs described in Theorems 1 and 2 yield identical values of $\mathfrak{BID}_\phi$. Examples of such indices include $\mathcal{F}$ and $\mathcal{Z}_1$ because

$$\mathcal{Z}_1(G) = \sum_{xy\in E(G)} (d_x + d_y) = \sum_{z\in V(G)} (d_z)^2$$

and

$$\mathcal{F}(G) = \sum_{xy\in E(G)} (d_x^2 + d_y^2) = \sum_{z\in V(G)} (d_z)^3.$$

Thus, for these types of indices, under specific conditions on ϕ, these theorems offer a complete characterization of graphs minimizing or maximizing $\mathfrak{BID}_\phi$ among fixed-order unicyclic graphs with prescribed maximum degree. For the case where $\mathfrak{BID}_\phi$ depends not only on the degree sequence but also on the adjacency relationships between vertices, we need to establish a few additional lemmas.

Lemma 11. *Let ϕ be the function defined in Lemma 1, satisfying condition (i) stated therein. Also, assume that*

$$\phi(3,1) - \phi(3,2) + \phi(2,2) - \phi(1,2) > 0. \tag{2.6}$$

(*We remark here that if the function Ψ, defined in condition (i) of Lemma 1, is strictly decreasing, then* (2.6) *holds.*) *Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the minimum value of $\mathfrak{BID}_\phi$ among all such graphs, where $3 \le \Delta \le n-2$. If U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle, then the graph U cannot have the pendent paths of both length 1 and length greater than 2 simultaneously.*

Proof. For the sake of contradiction, assume that the graph U has both a pendent path $P : zx$ of length 1 and a pendent path $Q : zz_1z_2 \dots z_{r-1}z_r$ of length $r \ge 3$. Certainly, $d_z(U) = \Delta$. Define $U^* := U - z_{r-1}z_r + z_r x$. Then, by condition (i) of Lemma 1 and inequality (2.6), we have

$$\begin{aligned}\mathfrak{BID}_\phi(U) - \mathfrak{BID}_\phi(U^*) &= \phi(\Delta,1) - \phi(\Delta,2) + \phi(2,2) - \phi(1,2)\\ &\ge \phi(3,1) - \phi(3,2) + \phi(2,2) - \phi(1,2) > 0,\end{aligned}$$

which leads to a contradiction. □

The next result's proof is completely analogous to that of Lemma 11, and is therefore omitted.

Lemma 12. *Let ϕ be the function defined in Lemma 2, satisfying condition (i) stated therein. Also, assume that*

$$\phi(3,1) - \phi(3,2) + \phi(2,2) - \phi(1,2) < 0. \tag{2.7}$$

(*We remark here that if the function Ψ, defined in condition (i) of Lemma 2, is strictly increasing, then* (2.7) *holds.*) *Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the maximum value of $\mathfrak{BID}_\phi$ among all such graphs, where $3 \le \Delta \le n-2$. If U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle, then the graph U cannot have the pendent paths of both length 1 and length greater than 2 simultaneously.*

Lemma 13. *Let ϕ be the function defined in Lemma 1, satisfying condition (i) stated therein. Also, assume that* (2.6) *holds. Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the minimum value of $\mathfrak{BID}_\phi$ among all such graphs, where $3 \le \Delta \le n-2$. If U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle such that at least one of these paths has length 1, then the cycle of U is a triangle.*

Proof. For the sake of contradiction, assume that U has a pendent path $P : zx$ with the length 1 and its cycle is not a triangle, where $d_z(U) = \Delta$. Let $z''z'z$ be a path located in the cycle of U. Then, $d_{z'}(U) = 2 = d_{z''}(U)$. Define $U^* := U - \{z''z', z'z\} + \{z'x, z''z\}$. Then, by condition (i) of Lemma 1 and inequality (2.6), we have

$$\begin{aligned}\mathfrak{BID}_\phi(U) - \mathfrak{BID}_\phi(U^*) &= \phi(\Delta, 1) - \phi(\Delta, 2) + \phi(2, 2) - \phi(1, 2)\\ &\ge \phi(3, 1) - \phi(3, 2) + \phi(2, 2) - \phi(1, 2) > 0,\end{aligned}$$

which leads to a contradiction. □

The following lemma's proof is fully analogous to that of Lemma 13, and is therefore omitted.

Lemma 14. *Let ϕ be the function defined in Lemma 2, satisfying condition (i) stated therein. Also, assume that* (2.7) *holds. Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the maximum value of $\mathfrak{BID}_\phi$ among all such graphs, where $3 \le \Delta \le n-2$. If U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle such that at least one of these paths has length 1, then the cycle of U is a triangle.*

Theorem 3. *Let ϕ be the function defined in Lemma 1, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 3 and 5 hold. Furthermore, assume that* (2.6) *holds. Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the minimum value of $\mathfrak{BID}_\phi$ among all such graphs, where $3 \le \Delta \le n - 2$. Then, the following statements hold.*

(a) *The graph U is constructed by attaching $\Delta - 2$ pendent paths having the length larger than 1 to a single vertex of a cycle, where $2 < \Delta < \lfloor (n+1)/2 \rfloor + 1$. As a result,*

$$\mathfrak{BID}_\phi(U) = (n - 2\Delta + 2)\,\phi(2, 2) + \Delta\,\phi(\Delta, 2) + (\Delta - 2)\,\phi(1, 2).$$

(b) *For $\lceil (n+1)/2 \rceil - 1 < \Delta < n - 1$, the graph U is uniquely determined by attaching $2\Delta - n - 1$ pendent vertices and $n - \Delta - 1$ pendent paths having the length 2 to a single vertex of the triangle C_3. Consequently,*

$$\mathfrak{BID}_\phi(U) = (n - \Delta + 1)\,\phi(\Delta, 2) + (n - \Delta - 1)\,\phi(2, 1) - (n - 2\Delta + 1)\,\phi(\Delta, 1) + \phi(2, 2).$$

Proof. By Theorem 1, U is constructed by attaching $\Delta - 2$ pendent paths to a single vertex on a cycle. Let p_1, p_2, and p_3 represent the counts of pendent paths (in U) of lengths 1, 2, and at least 3, respectively.

(a) We assume that $2 < \Delta < \lfloor (n+1)/2 \rfloor + 1$. Then, we obtain

$$2\Delta \le n + 1. \tag{2.8}$$

Assume, for contradiction, that $p_1 \geq 1$. Then, by Lemmas 11 and 13, the cycle of U is the triangle and $p_3 = 0$. Then, it holds that $p_2 < p_1 + p_2 = \Delta - 2$. Consequently, we have

$$n = p_1 + 2p_2 + |V(C)| = \Delta + p_2 + 1 < 2\Delta - 1,$$

which leads to a contradiction with (2.8). Therefore, $p_1 = 0$. A straightforward computation then yields the required expression for $\mathfrak{B}\mathfrak{I}\mathfrak{D}_\phi(U)$.

(b) Now consider the case $\lceil (n+1)/2 \rceil - 1 < \Delta < n - 1$. This implies the inequality

$$n \leq 2\Delta - 1. \tag{2.9}$$

Suppose, for contradiction, that $p_3 \geq 1$. Then, by Lemma 11, we have $p_1 = 0$, and so, $p_2 + p_3 = \Delta - 2$. Consequently,

$$2\Delta \leq 2\Delta + p_3 - 1 = 2p_2 + 3p_3 + 3 \leq 2p_2 + 3p_3 + |V(C)| \leq n,$$

which contradicts inequality (2.9). Therefore, $p_3 = 0$.

If $p_1 \neq 0$, then by Lemma 13, the cycle of U is the triangle. If $p_1 = 0$, then $n = |V(C)| + 2p_2 = |V(C)| + 2(\Delta - 2)$, which implies $|V(C)| = 3$ because of (2.9). Hence, in either of the two cases, we have $|V(C)| = 3$. The equations $p_1 + p_2 = \Delta - 2$ and $p_1 + 2p_2 = n - 3$ yield

$$p_1 = 2\Delta - n - 1 \quad \text{and} \quad p_2 = n - \Delta - 1.$$

These expressions make it possible to compute $\mathfrak{B}\mathfrak{I}\mathfrak{D}_\phi(U)$ directly. □

Remark 3. *Theorem 3 covers the indices $\mathcal{RSC}$, $\mathcal{SO}$, $\mathcal{RSO}$, $\mathcal{BSO}$, $\mathcal{CSO}$, $\mathcal{EU}$, and $\mathcal{REU}$, as their associated functions meet the required assumptions; where $\mathcal{RSC}$ is defined in Remark 1, and $\mathfrak{B}\mathfrak{I}\mathfrak{D}_\phi$ corresponds to the broadened Sombor index $\mathcal{BSO}$ or the cubic Sombor index $\mathcal{CSO}$ when $\phi(\xi_1, \xi_2) = \sqrt{\xi_1^2 + \xi_2^2 + \xi_1 + \xi_2}$ or $\phi(\xi_1, \xi_2) = \sqrt{\xi_1^3 + \xi_2^3}$, respectively, whereas all the remaining indices are defined in the introduction section.*

The next theorem's proof is fully analogous to that of Theorem 3, and is therefore omitted.

Theorem 4. *Let ϕ be the function defined in Lemma 2, satisfying conditions (i) and (ii) stated therein. Also, assume that the inequalities, involving ϕ, listed in Lemmas 4 and 6 hold. Furthermore, assume that* (2.7) *holds. Let U be a unicyclic graph with the order n and maximum degree Δ such that it yields the maximum value of $\mathfrak{B}\mathfrak{I}\mathfrak{D}_\phi$ among all such graphs, where $3 \leq \Delta \leq n - 2$. Then, the statements (a) and (b) of Theorem 3 hold.*

Remark 4. *Theorem 4 covers the indices $\mathcal{SC}$, $\mathcal{H}$, and ${}^m\mathcal{SO}$, as their associated functions meet the required assumptions, where ${}^m\mathcal{SO}$ is defined in Remark 2 and the definitions of the other two indices are given in the introduction section.*

3. Conclusions

In this paper, the problem of identifying the graphs that minimize or maximize $\mathfrak{B}\mathfrak{I}\mathfrak{D}_\phi$ among all unicyclic graphs of a given order and prescribed maximum degree, under specific conditions on the function ϕ, has been addressed. These conditions on ϕ are met by several classical and contemporary degree-based indices. Notably, one of the results obtained is applicable to the harmonic and sum-connectivity indices (see Remark 4), while another one covers the recently introduced Sombor and Euler–Sombor indices, along with their reduced versions (see Remark 3).

Among many open problems related to the present study, the one regarding the augmented Zagreb index seems to deserve more attention, where $\mathfrak{BID}_\phi$ corresponds to the augmented Zagreb index (see [1]) when $\phi(\xi_1, \xi_2) = (\xi_1\xi_2)^3(\xi_1 + \xi_2 - 2)^{-3}$.

Funding statement

This work was supported and funded by the Deanship of Scientific Research at Imam Mohammad Ibn Saud Islamic University (IMSIU) (grant number IMSIU-DDRSP2503).

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 have no conflict of interest to declare.

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