Research Article

On the Maximum Sombor Index of Unicyclic Graphs with a Fixed Girth

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Let \( G \) be a graph having the set of edges \( E(G) \). Represent by \( d_G(u) \) the degree of a vertex \( u \) of \( G \). The Sombor (SO) index of \( G \) is defined as

\[
SO(G) = \sum_{uv \in E(G)} \left( d_G(u)^2 + d_G(v)^2 \right).
\]

The length of a shortest cycle in a graph \( G \) is known as the girth of \( G \). A connected graph with the same order and size is usually referred to as a (connected) unicyclic graph. This paper reports the characterization of the graphs possessing the first-two maximum values of the SO index in the class of all (connected) unicyclic graphs with a fixed girth and order.

1. Introduction

In this paper, we are concerned with only connected and finite graphs. Thus, throughout this study, the term “graph” means a connected and finite graph. The graph-theoretical terminology utilized in this work without giving their definitions may be found in the books [1–3].

For a graph \( G \), represent by \( E(G) \) and \( V(G) \) the sets of edges and vertices, respectively. For a vertex \( u \in V(G) \), the set \( N_G(u) \) consists of all those vertices of \( G \) that are adjacent with \( u \). The degree of a vertex \( u \in V(G) \) is represented by \( d_G(u) \), which is equal to the number of elements of the set \( N_G(u) \). If \( d_G(u) = 1 \), then \( u \) is called a pendant vertex, and if \( d_G(u) \geq 3 \), then \( u \) is called a branching vertex. Denote by \( G - w \) the graph deduced from \( G \) by removing the vertex \( w \in V(G) \) as well as its incident edges. The length of a shortest cycle in a graph \( G \) is known as the girth of \( G \). A connected graph with the same order and size is usually referred to as a unicyclic graph. In other words, a connected cyclic graph having cyclomatic number one is known as a unicyclic graph [4].

The Sombor (SO) index for a graph \( G \) is defined [5] as

\[
SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.
\]

The SO index, although proposed recently [5], has received a lot of attention from academics and led to numerous articles; for instance, see the surveys [6, 7] and associated references are given therein. Possible chemical applications of the SO index may be found in the papers [8, 9].

In the present article, we are concerned with the solution to an extremal problem involving the SO index for unicyclic graphs with a fixed girth and order. The SO index of unicyclic graphs has been studied in several papers. The graphs possessing the least and largest values of the SO index among all unicyclic graphs with a fixed order were found independently in [10, 11]. Liu [12] (respectively, Alidadi et al. [13]) reported the graphs attained the highest value (respectively, least value) of the SO index among all unicyclic graphs with a fixed diameter and order. The graphs attaining the minimum (respectively, maximum) SO index over the class of all unicyclic graphs with a fixed maximum degree (respectively, matching number) and order were...
characterized in [14] (respectively, in [15]). In this paper, we give the characterization of the graphs possessing the first-two maximum values of the SO index in the class of all unicyclic graphs with a fixed girth and order.

2. Main Results

We start this section with an elementary lemma.

**Lemma 1.** For \( a > b \geq 1 \) and \( x \geq 1 \), the function \( f \) defined by

\[
f(x) = \sqrt{a^2 + x^2} - \sqrt{b^2 + x^2},
\]

is strictly decreasing.

Next, we provide a lemma that is crucial for proving our first main result.

**Lemma 2.** Let \( G \) be a connected graph of order at least 4. Let \( u \) and \( v \) be adjacent vertices of degrees at least 2 such that they do not have any neighbor in common. Let \( H \) be the graph deduced from \( G \) by dropping all the edges, except \( uv \), incident with \( v \) and inserting the edges \( ux \) for all \( x \in N_G(v) \setminus \{u\} \). Then, \( \text{SO}(G) < \text{SO}(H) \).

**Proof.** If \( N_G(v) = \{u, v_1, v_2, \ldots, v_s\} \), where \( s \geq 1 \), then

\[
\text{SO}(H) - \text{SO}(G) = \sum_{w \in N_G(u) \setminus \{v\}} \left[ \sqrt{(d_G(u) + s)^2 + (d_G(w))^2} - \sqrt{(d_G(u))^2 + (d_G(w))^2} \right] + \sum_{i=1}^{s} \left[ \sqrt{(d_G(u) + s)^2 + (d_G(v_i))^2} - \sqrt{(s + 1)^2 + (d_G(v_i))^2} \right] + \left[ \sqrt{(d_G(u) + s)^2 + 1} - \sqrt{(d_G(u))^2 + (s + 1)^2} \right] > 0,
\]

as desired.

The next result gives the characterization of the graphs possessing the first maximum value of the SO index in the class of all unicyclic graphs with a fixed girth and order.

**Theorem 1.** If \( G \) is a unicyclic graph with order \( n \) and girth \( k \), then

\[
\text{SO}(G) \leq (n - k) \sqrt{(n - k + 2)^2 + 1} + 2 \sqrt{(n - k + 2)^2 + 4 + (k - 2)\sqrt{8}},
\]

with equality if and only if \( G = C_{k,n-k} \), where \( C_{k,n-k} \) is the graph formed by attaching \( n - k \) pendant vertices to exactly one vertex of the cycle graph \( C_k \) of order \( k \).

**Proof.** In [11], it was proved that \( C_{3,n-3} \) is the unique graph having the maximum Sombor index among all unicyclic graphs of order \( n \); thus, our theorem follows from this result when \( k = 3 \). In the rest of the proof, we assume that \( 4 \leq k \leq n \). Also, suppose that \( \text{SO}(G) \) is as large as possible. By Lemma 2, every vertex that lies on the cycle of \( G \) has exactly two nonpendent neighbors. Note that \( n \) can be written in terms of \( k \); that is, \( n = k, k + 1, k + 2, \ldots \). Now, we apply induction on \( n \). The result trivially holds for \( n \in \{k, k + 1\} \), because there is only one graph in either of these two cases. Thence, the induction starts. Let \( w \in V(G) \) be a pendant vertex having the neighbor \( v \). Take \( N_G(v) = \{w, v_1, v_2, \ldots, v_q\} \) with \( d_G(v_i) = q_i \) for each \( i \in \{1, 2, \ldots, q - 1\} \) and \( d_G(v) = q \geq 3 \). Note that \( n - k + 2 \geq q \) and that exactly two members of \( N_G(v) \) are nonpendent. Observe that the graph \( G - w \) has order \( n - 1 \) and girth \( k \).

By Lemma 1, one has

\[
\text{SO}(G) = \text{SO}(G - w) + \sum_{i=1}^{q-1} \left( \sqrt{q_i^2 + q_i^2} - \sqrt{(q - 1)^2 + q_i^2} \right) + \sqrt{q^2 + 1} + \sum_{i=1}^{q-1} 2\left( \sqrt{q_i^2 + 2^2} - \sqrt{(q - 1)^2 + 2^2} \right) + (q - 3)\left( \sqrt{q^2 + 1} - \sqrt{(q - 1)^2 + 1} \right).
\]

(5)
\[ SO(G) \leq SO(G - \omega) + (n - k)\sqrt{(n - k + 2)^2 + 1} + 2\sqrt{(n - k + 2)^2 + 4} \]
\[ - (n - k - 1)\sqrt{(n - k + 1)^2 + 1} - 2\sqrt{(n - k + 1)^2 + 4}, \]

(6)

where the equality sign in (5) holds if and only if each of the two nonpendent neighbors of \( v \) has degree 2. Note that the function \( \psi \) defined by

\[ \psi(x) = (x - 2)\sqrt{x^2 + 1} + 2\sqrt{x^2 + 4} - (x - 3)\sqrt{(x - 1)^2 + 1} - 2\sqrt{(x - 1)^2 + 4}, \]

(7)

is strictly increasing for \( x \geq 3 \) because its derivative

\[ \psi'(x) = \frac{(x - 2)x}{\sqrt{x^2 + 1}} + \frac{2x}{\sqrt{x^2 + 4}} - \frac{(x - 3)(x - 1)}{\sqrt{(x - 1)^2 + 1}} - \frac{2(x - 1)}{\sqrt{(x - 1)^2 + 4}} - \sqrt{(x - 1)^2 + 1}, \]

(8)

is positive for \( x \geq 3 \) as the inequalities

\[ \frac{(x - 2)x}{\sqrt{x^2 + 1}} - \frac{(x - 3)(x - 1)}{\sqrt{(x - 1)^2 + 1}} > 0, \]

\[ \frac{2x}{\sqrt{x^2 + 4}} - \frac{2(x - 1)}{\sqrt{(x - 1)^2 + 4}} > 0, \]

(9)

\[ \sqrt{x^2 + 1} - \sqrt{(x - 1)^2 + 1} > 0, \]

hold for \( x \geq 3 \). Recall that \( n - k + 2 \geq q \geq 3 \). Consequently, it holds that

\[ \psi(q) \leq \psi(n - k + 2), \]

(10)

and hence, from (6), it follows that

\[ SO(G) \leq SO(G - \omega) + (n - k - 2)\sqrt{(n - k + 1)^2 + 1} + 2\sqrt{(n - k + 1)^2 + 4} \]

(11)

with equality if and only if each of the two nonpendent neighbors of \( v \) has degree 2 and \( n - k + 2 = q \). Now, by using the inductive hypothesis in (11), one arrives at

\[ SO(G) \leq (n - k)\sqrt{(n - k + 2)^2 + 1} + 2\sqrt{(n - k + 2)^2 + 2^2 + (k - 2)\sqrt{8}}, \]

(12)

with equality if and only if each of the two nonpendent neighbors of \( v \) has degree 2, \( n - k + 2 = q \), and \( G - \omega = C_{k,n-k-1} \). This completes the induction and thence the proof.

In order to prove our second main result, which gives the characterization of the graphs possessing the second-maximum value of the SO index in the class of all unicyclic graphs with a fixed girth and order, we prove a series of lemmas.

**Lemma 3.** Let \( G \) be a connected graph of order at least 5. Let \( uv \) be an edge of \( G \) such that each of its end vertices (i) has exactly two nonpendent neighbors and (ii) contains at least one pendent neighbor provided that \( d_{C_3}(u) \geq d_{C_3}(v) \geq 3 \). Let \( G' \)
be the graph obtained from $G$ by removing all the pendent neighbors of $v$ and then attaching them to the vertex $u$. It holds that $\text{SO}(G) < \text{SO}(G')$.

Proof. Let $\{v, w\}$ be the set of nonpendent neighbors of $u$ with $d_G(w) = s \geq 2$. Let $\{u, w'\}$ be the set of nonpendent neighbors of $(\text{HTML translation failed})$ with $d_G(w') = t \geq 2$. Also, assume that $d_G(u) = p$ and $d_G(v) = q$. Then, $p \geq q \geq 3$.

\[
\text{SO}(G) - \text{SO}(G') = \left( \sqrt{p^2 + s^2} - \sqrt{(p + q - 2)^2 + s^2} \right) + (p - 2)\left( \sqrt{p^2 + 1} - \sqrt{(p + q - 2)^2 + 1} \right) + (q - 2)\left( \sqrt{q^2 + 1} - \sqrt{(p + q - 2)^2 + 1} \right) + (q - 2)\left( \sqrt{q^2 + t^2} - \sqrt{t^2 + 4} \right)
\]

By Lemma 1, it holds that and hence, (13) yields

\[
\sqrt{q^2 + t^2} - \sqrt{t^2 + 4} \leq \sqrt{q^2 + 4} - \sqrt{8},
\]

\[
\text{SO}(G) - \text{SO}(G') < (q - 2)\left( \sqrt{q^2 + 1} - \sqrt{4(q - 1)^2 + 1} \right) + \sqrt{q^2 + 4} - \sqrt{8}
\]

\[
= \sqrt{q^2 + 1} - \sqrt{4(q - 1)^2 + 1} + \sqrt{q^2 + 4} - \sqrt{8} + (q - 3)\left( \sqrt{q^2 + 1} - \sqrt{4(q - 1)^2 + 1} \right)
\]

\[
\leq \sqrt{q^2 + 1} - \sqrt{4(q - 1)^2 + 1} + \sqrt{q^2 + 4} - \sqrt{8} < 0.
\]

Lemma 4. Let $G$ be a connected graph of order at least 5. Let $uv$ be an edge of $G$ such that each of its end vertices (i) has at least one pendent neighbor and (ii) contains exactly two nonpendent neighbors such that one of them has degree 2 and $d_G(u) \geq d_G(v) \geq 3$. (It is possible that the vertices $u$ and $v$ have a common neighbor.) Let $G'$ be the graph obtained from $G$ by removing a pendent neighbor of $v$ and then attaching it to $u$. It holds that $\text{SO}(G) < \text{SO}(G')$.

Proof. Let $d_G(u) = p$ and $d_G(v) = q$. Then, $p \geq q \geq 3$. Here, one has

\[
\text{SO}(G) - \text{SO}(G') = \left( \sqrt{p^2 + 4} - \sqrt{(p + 1)^2 + 4} \right) + (p - 2)\left( \sqrt{p^2 + 1} - \sqrt{(p + 1)^2 + 1} \right)
\]

\[
+ \left( \sqrt{p^2 + q^2} - \sqrt{(p + 1)^2 + (q - 1)^2} \right) + (q - 3)\left( \sqrt{q^2 + 1} - \sqrt{(q - 1)^2 + 1} \right) + \left( \sqrt{q^2 + t^2} - \sqrt{(q - 1)^2 + 1} \right)
\]

\[
\leq \left( \sqrt{q^2 + 1} - \sqrt{(q - 1)^2 + 1} \right) + (q - 3)\left( \sqrt{q^2 + 1} - \sqrt{(q - 1)^2 + 1} \right) + \left( \sqrt{q^2 + 4} - \sqrt{(q - 1)^2 + 1} \right) + \left( \sqrt{q^2 + 4} - \sqrt{(q - 1)^2 + 1} \right)
\]

\[
< 0.
\]

\[\Box\]
Lemma 5. Let $G$ be a connected graph of order at least 6. Let $u$ and $v$ be nonadjacent vertices of $G$ such that each of them (i) has at least one pendant neighbor and (ii) contains exactly two nonpendent neighbors such that each of them has degree 2 and $d_G(u) \geq d_G(v) \geq 3$. Let $G'$ be the graph obtained from $G$ by removing a pendant neighbor of $v$ and then attaching it to $u$. It holds that $SO(G) < SO(G')$.

Proof. If $d_G(u) = p$ and $d_G(v) = q$, then $p \geq q \geq 3$, and hence, we have

\[
SO(G) - SO(G') = 2\sqrt{p^2 + 4 - \sqrt{(p + 1)^2 + 4}} + 2\sqrt{q^2 + 4 - \sqrt{(q - 1)^2 + 4}}
\]

Here, it holds that $p^2 + 4 - \sqrt{(p + 1)^2 + 4} \geq q^2 + 4 - \sqrt{(q - 1)^2 + 4}$.

Lemma 6. Let $G$ be the graph deduced from the cycle $C_k$ of order $k$ by attaching $p$ pendant vertices to a vertex $u \in V(C_k)$ and attaching $q$ pendant vertices to another vertex $v \notin \{u\}$ of $C_k$, where $p \geq q \geq 1$ and $p + q = n - k$.

\[
SO(G) \leq (n - 4)\sqrt{(n - 2)^2 + 1 + \sqrt{(n - 2)^2 + 4 + \sqrt{(n - 2)^2 + 9 + \sqrt{10} + \sqrt{13}}}},
\]

with equality if and only if $p = n - 4$.

(i) If $k = 3$, then

(ii) If $4 \leq k \leq n - 2$, then

\[
SO(G) \leq (n - k - 1)\sqrt{(n - k + 1)^2 + 1 + 2\sqrt{(n - k + 1)^2 + 4}} + (k - 4)\sqrt{8 + 2\sqrt{13} + \sqrt{10}},
\]

with equality if and only if $p = n - k - 1$ and $uv \notin E(G)$.

Proof. (i) This part follows directly from Lemma 4 because $uv \in E(G)$ when $k = 3$.

(ii) If $uv \notin E(G)$, then the desired conclusion follows from Lemma 5. In the rest of the proof, assume that $uv \in E(G)$. By Lemma 4, we have

\[
SO(G) \leq (n - k - 1)\sqrt{(n - k + 1)^2 + 1 + \sqrt{(n - k + 1)^2 + 4 + \sqrt{(n - k + 1)^2 + 9 + \sqrt{8 + \sqrt{10} + \sqrt{13}}}}},
\]

with equality if and only if $p = n - k - 1$. Let

\[
\Theta_1 = (n - k - 1)\sqrt{(n - k + 1)^2 + 1 + 2\sqrt{(n - k + 1)^2 + 4}} + (k - 4)\sqrt{8 + 2\sqrt{13} + \sqrt{10}},
\]

\[
\Theta_2 = (n - k - 1)\sqrt{(n - k + 1)^2 + 1 + \sqrt{(n - k + 1)^2 + 4 + \sqrt{(n - k + 1)^2 + 9 + (k - 3)\sqrt{8 + \sqrt{10} + \sqrt{13}}}}}.
\]

Here, it holds that
\[ \Theta_2 - \Theta_1 = \sqrt{(n-k+1)^2 + 9} - \sqrt{(n-k+1)^2 + 4 + \sqrt{8} - \sqrt{13}}. \]  
(22)

Taking \( p = n-k-1 \), we have
\[ \Theta_2 - \Theta_1 = \sqrt{(p+3)^2 + 9} - \sqrt{(p+3)^2 + 4 + \sqrt{8} - \sqrt{13}} < 0, \]  
(23)

with equality if and only if \( q = 1 \).

For \( p \geq 1 \).

**Lemma 7.** For \( n-k-1 \geq q \geq 1 \) and \( k \leq n-2 \), if \( G \) is the graph deduced from the unicyclic graph \( C_{k,n-k-q} \) (see Theorem 1) by attaching \( q \) pendent vertices to exactly one pendent vertex of \( C_{k,n-k-q} \), then

\[ \text{SO}(G) \leq (n-k-2)\sqrt{(n-k+1)^2 + 1} + 3\sqrt{(n-k+1)^2 + 4 + (k-2)\sqrt{8} + \sqrt{5}}, \]  
(24)

Proof. The result trivially holds for \( k = n-2 \) because there is only one graph in this case. Thus, we suppose that \( k \leq n-3 \). Here, we have

\[ \text{SO}(G) = (n-k-q-1)\sqrt{(n-k-q+2)^2 + 1} + 2\sqrt{(n-k-q+2)^2 + 4} \]  
+ \( \sqrt{(n-k-q+2)^2 + (q+1)^2 + (k-2)\sqrt{8} + q\sqrt{(q+1)^2 + 1}} \).  
(25)

The substitution \( n-k = \alpha \) in equation (25) yields

\[ \text{SO}(G) = (\alpha - q - 1)\sqrt{(\alpha - q + 2)^2 + 1} + 2\sqrt{(\alpha - q + 2)^2 + 4} \]  
+ \( \sqrt{(\alpha - q + 2)^2 + (q+1)^2 + (k-2)\sqrt{8} + q\sqrt{(q+1)^2 + 1}} \).  
(26)

where \( \alpha \geq q + 1 \geq 2 \). By a computer program, it is checked that the maximum value of the right-hand-sixed expression of (26) under the given constraints is achieved if and only if \( q = 1 \).

Now, we determine the graph attaining the second-maximum value of the Sombor index in the class of all unicyclic graphs with a fixed order and girth.

**Theorem 2.** Let \( G \) be a unicyclic graph with order \( n \) and girth \( g \) such that \( G \neq C_{k,n-k} \) (see Theorem 1).  

(i) If \( k = 3 \), then

\[ \text{SO}(G) \leq \sqrt{(n-2)^2 + 4} + \sqrt{(n-2)^2 + 9} + (n-4)\sqrt{(n-2)^2 + 1} + \sqrt{10} + \sqrt{13}, \]  
(27)

with equality if and only if \( G \) is the graph deduced from \( C_{3,n-4} \) by attaching a pendent vertex to one of its vertices of degree 2.

(ii) If \( 4 \leq k \leq n-2 \), then

\[ \text{SO}(G) \leq (k-4)\sqrt{8} + 2\sqrt{(n-k+1)^2 + 4 + (n-k-1)\sqrt{(n-k+1)^2 + 1} + 2\sqrt{13} + \sqrt{10}}, \]  
(28)

with equality if and only if \( G \) is a graph deduced from \( C_{k,n-k-1} \) by attaching a pendent vertex to a vertex \( w \in V(C_{k,n-k-1}) \), where \( d_{C_{k,n-k-1}}(w) = 2 \) and \( w \) is not adjacent to the branching neighbor.
Proof. Suppose that $v_1 v_2 \ldots v_k v_1$ is the unique cycle of $G$. Let

\begin{align*}
a &= \sqrt{(n-2)^2 + 4 + \sqrt{(n-2)^2 + 9 + (n-4)\sqrt{(n-2)^2 + 1 + \sqrt{10} + \sqrt{13}}}} \quad \text{when } k = 3, \\
a &= (k - 4)\sqrt{8 + 2\sqrt{(n-k+1)^2 + 4 + (n-k+1)\sqrt{(n-k+1)^2 + 1 + 2\sqrt{13} + \sqrt{10}}}},
\end{align*}

(29)

when $4 \leq k \leq n - 2$.

If the set $\{v_1, v_2, \ldots, v_k\}$ contains at least three branching vertices, then by using Lemmas 2, 3 (or 5), and 6, we find a unicyclic graph $G'$ with order $n$ and girth $g$ such that $G' \neq C_{k,n-k}$ and satisfying $SO(G) < SO(G') \leq a$.

If the set $\{v_1, v_2, \ldots, v_k\}$ contains exactly two branching vertices, then by using Lemmas 2, 4 (or 5), and 6, we find a unicyclic graph $G''$ with order $n$ and girth $g$ such that $G'' \neq C_{k,n-k}$ and satisfying $SO(G) \leq SO(G'') \leq a$, where both the equality signs hold if and only if $G$ is one of the two extremal graphs defined in the statement of the theorem.

\begin{align*}
b &= (k - 2)\sqrt{8 + 3\sqrt{(n-k+1)^2 + 4 + (n-k-2)\sqrt{(n-k+1)^2 + 1 + \sqrt{5}}}}. 
\end{align*}

(30)

At the end of the proof, we will prove that $b - a < 0$. If $v_1$ has only three nonpendent neighbors such that one of them has only one nonpendent neighbor, then from Lemma 7, it follows that $SO(G) \leq b$ with equality if and only if $q = 1$.

In order to complete the proof, in the following, we prove that $b - a < 0$. First, we assume that $k = 3$. Then,

\begin{align*}
a - b &= \sqrt{(n-2)^2 + 9 - 2\sqrt{(n-2)^2 + 4 + \sqrt{(n-2)^2 + 1 + \sqrt{13} + \sqrt{10} - \sqrt{5} - \sqrt{8}}}} \\
&> \sqrt{(n-2)^2 + 9 - 2\sqrt{(n-2)^2 + 4 + \sqrt{(n-2)^2 + 1}}} \\
&> 0.
\end{align*}

(31)

Now, we suppose that $4 \leq k \leq n - 2$. Then,

\begin{align*}
a - b &= \sqrt{(n-k+1)^2 + 1 - \sqrt{(n-k+1)^2 + 4 + 2\sqrt{13} + \sqrt{10} - 2\sqrt{8} - \sqrt{5}}} \\
&= \sqrt{x^2 + 1 - \sqrt{x^2 + 4 + 2\sqrt{13} + \sqrt{10} - 2\sqrt{8} - \sqrt{5}}} > 0,
\end{align*}

(32)

for $x = n - k + 1 \geq 3$. \hfill \Box

Data Availability
The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest
The authors declare that they have no conflicts of interest.

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