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On Unicyclic Graphs with a Given Number of Pendent Vertices or Matching Number and Their Graphical Edge-Weight-Function Indices

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Abstract: Consider a unicyclic graph G with edge set $E(G)$. Let $\mathfrak{f}$ be a real-valued symmetric function defined on the Cartesian square of the set of all distinct elements of G's degree sequence. A graphical edge-weight-function index of G is defined as $\mathcal{I}_{\mathfrak{f}}(G) = \sum_{xy \in E(G)} \mathfrak{f}(d_G(x), d_G(y))$, where $d_G(x)$ denotes the degree a vertex x in G. This paper determines optimal bounds for $\mathcal{I}_{\mathfrak{f}}(G)$ in terms of the order of G and a parameter $\mathfrak{z}$, where $\mathfrak{z}$ is either the number of pendent vertices of G or the matching number of G. The paper also fully characterizes all unicyclic graphs that achieve these bounds. The function $\mathfrak{f}$ must satisfy specific requirements, which are met by several popular indices, including the Sombor index (and its reduced version), arithmetic–geometric index, sigma index, and symmetric division degree index. Consequently, the general results obtained provide bounds for several well-known indices.

Keywords: topological index; bond incident degree index; graphical edge-weight-function index; degree-based index; unicyclic graph; matching number, pendent vertex; bound

MSC: 05C07; 05C09

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1. Introduction

For definitions of the graph-theoretical terms used in this paper but not defined here, we refer the reader to the books [1–3]. For chemical-graph-theoretical terms, the books [4–6] can be consulted.

We only consider nontrivial and connected graphs in this study. A graph of order n is referred to as an n-order graph. The edge set of a graph G is represented by the notation $E(G)$, and its vertex set is represented by the notation $V(G)$. The notation $d_G(x)$ is chosen to represent the degree of $x \in V(G)$. Particularly, if $d_G(x) = 1$, then x is called a pendent vertex. A nonempty subset M of $E(G)$ is said to be a matching in G if the elements of M are pairwise nonadjacent. A matching is called a β-matching when it has precisely β edges. A maximum matching of G is a matching that consists of the maximum possible edges. If M^* is a maximum matching of G, then $|M^*|$ (the number of its elements) is known as its matching number.

A property of a graph that does not change with respect to graph isomorphism is called a graph invariant [3]. The graph invariants that take only numerical quantities are also known as topological indices or molecular descriptors in the field of chemical graph theory [4–6]. Numerous studies, like [4,7–10], have discussed how useful these topological indices are in predicting distinct properties of chemical compounds. Graphical edge-weight-function indices are particular topological indices that are expressed in the way described below [11]:

$$\mathcal{I}_{\mathfrak{f}}(G) = \sum_{st \in E(G)} \mathfrak{f}(d_G(s), d_G(t)), \tag{1}$$

where $\mathfrak{f}$ is a real-valued symmetric function defined on the Cartesian square of the set consisting of all different members of the degree sequence of a graph G. As seen in studies like [12–14], these indices have also been studied under the terminology "bond incident degree indices". The graphical edge-weight-function indices' class is a subclass of a larger class of certain indices known as degree-based topological indices [15].

By a unicyclic graph, we mean a connected graph with the same size and order; let G be such a graph. The goal of this work is to find the best possible bounds on $\mathcal{I}_{\mathfrak{f}}(G)$ in terms of the order of G and a parameter $\mathfrak{z}$, under certain restrictions on the function $\mathfrak{f}$, where $\mathfrak{z}$ is either the number of pendent vertices or the matching number. All graphs achieving the obtained bounds are also characterized. The restrictions taken into account for $\mathfrak{f}$ are satisfied by a number of popular existing indices, including the Sombor index (together with its reduced version) [16–18], arithmetic–geometric index (for example, see [19]), sigma index [20,21], and symmetric division deg index [22,23]. Consequently, the obtained general results yield bounds on several well-known existing indices. In other words, the obtained results generalize many existing results and provide particular new cases for many existing indices. As there are a lot of particular graphical edge-weight-function indices and, in many cases, the extremal results with respect to them, including their proofs, are considerably similar to one another; it is natural to adopt a unified technique to obtain those results and hence generalize them. The present paper is a contribution to this research direction.

2. Preliminaries

In this section, the basic concepts and notations that will be used in the next sections are given.

The n-order cycle graph is represented by C_n. Given a subset $S \subset V(G)$, the graph obtained by deleting all the elements of S and their corresponding incident edges from G is represented by $G - S$. In the case when S consists of a single vertex, say $S = \{x\}$, the notation can be simplified to $G - x$ for ease of reference. An edge xy in G is said to be pendent if either $d_G(x) = 1$ or $d_G(y) = 1$. Define $N_G(x) := \{v \in V(G) : vx \in E(G)\}$; particularly, the vertices of $N_G(x)$ are referred to as neighbors of x.

Table 1 gives some special cases of Equation (1) considered in this study. The topological indices given in this table will be used in the subsequent sections.

Let S_n^+ be the unicyclic graph formed by inserting exactly one edge in the n-order star graph, where $n \geq 4$. Denote by $U_{n,\beta}$ the graph formed by subdividing $\beta - 2$ pendent edge(s) of $S^+_{n-\beta+2}$, where $n \geq 2\beta \geq 4$. The graph $U_{n,\beta}$ is depicted in Figure 1. We note that the matching number of $U_{n,\beta}$ is β.

For a graph G, a vertex $x \in V(G)$ incident with an element of a matching M in G is termed M-saturated; moreover, if all the vertices of G are M-saturated, then M is called a perfect matching. A vertex of G that is not M-saturated is known as an M-unsaturated vertex. One can observe from Figure 1 that for any $\beta \geq 2$, there exists a perfect matching in $U_{2\beta,\beta}$.

Table 1. Some special cases of Equation (1) considered in this study.

Function $\mathfrak{f}(q_1, q_2)$	$\mathcal{I}_{\mathfrak{f}}$ in Equation (1) Corresponds to
$\sqrt{q_1^2 + q_2^2}$	Sombor (SO) index [16–18]
$\sqrt{q_1^2 + q_2^2 + q_1 q_2}$	Euler–Sombor (ES) index [24]
$\sqrt{(q_1 - 1)^2 + (q_2 - 1)^2}$	reduced Sombor (RSO) index [16]
$(2\sqrt{q_1 q_2})^{-1}(q_1 + q_2)$	arithmetic-geometric (AG) index [19]
$\sqrt{(2q_1 q_2)^{-1}(q_1^2 + q_2^2)}$	modified symmetric division deg (MSDD) index [25]
$(q_1 q_2)^{-1}(q_1^2 + q_2^2)$	symmetric division deg (SDD) index [22,23]
$(\sqrt{q_1} - \sqrt{q_2})^2$	modified misbalance rodeg (MMR) index [26]
$(q_1 - q_2)^2$	sigma index [20,21]
$2(q_1 + q_2)^{-1}$	harmonic index [27,28]
$(a_1 a_2)^{-1/2}$	Randić index [29–31]
$(a_1 + a_2)^{-1/2}$	sum-connectivity (SC) index [27,32]

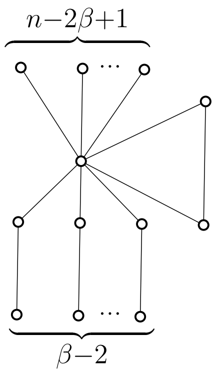

Figure 1. The unicyclic graph $U_{n,\beta}$.

Denote by $U'_{n,p}$ the unicyclic graph shown in Figure 2, where $0 \le p \le n-3$.

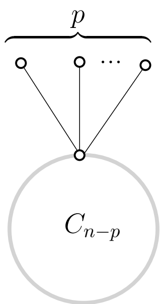

Figure 2. The unicyclic graph $U'_{n,p}$.

Finally, we define $\mathbb{R}^2_{\ge 1} := \{(q_1, q_2) \in \mathbb{R}^2 : q_1 \ge 1 \text{ and } q_2 \ge 1\}$, where $\mathbb{R}$ is the set of real numbers.

3. Results About Matching Number

We give the following known result before demonstrating the very first main result of the current section:

Lemma 1 (see Lemma 3.1 in [33]). *If G is a unicyclic n-order graph with a matching number β, such that $G \ncong C_n$ and $n > 2\beta \geq 4$, then G has a β-matching M and a pendent vertex x that is not M-saturated.*

Theorem 1. *Let $\mathfrak{f} : \mathbb{R}^2_{\geq 1} \to \mathbb{R}$ be a symmetric function, such that*

(i) $\mathfrak{f}(q_1, 2) - \mathfrak{f}(q_1, 3) + \mathfrak{f}(q_2, 2) - \mathfrak{f}(q_2, 3) + \mathfrak{f}(2, 2) - \mathfrak{f}(1, 3) < 0$ *for* $q_1, q_2 \in \{2, 3\}$,

(ii) $q_1[\mathfrak{f}(1, 3) + \mathfrak{f}(3, 3)] < q_1 \mathfrak{f}(q_1 + 1, 2) + (q_1 - 2)\mathfrak{f}(1, 2) + \mathfrak{f}(q_1 + 1, 1) + \mathfrak{f}(2, 2)$ *for* $q_1 \geq 3$,

(iii) the function g defined as $g(q_1, q_2) = \mathfrak{f}(q_1, q_2) - \mathfrak{f}(q_1, q_2 - 1)$, is strictly decreasing in q_1 for $q_2 \geq 2$ and $q_1 \geq 1$,

(iv) the function $\hbar$ defined as

$$\hbar(q_1) = \mathfrak{f}(q_1, 2) + \mathfrak{f}(q_1, 1) - \mathfrak{f}(q_1 - 1, 1) + (q_1 - 2)[\mathfrak{f}(q_1, 2) - \mathfrak{f}(q_1 - 1, 2)]$$

is strictly increasing for $q_1 \geq 2$,

then the inequality

$$\mathcal{I}_{\mathfrak{f}}(G) \leq \beta\, \mathfrak{f}(\beta + 1, 2) + (\beta - 2)\mathfrak{f}(1, 2) + \mathfrak{f}(\beta + 1, 1) + \mathfrak{f}(2, 2) \tag{2}$$

is valid for every 2β-order unicyclic graph G with a matching number $\beta(\geq 2)$. Inequality (2) becomes equation iff $G \cong U_{2\beta,\beta}$ (see Figure 1).

Proof. We assume that the right-hand side of (2) is $\varphi(\beta)$, and we use induction on β. The result is valid for $\beta = 2$ as $G \in \{U_{4,2}, C_4\}$ and because of condition (i) with $r = 2 = s$, we have

$$\mathcal{I}_{\mathfrak{f}}(C_4) = 4\mathfrak{f}(2, 2) < \mathfrak{f}(2, 2) + \mathfrak{f}(1, 3) + 2\mathfrak{f}(2, 3) = \mathcal{I}_{\mathfrak{f}}(U_{4,2}).$$

Next, suppose that $\beta > 2$ and that the result is valid for all unicyclic graphs with order $2(\beta - 1)$ and matching number $\beta - 1$. Next, let G be a 2β-order unicyclic graph with matching number $\beta(> 2)$.

Case 1. The graph G contains no pendent vertex having a neighbor of degree 2.

As no two pendent edges of G can be adjacent, G has a maximum degree not more than 3; particularly, G is the graph formed by attaching at most one pendent vertex to every vertex of its unique cycle, say C_t, where $\beta \leq t \leq 2\beta$. Let $G^\star$ be the graph maximizing $\mathcal{I}_{\mathfrak{f}}$ among all graphs of the present case. Then

$$\mathcal{I}_{\mathfrak{f}}(G) \leq \mathcal{I}_{\mathfrak{f}}(G^\star) \tag{3}$$

Let M be the maximum matching of $G^\star$ and C be its unique cycle.

If $\beta + 1 \leq t \leq 2\beta$, then there exists $w_1 w_2 \in M$ on C, such that $d_{G^\star}(w_1) = 2 = d_{G^\star}(w_2)$. Let $N_{G^\star}(w_1) = \{w', w_2\}$ and $N_{G^\star}(w_2) = \{w'', w_1\}$. Evidently, $w' \neq w''$ because $\beta > 2$. Form a new graph $G^{\star\star}$ from $G^\star$ by dropping $w_1 w'$ and inserting $w_2 w'$. Certainly, $G^{\star\star}$ has matching number β. As $d_{G^\star}(w'), d_{G^\star}(w'') \in \{2, 3\}$, by condition (i), we have

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G^\star) - \mathcal{I}_{\mathfrak{f}}(G^{\star\star}) = {} & \mathfrak{f}(d_{G^\star}(w''), 2) - \mathfrak{f}(d_{G^\star}(w''), 3) + \mathfrak{f}(d_{G^\star}(w'), 2) - \mathfrak{f}(d_{G^\star}(w'), 3) \\ & + \mathfrak{f}(2, 2) - \mathfrak{f}(1, 3) < 0,\end{aligned}$$

a contradiction. Hence, $t = \beta$; that is, each vertex of C has a degree 3 in $G^\star$. Therefore, by condition (ii), we have

$$\mathcal{I}_{\mathfrak{f}}(G^\star) = \beta[\mathfrak{f}(3, 3) + \mathfrak{f}(1, 3)] < \beta\, \mathfrak{f}(2, \beta + 1) + (\beta - 2)\mathfrak{f}(2, 1) + \mathfrak{f}(\beta + 1, 1) + \mathfrak{f}(2, 2). \tag{4}$$

From (3) and (4), the required inequality follows.

Case 2. The graph G has at least one pendent vertex with a neighbor of a degree 2.

Let $x \in V(G)$ be a pendent vertex having the neighbor y with degree two. Certainly, xy belongs to every maximum matching of G. Because the unicyclic graph $G' := G - \{x, y\}$ is of order $2(\beta - 1)$ and possesses matching number $\beta - 1$, we have by inductive hypothesis:

$$\mathcal{I}_{\mathfrak{f}}(G') \le \varphi(\beta - 1) \tag{5}$$

with equality iff $G \cong U_{2(\beta-1),\beta-1}$. Let $N_G(y) = \{x, z\}$. Since z cannot have more than one pendent neighbor and because it can lie on at most one triangle, we have $2 \le d_G(z) \le \beta + 1$. Take $N_G(z) := \{z_0(= y), z_1, \cdots, z_{t-1}\}$, provided that z_{p+1}, z_{p+2}, $\cdots$, z_{t-1} have degree at least 2, where p is either 0 or 1, and the degree of z_1 is 1 when $p = 1$. Because of condition (iii), one has

$$\begin{aligned}
\mathcal{I}_{\mathfrak{f}}(G) = {} & \mathcal{I}_{\mathfrak{f}}(G') + \mathfrak{f}(1,2) + \mathfrak{f}(2,t) + p[\mathfrak{f}(1,t) - \mathfrak{f}(1,t-1)] \\
& + \sum_{i=p+1}^{t-1} [\mathfrak{f}(d_G(z_i), t) - \mathfrak{f}(d_G(z_i), t-1)] \\
\le {} & \mathcal{I}_{\mathfrak{f}}(G') + \mathfrak{f}(1,2) + \mathfrak{f}(2,t) + p[\mathfrak{f}(1,t) - \mathfrak{f}(1,t-1)] \\
& + (t-p-1)[\mathfrak{f}(2,t) - \mathfrak{f}(2,t-1)].
\end{aligned} \tag{6}$$

Since $t \ge 2$, again by condition (iii), we have

$$\mathfrak{f}(1,t) - \mathfrak{f}(1,t-1) - [\mathfrak{f}(2,t) - \mathfrak{f}(2,t-1)] > 0$$

and hence (6) yields

$$\begin{aligned}
\mathcal{I}_{\mathfrak{f}}(G) \le {} & \mathcal{I}_{\mathfrak{f}}(G') + \mathfrak{f}(1,2) + \mathfrak{f}(2,t) + \mathfrak{f}(1,t) - \mathfrak{f}(1,t-1) \\
& + (t-2)[\mathfrak{f}(2,t) - \mathfrak{f}(2,t-1)].
\end{aligned} \tag{7}$$

Since $2 \le t \le \beta + 1$, by condition (iv), one has

$$\begin{aligned}
& \mathfrak{f}(2,t) + \mathfrak{f}(1,t) - \mathfrak{f}(1,t-1) + (t-2)[\mathfrak{f}(2,t) - \mathfrak{f}(2,t-1)] \\
& \le \mathfrak{f}(\beta+1,2) + \mathfrak{f}(\beta+1,1) - \mathfrak{f}(\beta,1) + (\beta-1)[\mathfrak{f}(2,\beta+1) - \mathfrak{f}(2,\beta)].
\end{aligned} \tag{8}$$

From (5), (7) and (8), one has $\mathcal{I}_{\mathfrak{f}}(G) \le \varphi(\beta)$ with equality iff $G \cong U_{2\beta,\beta}$. $\square$

The following theorem's proof is fully analogous to that of Theorem 1 and, therefore, we omit it.

Theorem 2. *Let $\mathfrak{f} : \mathbb{R}^2_{\ge 1} \to \mathbb{R}$ be a symmetric function such that*

(i) $\mathfrak{f}(q_1,2) - \mathfrak{f}(q_1,3) + \mathfrak{f}(q_2,2) - \mathfrak{f}(q_2,3) + \mathfrak{f}(2,2) - \mathfrak{f}(1,3) > 0$ *for* $q_1, q_2 \in \{2,3\}$,
(ii) $q_1[\mathfrak{f}(1,3) + \mathfrak{f}(3,3)] > q_1\,\mathfrak{f}(q_1+1,2) + (q_1-2)\mathfrak{f}(1,2) + \mathfrak{f}(q_1+1,1) + \mathfrak{f}(2,2)$ *for* $q_1 \ge 3$,
(iii) *the function g defined as $g(q_1,q_2) = \mathfrak{f}(q_1,q_2) - \mathfrak{f}(q_1,q_2-1)$, is strictly increasing in q_1 for $q_2 \ge 2$ and $q_1 \ge 1$,*
(iv) *the function $\hbar$ defined as*

$$\hbar(q_1) = \mathfrak{f}(q_1,2) + \mathfrak{f}(q_1,1) - \mathfrak{f}(q_1-1,1) + (q_1-2)[\mathfrak{f}(q_1,2) - \mathfrak{f}(q_1-1,2)]$$

is strictly decreasing for $q_1 \ge 2$,

then the inequality

$$\mathcal{I}_{\mathfrak{f}}(G) \ge \beta\,\mathfrak{f}(\beta+1,2) + (\beta-2)\mathfrak{f}(1,2) + \mathfrak{f}(\beta+1,1) + \mathfrak{f}(2,2) \tag{9}$$

is valid for every 2β-order unicyclic graph G with a matching number $\beta(\ge 2)$. Inequality (9) becomes equation iff $G \cong U_{2\beta,\beta}$ (see Figure 1).

Theorem 1 is about the n-order unicyclic graphs with a matching number β (≥ 2) for $n = 2\beta$. In the next result, we extend this theorem to the case when $n \geq 2\beta$.

Theorem 3. *Let $\mathfrak{f} : \mathbb{R}^2_{\geq 1} \to \mathbb{R}$ be a symmetric function, such that*

(i) $\mathfrak{f}(s_1, 2) - \mathfrak{f}(s_1, 3) + \mathfrak{f}(s_2, 2) - \mathfrak{f}(s_2, 3) + \mathfrak{f}(2, 2) - \mathfrak{f}(1, 3) < 0$ *for* $s_1, s_2 \in \{2, 3\}$,

(ii) $s_1[\mathfrak{f}(3, 3) + \mathfrak{f}(1, 3)] < s_1 \mathfrak{f}(s_1 + 1, 2) + (s_1 - 2)\mathfrak{f}(1, 2) + \mathfrak{f}(s_1 + 1, 1) + \mathfrak{f}(2, 2)$ *for* $s_1 \geq 3$,

(iii) *the function g defined as $g(s_1, s_2) = \mathfrak{f}(s_1, s_2) - \mathfrak{f}(s_1, s_2 - 1)$, is strictly decreasing in s_1 for $s_2 \geq 2$ and $s_1 \geq 1$,*

(iv) *the function $\hbar$ defined as*

$$\hbar(s_1) = \mathfrak{f}(s_1, 2) + \mathfrak{f}(s_1, 1) - \mathfrak{f}(s_1 - 1, 1) + (s_1 - 2)[\mathfrak{f}(s_1, 2) - \mathfrak{f}(s_1 - 1, 2)]$$

is strictly increasing for $s_1 \geq 2$,

(v) *the inequality $2\mathfrak{f}(s_1 + 2, 1) + s_1 \mathfrak{f}(s_1 + 2, 2) + (s_1 - 2)\mathfrak{f}(1, 2) - 2s_1 \mathfrak{f}(2, 2) > 0$ holds for $s_1 \geq 2$, and*

(vi) *the function Φ defined as*

$$\Phi(s_1, s_2) = \mathfrak{f}(s_1 - 1, 1) + s_2[\mathfrak{f}(s_1, 1) - \mathfrak{f}(s_1 - 1, 1)] + (s_1 - s_2)[\mathfrak{f}(s_1, 2) - \mathfrak{f}(s_1 - 1, 2)]$$

is strictly increasing in s_1 for $s_1 \geq s_2 + 1 \geq 2$,

then the inequality

$$\mathcal{I}_{\mathfrak{f}}(G) \leq (n - 2\beta + 1) \cdot \mathfrak{f}(n - \beta + 1, 1) + \beta \mathfrak{f}(n - \beta + 1, 2) + (\beta - 2)\mathfrak{f}(1, 2) + \mathfrak{f}(2, 2) \tag{10}$$

holds for every n-order unicyclic graph G having a matching number $\beta(\geq 2)$. Inequality (10) becomes equation iff $G \cong U_{n,\beta}$ (see Figure 1).

Proof. We set

$$\Psi(n, \beta) := (n - 2\beta + 1) \cdot \mathfrak{f}(n - \beta + 1, 1) + \beta \mathfrak{f}(n - \beta + 1, 2) + (\beta - 2)\mathfrak{f}(1, 2) + \mathfrak{f}(2, 2).$$

We use induction on n. For $n = 2\beta$, the required conclusion holds due to Theorem 1. This starts the induction. Now, suppose that $n > 2\beta$ and let G be an n-order unicyclic graph with a matching number β. If $G \cong C_n$, then $n = 2\beta + 1$ and, hence, we have $\mathcal{I}_{\mathfrak{f}}(G) = (2\beta + 1)\mathfrak{f}(2, 2) < \Psi(2\beta + 1, \beta)$ because of condition (v). In what follows, suppose that $G \ncong C_n$. Then, due to Lemma 1, G possesses a pendent vertex x and a β-matching M, such that x is not M-saturated. Hence, $G - x$ also has a matching number β. Consequently, we apply the induction hypothesis on $G - x$:

$$\mathcal{I}_{\mathfrak{f}}(G - x) \leq \Psi(n - 1, \beta) \tag{11}$$

with equality iff $G - x \cong U_{n-1,\beta}$. Let $N_G(x) = \{y\}$. We note that M has an edge incident with y because $xy \notin M$ (a maximum matching). This implies that the count of those edges incident with y that are not the members of M is $d_G(y) - 1$, which further implies that $d_G(y) - 1 \leq |E(G)| - |M|$; that is, $d_G(y) \leq n - \beta + 1$. Suppose that p is the count of the pendent neighbors of y. Then, $1 \leq p \leq d_G(y) - 1$. Because at least $p - 1$ pendent neighbors of y are M-unsaturated and the count of M-unsaturated vertices of G is $n - 2\beta$, it holds that $p - 1 \leq n - 2\beta$, which means that y has at most $n - 2\beta + 1$ pendant neighbors. Set

$N_G(y) := \{y_1(=x), y_2, \cdots, y_p, y_{p+1}, \cdots, y_s\}$, where $y_1, \cdots, y_p$ are pendent vertices and $y_{p+1}, \cdots, y_s$ are non-pendent vertices. By condition (iii), we have

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) &= \mathcal{I}_{\mathfrak{f}}(G-x) + \mathfrak{f}(s,1) + (p-1)[\mathfrak{f}(s,1) - \mathfrak{f}(s-1,1)] \\ &\quad + \sum_{i=p+1}^{s} \Big(\mathfrak{f}(s, d_G(y_i)) - \mathfrak{f}(s-1, d_G(y_i))\Big) \\ &\le \mathcal{I}_{\mathfrak{f}}(G-x) + \mathfrak{f}(s-1,1) + p[\mathfrak{f}(s,1) - \mathfrak{f}(s-1,1)] \\ &\quad + (s-p)\Big(\mathfrak{f}(s,2) - \mathfrak{f}(s-1,2)\Big). \end{aligned} \tag{12}$$

As $2 \le p+1 \le s \le n-\beta+1$, because of condition (vi), the inequality (12) yields

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) &\le \mathcal{I}_{\mathfrak{f}}(G-x) + \mathfrak{f}(n-\beta,1) + p\Big(\mathfrak{f}(n-\beta+1,1) - \mathfrak{f}(n-\beta,1)\Big) \\ &\quad + (n-\beta-p+1)\Big(\mathfrak{f}(n-\beta+1,2) - \mathfrak{f}(n-\beta,2)\Big). \end{aligned} \tag{13}$$

Since $p \le n-2\beta+1$ and $n-\beta \ge 2$, because of condition (iii), the inequality (13) yields

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) &\le \mathcal{I}_{\mathfrak{f}}(G-x) + \mathfrak{f}(n-\beta,1) + (n-2\beta+1)\Big(\mathfrak{f}(n-\beta+1,1) - \mathfrak{f}(n-\beta,1)\Big) \\ &\quad + \beta\Big(\mathfrak{f}(n-\beta+1,2) - \mathfrak{f}(n-\beta,2)\Big). \end{aligned} \tag{14}$$

By (11) and (14), we now have $\mathcal{I}_{\mathfrak{f}}(G) \le \Psi(n,\beta)$ with equality iff all equalities in (11), (12), (13) and (14) hold; that is, iff $G-x \cong U_{n-1,\beta}$, $d_G(y_{p+1}) = \cdots = d_G(y_s) = 2$, $s = n-\beta+1$ and $p = n-2\beta+1$. Consequently, we have $\mathcal{I}_{\mathfrak{f}}(G) = \Psi(n,\beta)$ iff $G \cong U_{n,\beta}$. □

As the following theorem's proof (which utilizes Theorem 2) is completely similar to that of Theorem 3, we omit it.

Theorem 4. *Let $\mathfrak{f} : \mathbb{R}^2_{\ge 1} \to \mathbb{R}$ be a symmetric function such that*

(i) $\mathfrak{f}(s_1,2) - \mathfrak{f}(s_1,3) + \mathfrak{f}(s_2,2) - \mathfrak{f}(s_2,3) + \mathfrak{f}(2,2) - \mathfrak{f}(1,3) > 0$ *for* $s_1, s_2 \in \{2,3\}$,

(ii) $s_1[\mathfrak{f}(3,3) + \mathfrak{f}(1,3)] > s_1\,\mathfrak{f}(s_1+1,2) + (s_1-2)\mathfrak{f}(1,2) + \mathfrak{f}(s_1+1,1) + \mathfrak{f}(2,2)$ *for* $s_1 \ge 3$,

(iii) the function g defined as $g(s_1,s_2) = \mathfrak{f}(s_1,s_2) - \mathfrak{f}(s_1,s_2-1)$, is strictly increasing in s_1 for $s_2 \ge 2$ and $s_1 \ge 1$,

(iv) the function $\hbar$ defined as

$$\hbar(s_1) = \mathfrak{f}(s_1,2) + \mathfrak{f}(s_1,1) - \mathfrak{f}(s_1-1,1) + (s_1-2)[\mathfrak{f}(s_1,2) - \mathfrak{f}(s_1-1,2)]$$

is strictly decreasing for $s_1 \ge 2$,

(v) the inequality $2\mathfrak{f}(s_1+2,1) + s_1\,\mathfrak{f}(s_1+2,2) + (s_1-2)\mathfrak{f}(1,2) - 2s_1\,\mathfrak{f}(2,2) < 0$ *holds for* $s_1 \ge 2$, *and*

(vi) the function Φ defined as

$$\Phi(s_1,s_2) = \mathfrak{f}(s_1-1,1) + s_2[\mathfrak{f}(s_1,1) - \mathfrak{f}(s_1-1,1)] + (s_1-s_2)[\mathfrak{f}(s_1,2) - \mathfrak{f}(s_1-1,2)]$$

is strictly decreasing in s_1 for $s_1 \ge s_2+1 \ge 2$,

then the inequality

$$\mathcal{I}_{\mathfrak{f}}(G) \ge (n-2\beta+1)\cdot\mathfrak{f}(n-\beta+1,1) + \beta\,\mathfrak{f}(n-\beta+1,2) + (\beta-2)\mathfrak{f}(1,2) + \mathfrak{f}(2,2) \tag{15}$$

holds for every n-order unicyclic graph G having a matching number $\beta(\ge 2)$. Inequality (15) becomes equation iff $G \cong U_{n,\beta}$ (see Figure 1).

Remark 1. *As all the conditions of Theorem 3 are satisfied by the functions associated with each of the following topological indices, the conclusion of this theorem holds for all these indices: SO index, RSO index, ES index, MMR index, sigma index, SDD index, and AG index (the definitions of these indices are given in Table 1).*

4. Results About Pendent Vertices

In the present section, we derive two optimal bounds on $\mathcal{I}_{\mathfrak{f}}(G)$ in terms of G's order and its number of pendent vertices, where is G is a unicyclic graph.

Theorem 5. *Let* $\mathfrak{f} : \mathbb{R}^2_{\geq 1} \to \mathbb{R}$ *be a symmetric function. Let* $s_1 \geq 2$ *and* $s_2 \geq 2$*. If*

(i) *the function* g *defined by* $g(s_1, s_2) = \mathfrak{f}(s_1, s_2) - \mathfrak{f}(s_1 - 1, s_2)$*, is strictly decreasing in* s_2*,*

(ii) *the function* j_a *defined by*

$$j_a(s_1) = \mathfrak{f}(1, s_1) + (s_1 - a - 1)[\mathfrak{f}(1, s_1) - \mathfrak{f}(1, s_1 - 1)] + a[\mathfrak{f}(2, s_1) - \mathfrak{f}(2, s_1 - 1)],$$

is strictly increasing for $s_1 \geq 3$*, where* $a \in \{1, 2\}$*, and*

(iii) *the strict inequality* $(2s_3 - 1)\mathfrak{f}(s_3 + 1, 1) - (s_3 - 1)\mathfrak{f}(s_3, 1) + 3\mathfrak{f}(s_3 + 1, 2) - \mathfrak{f}(s_3, 2) - 2\mathfrak{f}(s_3 + 2, 2) - s_3\, \mathfrak{f}(s_3 + 2, 1) < 0$ *holds for every positive integer* s_3*,*

then

$$\mathcal{I}_{\mathfrak{f}}(G) \leq p\, \mathfrak{f}(p + 2, 1) + (n - p - 2)\mathfrak{f}(2, 2) + 2\mathfrak{f}(p + 2, 2) \tag{16}$$

for every n*-order unicyclic graph* G *possessing* p *pendent vertices, such that* $0 \leq p \leq n - 3$*. The equality in* (16) *holds iff* $G \cong U'_{n,p}$ *(see Figure 2).*

Proof. We use induction on n. For $n \in \{3, 4\}$, we have the required conclusion, because for any case, the graph must be $U'_{n,p}$. Assume that $n \geq 5$ and suppose that the theorem is valid for every $(n - 1)$-order unicyclic graph having p' pendent vertices provided that $0 \leq p' \leq (n - 1) - 3$.

Let G be an n-order unicyclic graph possessing p pendent vertices, provided that the inequality $0 \leq p \leq n - 3$ holds. If $p = 0$, then $G \cong U'_{n,p}$ and thus we are done. In the following, we assume $1 \leq p \leq n - 3$. Let C be the unique cycle of G and let $c_1, c_2, \ldots, c_k$ be all vertices of C. For $i \in \{1, 2, \ldots, k\}$, let $\mathcal{P}(c_i)$ be the class of all those paths of G whose one end vertex is c_i and the other end vertex is a pendent vertex of G, such that none of these paths contain any vertex from the set $\{c_1, c_2, \ldots, c_k\} \setminus \{c_i\}$. It is possible that $\mathcal{P}(c_j)$ is empty for some j. We suppose, without loss of generality, that $\mathcal{P}(c_1)$ is non-empty. Let w be the pendent end vertex of a longest path in $\mathcal{P}(c_1)$. Let $v \in V(G)$ be the unique neighbor of w, and take $N_G(v) := \{w, v_1, v_2, \cdots, v_{d-1}\}$, such that $d_G(v_1) \geq d_G(v_2) \geq \cdots \geq d_G(v_{d-1})$.

Case 1. The vertices v and c_1 are the same.

In this case, $d \geq 3$. We observe that v_1 and v_2 are the only non-pendent vertices in $N_G(v)$. Because of condition (i), we have

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) - \mathcal{I}_{\mathfrak{f}}(G - w) &= \mathfrak{f}(1, d) + \sum_{i=1}^{d-1} [\mathfrak{f}(d_G(v_i), d) - \mathfrak{f}(d_G(v_i), d - 1)] \\ &\leq \mathfrak{f}(1, d) + (d - 3)[\mathfrak{f}(1, d) - \mathfrak{f}(1, d - 1)] + 2[\mathfrak{f}(2, d) - \mathfrak{f}(2, d - 1)] \end{aligned} \tag{17}$$

where the equality in (17) holds iff $d_G(v_1) = d_G(v_2) = 2$. As $d \leq p + 2$, because of condition (ii) with $a = 2$, the inequality (17) yields

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) - \mathcal{I}_{\mathfrak{f}}(G - w) \leq{}& \mathfrak{f}(1, p + 2) + (p - 1)[\mathfrak{f}(1, p + 2) - \mathfrak{f}(1, p + 1)] \\ &+ 2[\mathfrak{f}(2, p + 2) - \mathfrak{f}(2, p + 1)] \end{aligned} \tag{18}$$

where the equality in (18) holds iff $d_G(v_1) = d_G(v_2) = 2$ and $d = p + 2$. In the present case, the graph $G - w$ has exactly $p - 1$ pendent vertices. As $1 \leq p \leq n - 3$, we have

$0 \leq p-1 \leq (n-1)-3$ and thus we are allowed to apply the induction hypothesis on $G-w$, and, therefore,

$$\mathcal{I}_{\mathfrak{f}}(G-w) \leq (p-1)\,\mathfrak{f}(p+1,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+1,2), \tag{19}$$

where the equality in (19) holds iff $G-w \cong U'_{n-1,p-1}$. Now, (16) follows from (18) and (19).

Case 2. The vertices v and c_1 are not the same.

In the current case, we observe that $d_G(v_1) \geq 2$ and $d_G(v_i) = 1$ when $2 \leq i \leq d-1$. Also, $2 \leq d \leq p+1$.

Subcase 2.1. $d = 2$.

In the present subcase, the inequality $p \leq n-4$ holds. We also note that, in the current subcase, the graph $G-w$ has p pendent vertices. As $1 \leq p \leq (n-1)-3$, the induction hypothesis is applicable on $G-w$:

$$\mathcal{I}_{\mathfrak{f}}(G-w) \leq p\,\mathfrak{f}(p+2,1) + (n-p-3)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+2,2), \tag{20}$$

where the equality in (20) holds iff $G-w \cong U'_{n-1,p}$. On the other hand, by condition (i), we have

$$\mathcal{I}_{\mathfrak{f}}(G) - \mathcal{I}_{\mathfrak{f}}(G-w) = \mathfrak{f}(1,2) + \mathfrak{f}(2,d_G(v_1)) - \mathfrak{f}(1,d_G(v_1)) \leq \mathfrak{f}(2,2) \tag{21}$$

with the right equality iff $d_G(v_1) = 2$. By (20) and (21), we obtain

$$\mathcal{I}_{\mathfrak{f}}(G) \leq p\,\mathfrak{f}(p+2,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+2,2),$$

with equality iff $G-w \cong U'_{n-1,p}$ and $d_G(v_1) = 2$; particularly, these two constraints do not hold simultaneously, and hence in the current subcase, we have

$$\mathcal{I}_{\mathfrak{f}}(G) < p\,\mathfrak{f}(p+2,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+2,2).$$

Subcase 2.2. $d > 2$.

By condition (i), we have

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) - \mathcal{I}_{\mathfrak{f}}(G-w) &= \mathfrak{f}(1,d) + \sum_{i=1}^{d-1}[\mathfrak{f}(d_G(v_i),d) - \mathfrak{f}(d_G(v_i),d-1)] \\ &\leq \mathfrak{f}(1,d) + (d-2)[\mathfrak{f}(1,d) - \mathfrak{f}(1,d-1)] + [\mathfrak{f}(2,d) - \mathfrak{f}(2,d-1)]\end{aligned} \tag{22}$$

where the equality in (22) holds iff $d_G(v_1) = 2$. As $d \leq p+1$, by condition (ii) with $a = 1$, the inequality (22) yields

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) - \mathcal{I}_{\mathfrak{f}}(G-w) \leq \mathfrak{f}(1,p+1) + (p-1)\,[\mathfrak{f}(1,p+1) - \mathfrak{f}(1,p)] \\ + [\mathfrak{f}(2,p+1) - \mathfrak{f}(2,p)].\end{aligned} \tag{23}$$

In the present case, $G-w$ has exactly $p-1$ pendent vertices. As $0 \leq p-1 \leq (n-1)-3$, the induction hypothesis is applicable here, and, therefore,

$$\mathcal{I}_{\mathfrak{f}}(G-w) \leq (p-1)\,\mathfrak{f}(p+1,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+1,2), \tag{24}$$

with equality iff $G - w \cong U'_{n-1,p-1}$. Now, because of condition (iii), from (23) and (24) we obtain

$$\begin{aligned}\mathcal{I}_{\mathfrak{f}}(G) \leq\ & (n-p-2)\mathfrak{f}(2,2) + (2p-1)\mathfrak{f}(p+1,1) - (p-1)\mathfrak{f}(p,1) \\ & + 3\mathfrak{f}(p+1,2) - \mathfrak{f}(p,2) \\ & < p\,\mathfrak{f}(p+2,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+2,2),\end{aligned}$$

as required. This completes the induction and, thus, the proof. □

Because the proof of the following result is completely similar to that of Theorem 5, we omit it:

Theorem 6. *Let $\mathfrak{f} : \mathbb{R}^2_{\geq 1} \to \mathbb{R}$ be a symmetric function. Let $s_1 \geq 2$ and $s_2 \geq 2$. If*

(i) the function g defined by $g(s_1, s_2) = \mathfrak{f}(s_1, s_2) - \mathfrak{f}(s_1 - 1, s_2)$, is strictly increasing in s_2,

(ii) the function j_a defined by

$$j_a(s_1) = \mathfrak{f}(1, s_1) + (s_1 - a - 1)[\mathfrak{f}(1, s_1) - \mathfrak{f}(1, s_1 - 1)] + a[\mathfrak{f}(2, s_1) - \mathfrak{f}(2, s_1 - 1)],$$

is strictly decreasing for $s_1 \geq 3$, where $a \in \{1, 2\}$, and

(iii) the strict inequality $(2s_3 - 1)\mathfrak{f}(s_3 + 1, 1) - (s_3 - 1)\mathfrak{f}(s_3, 1) + 3\mathfrak{f}(s_3 + 1, 2) - \mathfrak{f}(s_3, 2) - 2\mathfrak{f}(s_3 + 2, 2) - s_3\,\mathfrak{f}(s_3 + 2, 1) > 0$ holds for every positive integer s_3,

then

$$\mathcal{I}_{\mathfrak{f}}(G) \geq p\,\mathfrak{f}(p+2,1) + (n-p-2)\mathfrak{f}(2,2) + 2\mathfrak{f}(p+2,2) \tag{25}$$

for every n-order unicyclic graph G possessing p pendent vertices, such that $0 \leq p \leq n-3$. The equality in (25) holds iff $G \cong U'_{n,p}$ (see Figure 2).

Remark 2. *As all the conditions of Theorem 5 hold for each of the functions corresponding to the following topological indices, the conclusion of this theorem holds for all these indices: SO index, RSO index, ES index, MMR index, sigma index, SDD index, MSDD index, AG index (the definitions of these indices are given in Table 1).*

Remark 3. *As all the conditions of Theorem 6 are satisfied for each of the functions associated with the following three topological indices, the conclusion of this theorem holds for these three indices: harmonic index, SC index, Randić index (the definitions of these indices are given in Table 1).*

Remark 4. *One of the referees asked to check whether Theorem 5 or Theorem 6 is applicable to the first Zagreb index Z_1 or second Zagreb index Z_2, where Equation (1) gives Z_1 or Z_2 if one takes $\mathfrak{f}(q_1, q_2) = q_1 + q_2$ or $\mathfrak{f}(q_1, q_2) = q_1 q_2$, respectively (see the survey [34], for details on these Zagreb indices). We observe that neither of the aforementioned theorems is applicable to either of these Zagreb indices. By Theorem 2 of [35], the graph attaining the greatest possible value of Z_1 among all fixed-order unicyclic graphs with a given number of pendent vertices is not generally unique; such extremal graphs include $U'_{n,p}$ (see Figure 2) in addition to other graphs. Similarly, by Theorems 1 and 2 of [36], none of the sets of extremal graphs with respect to Z_2 over the aforementioned graph class is equal to $\{U'_{n,p}\}$.*

5. Conclusions

In this paper, we have addressed the question of establishing the best possible bounds on the topological index $\mathcal{I}_{\mathfrak{f}}$ of unicyclic graphs in terms of their order and an additional parameter $\mathfrak{z}$, under certain restrictions on the function $\mathfrak{f}$, where $\mathfrak{z}$ is either the number of pendent vertices or the matching number. All graphs achieving the obtained bounds are also characterized. The restrictions taken into account for $\mathfrak{f}$ are satisfied by a number of popular existing indices, including the Sombor index (together with its reduced version), arithmetic–geometric index, sigma index, and symmetric division deg index (see Table 1 for the definitions of these indices). Consequently, the obtained general results yield bounds on several well-known existing indices. In other words, the obtained results generalize many existing results and provide particular new cases for many existing indices. As there are a lot of particular graphical edge-weight-function indices and, in many cases, the extremal results with respect to them, including their proofs, are considerably similar to one another; it is natural to adopt a unified technique to obtain those results and, hence, generalize them. The present paper is a contribution to this research direction.

There are many existing (particular) graphical edge-weight-function indices for which our results are not applicable; for instance, the first and second Zagreb indices are not covered by our results (see Remark 4). Therefore, it is natural to extend the present study to obtain similar results that cover additional (particular) graphical edge-weight-function indices.

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