Maximizing general first Zagreb and sum-connectivity indices for unicyclic graphs with given independence number

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Abstract

In this paper it is shown that in the class of unicyclic graphs of order \( n \) and independence number \( s \), the spider graph \( S_{\Delta}(n,s) \) is the unique graph maximizing general first Zagreb index \( 0_R^\alpha(G) \) for \( \alpha > 1 \) and general sum-connectivity index \( \chi_\alpha(G) \) for \( \alpha \geq 1 \).

Keywords: Unicyclic graph, independence number, general first Zagreb index, general sum-connectivity number, spider graph, Jensen inequality.

Math. Subj. Class.: 05C35, 05C69

1 Introduction

Let \( G \) be a simple graph having vertex set \( V(G) \) and edge set \( E(G) \). For a vertex \( u \in V(G) \), \( d(u) \) denotes the degree of \( u \) and \( N(u) \) the set of vertices adjacent with \( u \). The maximum vertex degree of \( G \) is denoted by \( \Delta(G) \). \( K_{1,n-1} \) and \( C_n \) will denote, respectively, the star and the cycle on \( n \) vertices. The distance between vertices \( u \) and \( v \) of a connected graph, denoted by \( d(u,v) \), is the length of a shortest path between them. For \( x \in V(G) \) and \( A \subset V(G) \), the distance \( d(x,A) \) between \( x \) and \( A \) is \( \min_{y \in A} d(x,y) \). If \( x \in V(G) \), \( G-x \) denotes the subgraph of \( G \) obtained by deleting \( x \) and its incident edges. Similar notations are \( G-xy \) and \( G+xy \), where \( xy \in E(G) \) and \( xy \notin E(G) \), respectively.

Given a graph \( G \), a subset \( S \) of \( V(G) \) is said to be an independent set of \( G \) if every two vertices of \( S \) are not adjacent. The maximum number of vertices in an independent set of \( G \) is called the independence number of \( G \) and is denoted by \( \alpha(G) \). A unicyclic graph \( G \) of order \( n \) is connected, has \( n \) edges and it consists of a cycle \( C_r \), where \( 3 \leq r \leq n \) and some vertex-disjoint trees having each a vertex common with \( C_r \). It is not difficult to see that if
$G$ is a unicyclic graph of order $n \geq 3$, then $\lfloor n/2 \rfloor \leq \alpha(G) \leq n - 2$. The lower bound can be deduced since a unicyclic graph can be obtained from a tree, which is a bipartite graph, by adding a new edge. The validity of the upper bound follows from the property that if $3 \leq r \leq n$ then $\alpha(C_r) \leq r - 2$ (equality holds only for $r = 3$ and $r = 4$).

For every $n \geq 3$ and $\lfloor n/2 \rfloor \leq s \leq n - 2$, the spider graph denoted by $S_\Delta(n, s)$ is a unicyclic graph of order $n$ consisting of $2s - n + 1$ edges and $n - s - 2$ paths of length 2 having a common endvertex with a triangle $K_3$; in other words, it is obtained from $K_{1,s+1} + e$ by attaching a pendant edge to $n - s - 2$ pendant vertices of $K_{1,s+1} + e$. We have $\alpha(S_\Delta(n, s)) = s$.

The graph, denoted by $H_n$, is defined as follows: for $n = 2k$ it consists of a cycle $C_k$ and $k$ pendant vertices adjacent each to a single vertex of $C_k$ such that each vertex of $C_k$ has degree three. For $n = 2k + 1$, $H_n$ is composed from $C_{k+1}$ and $k$ pendant vertices adjacent each to a single vertex of $C_{k+1}$ such that $k$ vertices of $C_k$ have degree three and one vertex has degree two.

For other notations in graph theory, we refer [16].

The Randić index $R(G)$ [12], one of the most used molecular descriptors in structure-property and structure-activity relationship studies [5, 6, 7, 11, 13, 14], was defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}. $$

The general Randić connectivity index (or general product-connectivity index) of $G$, denoted by $R_\alpha$, was defined by Bollobás and Erdős [1] as

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha, $$

where $\alpha$ is a real number. Then $R_{-1/2}$ is the classical Randić connectivity index and for $\alpha = 1$ it is also known as second Zagreb index and denoted by $M_2(G)$.

This concept was extended to the general sum-connectivity index $\chi_\alpha(G)$ in [20], which is defined by

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha, $$

where $\alpha$ is a real number. The sum-connectivity index $\chi_{-1/2}(G)$ was proposed in [19].

The general first Zagreb index (sometimes referred as “zeroth-order general Randić index”), denoted by $^0R_\alpha(G)$ was defined as

$$^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha, $$

where $\alpha$ is a real number. For $\alpha = -1/2$ this index was defined in [9] and [10] and for $\alpha = 2$ it is also known as first Zagreb index and denoted by $M_1(G)$. Notice that $\chi_1(G) = ^0R_2(G) = M_1(G)$.

Thus, the general Randić connectivity index generalizes both the ordinary Randić connectivity index and the second Zagreb index, while the general sum-connectivity index generalizes both the ordinary sum-connectivity index and the first Zagreb index [20].

Several extremal properties of the sum-connectivity and general sum-connectivity indices for trees, unicyclic graphs and general graphs were given in [3, 4, 19, 20].
Das, Xu and Gutman [2] proved that in the class of trees of order \( n \) and independence number \( s \), the spur \( S_{n,s} \) maximizes both first and second Zagreb indices and this graph is unique with these properties. Tomescu and Jamil [15] showed that in the same class of trees \( T \), \( S_{n,s} \) is the unique graph maximizing general first Zagreb index \( 0 R_\alpha(T) \) for \( \alpha > 1 \) and general sum-connectivity index \( \chi_\alpha(T) \) for \( \alpha \geq 1 \).

In this paper, we show that the spider graph \( S_\Delta(n, s) \) is the unique graph maximizing general first Zagreb index \( 0 R_\alpha(G) \) for \( \alpha > 1 \) and general sum-connectivity index \( \chi_\alpha(G) \) for \( \alpha \geq 1 \) in the set of unicyclic graphs of order \( n \) and independence number \( s (\lfloor n/2 \rfloor \leq s \leq n - 2) \).

2 Preliminary results

The following inequality may be deduced in a straightforward way:

Lemma 2.1. Let \( x > 0 \). If \( \beta < 0 \) then \((1 + x)^\beta > 1 + \beta x\).

The general first Zagreb index and general sum-connectivity index of \( S_\Delta(n, s) \) are given by:

\[
0 R_\alpha(S_\Delta(n, s)) = (s + 1)^\alpha + s(1 - 2^\alpha) + 2^\alpha n - 1;
\]

\[
\chi_\alpha(S_\Delta(n, s)) = (n - s)(s + 3)^\alpha + (2s - n + 1)(s + 2)^\alpha + (n - s - 2)3^\alpha + 4^\alpha.
\]

The cycle \( C_n \) has independence number equal to \( \lfloor n/2 \rfloor \).

Lemma 2.2. Let \( n \geq 5 \). Then (2.1) holds for \( \alpha > 1 \) and (2.2) holds for \( \alpha \geq 1 \):

\[
0 R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > 0 R_\alpha(C_n)
\]

\[
\chi_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > \chi_\alpha(C_n).
\]

Proof. We get \( 0 R_\alpha(C_n) = n2^\alpha \) and \( \chi_\alpha(C_n) = n4^\alpha \). If \( n \) is even, \( n = 2k \), (2.1) can be written as

\[
(k + 1)^\alpha - 2^\alpha k + k - 1 > 0,
\]

where \( k \geq 3 \) and \( \alpha > 1 \). Consider the function \( \varphi(x) = (x + 1)^\alpha - 2^\alpha x + x - 1 \), where \( x \geq 3 \). We get \( \varphi'(x) = \alpha(x + 1)^{\alpha - 1} - 2^\alpha + 1 \geq \alpha4^{\alpha - 1} - 2^\alpha + 1 \). By letting \( \psi(y) = y4^{y-1} - 2^y + 1 \), where \( y > 1 \), we have \( \psi'(y) = 4^{y-1}(1 + y \ln 4) - \ln 2 \cdot 2^y \). Since \( 2^y > 2 \) we deduce

\[
\psi'(y) > 2^y \left( \frac{1 + y \ln 4}{2} - \ln 2 \right) > 2^y \left( \frac{1 + \ln 4}{2} - \ln 2 \right) = 2^{y-1} > 0.
\]

Because \( \psi(1) = 0 \) we have \( \psi(y) > 0 \) for \( y > 1 \), thus \( \varphi(x) \) is strictly increasing for \( x \geq 3 \) and \( \alpha > 1 \). It follows that it is sufficient to prove (2.3) for \( k = 3 \). For \( k = 3 \) (2.3) becomes

\[
4^\alpha - 3 \cdot 2^\alpha + 2 > 0,
\]

or \( (2^\alpha - 1)(2^\alpha - 2) > 0 \), which is true for \( \alpha > 1 \).

If \( n = 2k + 1 \), where \( k \geq 2 \), (2.1) becomes (2.3) in which \( k \geq 2 \). For \( k = 2 \) (2.3) yields \( 3^\alpha - 2 \cdot 2^\alpha + 1 > 0 \), which holds by Jensen inequality since function \( x^\alpha \) is strictly convex for \( \alpha > 1 \).
In order to prove (2.2) consider first the case \( n \) even, \( n = 2k \). In this case (2.2) is
\[
k(k + 3)^\alpha + (k + 2)^\alpha + (k - 2)3^\alpha - (2k - 1)4^\alpha > 0, \tag{2.5}
\]
where \( k \geq 3 \) and \( \alpha \geq 1 \). For \( k = 3 \) (2.5) becomes \( 3 \cdot 6^\alpha + 5^\alpha + 3^\alpha - 5 \cdot 4^\alpha > 0 \), which is true since \( 5^\alpha + 3^\alpha \geq 2 \cdot 4^\alpha \) by Jensen inequality and \( 3 \cdot 6^\alpha > 3 \cdot 4^\alpha \).

Consider the function \( \xi(x) = x(x + 3)^\alpha + (x + 2)^\alpha + (x - 2)3^\alpha - (2x - 1)4^\alpha \), where \( x \geq 3 \). We get \( \xi'(x) = (x + 3)^\alpha + ax(x + 3)^{\alpha - 1} + \alpha(x + 2)^{\alpha - 1} + 3^\alpha - 2 \cdot 4^\alpha \). We have \( (x + 3)^\alpha + 3^\alpha - 2 \cdot 4^\alpha \geq 6^\alpha + 3^\alpha - 2 \cdot 4^\alpha \geq 2 \cdot 4.5^\alpha - 2 \cdot 4^\alpha > 0 \) by Jensen inequality. This implies that \( \xi'(x) > 0 \), hence \( \xi(x) \) is strictly increasing. Thus (2.5) is valid since it holds for \( k = 3 \). If \( n = 2k + 1 \), where \( k \geq 2 \), the proof is similar, using in the same way Jensen inequality.

\[ \square \]

**Lemma 2.3.** If \( n \geq 5 \) and \( \alpha \geq 1 \), \( \chi_\alpha(S_\Delta(n, s)) \) is strictly increasing in \( s \) for \( \lfloor n/2 \rfloor \leq s \leq n - 2 \).

**Proof.** Let
\[
f(x) = (n - x)(x + 3)^\alpha + (2x - n + 1)(x + 2)^\alpha + (n - x)3^\alpha.
\]
We have \( \chi_\alpha(S_\Delta(n, s)) = f(s) - 2 \cdot 3^\alpha + 4^\alpha \). We will show that \( f(x) \) is strictly increasing in \( x \) for \( n \geq 5 \) and \( 2 \leq (n - 1)/2 \leq x \leq n - 2 \). We have
\[
f'(x) = (x + 3)^\alpha - 1(\alpha(n - x) - x - 3) + (x + 2)^\alpha - 1(2x + 4 + 2\alpha x - \alpha n + \alpha) - 3^\alpha.
\]
If the coefficient of \( (x + 3)^\alpha - 1 \) is greater than or equal to zero, then \( f'(x) > 0 \) since \( 2\alpha x - \alpha n + \alpha \geq 0 \), which implies
\[
(x + 2)^\alpha - 1(2x + 4 + 2\alpha x - \alpha n + \alpha) - 3^\alpha \geq 2(x + 2)^\alpha - 3^\alpha \geq 2 \cdot 4^\alpha - 3^\alpha > 0.
\]
The coefficient of \( (x + 3)^\alpha - 1 \) is
\[
x(-\alpha - 1) + \alpha n - 3 \geq (n - 2)(-\alpha - 1) + \alpha n - 3 = -n + 2\alpha - 1 \geq 0
\]
for \( \alpha \geq (n + 1)/2 \).

Suppose that \( 1 \leq \alpha < (n + 1)/2 \). We will also prove that \( f'(x) > 0 \) in this case. We can write \( f'(x) = (x + 3)^\alpha - 1E(n, x, \alpha) \), where
\[
E(n, x, \alpha) = \alpha(n - x) - x - 3 + \left(1 + \frac{1}{x + 2}\right)^{1-\alpha(2x + 4 + 2\alpha x - \alpha n + \alpha)} - \frac{3^\alpha}{(x + 3)^\alpha - 1}.
\]

Lemma 2.1 yields
\[
\left(1 + \frac{1}{x + 2}\right)^{1-\alpha} > 1 + \frac{1 - \alpha}{x + 2},
\]
which implies
\[
E(n, x, \alpha) > (x + 1)(\alpha + 1) + 2 - 2\alpha^2 + \frac{\alpha(\alpha - 1)(n + 3)}{x + 2} - \frac{3^\alpha}{(x + 3)^\alpha - 1}. \tag{2.6}
\]
Since \( \alpha - 1 < \frac{n-1}{2} \) and \( x \geq \frac{n-1}{2} \) it follows that \( x > \alpha - 1 \), which implies \( (x+1)(\alpha+1) > \alpha^2 + \alpha \). Since \( x+2 < n+3 \) we get \( \frac{\alpha(x-1)(\alpha+3)}{x+2} \geq \frac{\alpha(x-1)(\alpha+3)}{x+2} \) and from (2.6) we obtain

\[
E(n, x, \alpha) > 2 - \frac{3\alpha}{(x+3)^{\alpha-1}}.
\]

If \( \alpha \geq 2 \) then \( \max_{x \geq 2} \frac{3\alpha}{(x+3)^{\alpha-1}} = 5\left(\frac{3}{5}\right)^\alpha \leq \frac{9}{5} \), which implies \( E(n, x, \alpha) > 0 \). The same conclusion holds if \( 1 \leq \alpha < 2 \) since in this case we have

\[
x \geq 2 > \alpha, \quad (x+1)(\alpha+1) > (\alpha+1)^2, \quad \frac{3\alpha}{(x+3)^{\alpha-1}} = 3 \left(\frac{3}{x+3}\right)^{\alpha-1} \leq 3
\]

and (2.6) yields \( E(n, x, \alpha) > (\alpha+1)^2 + 2 - 2\alpha^2 + \alpha(\alpha - 1) - 3 = \alpha \geq 1 \).

The following observation will be useful.

**Lemma 2.4.** Let \( G \) be a graph and \( x \in V(G) \), which is adjacent to pendant vertices \( v_1, \ldots, v_r \). If \( r \geq 2 \) then any maximum independent subset of \( V(G) \) contains \( v_1, \ldots, v_r \).

**Lemma 2.5.** The function

\[
h(x) = (x - 2)((x + a)^\alpha - (x + a - 1)^\alpha)
\]

is strictly increasing for \( x \geq 2, a \geq 1 \) and \( \alpha \geq 1 \).

**Proof.** We get

\[
h'(x) = (x + a)^\alpha - (x + a - 1)^\alpha + \alpha(x - 2)((x + a)^{\alpha-1} - (x + a - 1)^{\alpha-1}) > 0
\]

for \( x \geq 2, a \geq 1 \) and \( \alpha \geq 1 \).

\[\square\]

## 3 Main results

By simple inspection we can see that for \( n = 6 \) spider graph \( S_\Delta(6, s) \) is the unique extremal graph \( G \) of order six and independence number \( s, 3 \leq s \leq 4 \), having maximum \( 0R_\alpha(G) \) unless \( s = 3 \) and \( 1 < \alpha < 2 \), when \( 0R_\alpha(S_\Delta(6, 3)) < 0R_\alpha(H_6) \) (note that \( H_6 \) consists of a triangle \( K_3 \) and three pendant vertices adjacent to different vertices of \( K_3 \)). For \( n = 6, s = 3 \) and \( \alpha \in \{1, 2\} \) both graphs \( H_6 \) and \( S_\Delta(6, 3) \) are extremal. The case \( n \geq 7 \) is settled below.

**Theorem 3.1.** Let \( n \geq 7, \lfloor n/2 \rfloor \leq s \leq n - 2 \) and \( G \) be a unicyclic graph of order \( n \) with independence number \( s \). Then for every \( \alpha > 1, 0R_\alpha(G) \) is maximum if and only if \( G = S_\Delta(n, s) \).

**Proof.** The proof is by induction on \( n \). For \( n = 7 \) the proof is by inspection, using Jensen inequality or mathematical software [17]; there are 4 graphs with \( s = 3 \), 15 graphs with \( s = 4 \) and 5 graphs having \( s = 5 \).

Let \( n \geq 8 \) and suppose that the property is true for all unicyclic graphs of order \( n - 1 \). Let \( G \) be a unicyclic graph of order \( n \) and independence number \( s \) having maximum general first Zagreb index. By Lemma 2.2 \( 0R_\alpha(C_n) \) cannot be maximum; it follows that \( \Delta(G) \geq 3 \). Its independence number verifies \( s \geq 4 \). Denote by \( C \) the unique cycle of \( G \), whose length is at most \( n - 1 \). \( G \) has at least one pendant vertex. Let \( x_1 \) be a pendant vertex such that the distance \( d(x_1, C) \) is maximum. We shall consider two cases:
Case 1. Let $x_1, x_2, \ldots, x_p$, where $p \geq 3$ and $x_p \in C$ be the unique path from $x_1$ to $C$. By letting $d(x_2) = d_2$, since for every vertex $u$ in $N(u)$ at most two vertices are adjacent, we obtain $s \geq \Delta(G) - 1 \geq d_2 - 1$, or $d_2 \leq s + 1$. Other two subcases may hold:

\begin{itemize}
  \item Subcase 1.1: $\alpha(G - x_1) = \alpha(G) - 1$
  \item Subcase 1.2: $\alpha(G - x_1) = \alpha(G)$.
\end{itemize}

Subcase 1.1. By the induction hypothesis we can write

$$0 R_\alpha(G) = 0 R_\alpha(G - x_1) + 1 + d_2^\alpha - (d_2 - 1)^\alpha$$

$$\leq 0 R_\alpha(S_\Delta(n - 1, s - 1)) + 1 + d_2^\alpha - (d_2 - 1)^\alpha$$

$$= s^\alpha + 2^\alpha(n - s) + s - 2 + 1 + d_2^\alpha - (d_2 - 1)^\alpha.$$ 

Since the function $x^\alpha - (x - 1)^\alpha$ is strictly increasing for $x \geq 1$ and $\alpha > 1$, it follows that $d_2^\alpha - (d_2 - 1)^\alpha \leq (s + 1)^\alpha - s^\alpha$, which implies $0 R_\alpha(G) \leq 0 R_\alpha(S_\Delta(n, s))$, equality holding if and only if $d_2 = s + 1$. But this equality is not possible. If $d_2 = s + 1$ holds, then two vertices in $N(x_2)$ are adjacent since otherwise we would have $s \geq d_2$. In this case, since $x_2 \notin C$, $G$ would have at least two cycles, a contradiction.

Consequently, $0 R_\alpha(G) < (s + 1)^\alpha + 2^\alpha(n - s) + s - 1 = 0 R_\alpha(S_\Delta(n, s))$, a contradiction.

Subcase 1.2. Next we assume that $\alpha(G - x_1) = \alpha(G)$. If $x_2$ would be adjacent to a vertex $w \neq x_1, x_3$, the degree of $w$ cannot be greater than one, since in this case the path $x_1, \ldots, x_p$ would not have maximum length. It follows that $d(w) = 1$ and by Lemma 2.4 every maximum independent set of vertices of $G$ includes both $x_1$ and $w$. This implies $\alpha(G - x_1) = \alpha(G) - 1$, which contradicts the hypothesis. It follows that $d_2 = 2$. We can write

$$0 R_\alpha(G) = 0 R_\alpha(G - x_1) + 2^\alpha$$

$$\leq 0 R_\alpha(S_\Delta(n - 1, s)) + 2^\alpha$$

$$= (s + 1)^\alpha + 2^\alpha(n - 1 - s) + s - 1 + 2^\alpha$$

$$= 0 R_\alpha(S_\Delta(n, s)).$$

The equality holds if and only if $G - x_1 = S_\Delta(n - 1, s)$ and pendant vertex $x_1$ is adjacent to a pendant vertex of $S_\Delta(n - 1, s)$. Let $u$ be the vertex of degree $s + 1$ of $S_\Delta(n - 1, s)$. If $x_1$ is adjacent to a pendant vertex $v_2$ of $S_\Delta(n - 1, s)$ such that $d(v_2, u) = 2$, the resulting graph $G$ has $\alpha(G) = s + 1$, which contradicts the hypothesis. We deduce that $x_1$ is adjacent to a pendant vertex which is adjacent to $u$ in $S_\Delta(n - 1, s)$, which implies that $G = S_\Delta(n, s)$.

Case 2. In this case we shall also consider two subcases:

\begin{itemize}
  \item Subcase 2.1: There exists a pendant vertex $x_1$ such that $d(x_1, C) = 1$ and $\alpha(G - x_1) = \alpha(G) - 1$; and
  \item Subcase 2.2: For all pendant vertices $x$ we have $d(x, C) = 1$ and $\alpha(G - x) = \alpha(G)$.
\end{itemize}
Subcase 2.1. As for Subcase 1.1 we get \( d_2 = d(x_2) \leq s + 1 \) and by the same arguments \( 0 R_{\alpha}(G) \leq (s + 1)^{\alpha} + 2^{\alpha}(n - s) + s - 1 = 0 R_{\alpha}(S_\Delta(n, s)) \) holds, with equality if and only if \( d(x_2) = s + 1 \) and \( G - x_1 = S_\Delta(n - 1, s - 1) \). It follows that \( x_1 \) is adjacent to the vertex of degree \( s \) in \( S_\Delta(n - 1, s - 1) \), i.e., \( G = S_\Delta(n, s) \). Since \( d(x_1, C) = \max\{d(x, C) : d(x) = 1\} = 1 \), this equality is possible only for \( n = s + 2 \).

Subcase 2.2. In this case a vertex of \( C \) may be adjacent to a single pendant vertex \( x \), since otherwise we would have \( \alpha(G - x) = \alpha(G) - 1 \) by Lemma 2.4. We deduce that \( G \) consists of \( C \) and some pendant vertices adjacent to vertices of \( C \) such that each vertex \( y \in C \) has its degree \( d(y) \in \{2, 3\} \). We shall prove that in this case \( 0 R_{\alpha}(G) < 0 R_{\alpha}(S_\Delta(n, s)) \), a contradiction.

Suppose that on \( C \) there exist four consecutive vertices \( x, u, v, y \) such that \( d(u) = d(v) = 2 \). In this case we shall define a new unicyclic graph \( G_1 \) of order \( n \) by \( G_1 = G - vy + uy \). We deduce \( 0 R_{\alpha}(G_1) - 0 R_{\alpha}(G) = 3^{\alpha} + 1^{\alpha} - 2 \cdot 2^{\alpha} > 0 \) by Jensen inequality since \( \alpha > 1 \). If on \( C \) there exist six vertices \( x, r, y, p, s, q \) (\( y \) may coincide with \( p \)) such that \( d(x) = d(y) = d(p) = d(q) = 3 \) and \( d(r) = d(s) = 2 \), we define a new unicyclic graph \( G_2 \) with the same vertex set as follows: \( G_2 = G - \{xr, ry\} \cup \{xy, rs\} \). By the same argument we obtain \( 0 R_{\alpha}(G_2) > 0 R_{\alpha}(G) \). If \( G \neq H_n \), by applying step by step this type of transformations we get \( H_n \), such that \( 0 R_{\alpha}(H_n) > 0 R_{\alpha}(G) \).

We have \( 0 R_{\alpha}(H_n) = k \cdot 3^\alpha + k \) for \( n = 2k \) and \( k \cdot 3^\alpha + 2^\alpha + k \) for \( n = 2k + 1 \) and
\[
\begin{align*}
0 R_{\alpha}(S_\Delta(2k, k)) &= (k + 1)^\alpha + k 2^\alpha + k - 1 \\
0 R_{\alpha}(S_\Delta(2k + 1, k)) &= (k + 1)^\alpha + (k + 1) 2^\alpha + k - 1.
\end{align*}
\]
In both cases, \( n = 2k \) or \( n = 2k + 1 \) the inequalities \( 0 R_{\alpha}(S_\Delta(n, \lfloor n/2 \rfloor)) > 0 R_{\alpha}(H_n) \) coincide with
\[
(k + 1)^\alpha - k(3^\alpha - 2^\alpha) - 1 > 0 \tag{3.1}
\]
for every \( k \geq 4 \) and \( \alpha > 1 \). Let \( g(x) = (x + 1)^\alpha - x(3^\alpha - 2^\alpha) - 1 \). We have
\[
\begin{align*}
g(4) &= 5^\alpha - 4 \cdot 3^\alpha + 4 \cdot 2^\alpha - 1 > 0 \text{ for } \alpha > 1 \tag{17} \text{ and} \\
g'(x) &= \alpha(x + 1)^{\alpha - 1} - 3^\alpha + 2^\alpha.
\end{align*}
\]
\( g'(x) \) is strictly increasing and \( g'(4) = \alpha 5^{\alpha - 1} - 3^\alpha + 2^\alpha > 0 \) for \( \alpha > 1 \) [17]. It follows that \( g'(x) > 0 \), hence \( g(x) \) is strictly increasing for \( x \geq 4 \) and \( \alpha > 1 \) and (3.1) is proved. Consequently, we can write \( 0 R_{\alpha}(G) \leq 0 R_{\alpha}(H_n) \leq 0 R_{\alpha}(S_\Delta(n, \lfloor n/2 \rfloor)) \leq 0 R_{\alpha}(S_\Delta(n, s)) \) since the last term is strictly increasing in \( s \), a contradiction.

Since the function \( 0 R_{\alpha}(S_\Delta(n, s)) \) is strictly increasing in \( s \), \( \lfloor n/2 \rfloor \leq s \leq n - 2 \), we deduce:

**Corollary 3.2 ([8, 18]).** Let \( G \) be a unicyclic graph of order \( n \geq 7 \). Then for every \( \alpha > 1 \), \( 0 R_{\alpha}(G) \) is maximum if and only if \( G = S_\Delta(n, n - 2) = K_{1,n-1} + e \).

A similar result holds for general sum-connectivity index.

**Theorem 3.3.** Let \( n \geq 3 \), \( \lfloor n/2 \rfloor \leq s \leq n - 2 \) and \( G \) be a unicyclic graph of order \( n \) with independence number \( s \). Then for every \( \alpha \geq 1 \), \( \chi_{\alpha}(G) \) is maximum if and only if \( G = S_\Delta(n, s) \). For \( n = 6 \) and \( \alpha = 1 \) there exists another extremal graph, \( H_6 \).
Proof. We shall use induction on \( n \) in the same way as in the proof of Theorem 3.1. For \( n = 3 \) there is a unique unicyclic graph on three vertices, \( S_\Delta(3,1) = K_3 \). For \( n = 4 \) there are two unicyclic graphs, \( C_4 \) and \( K_{1,3} + e = S_\Delta(4,2) \) and the theorem is verified.

Let \( n \geq 5 \) and suppose that the theorem is true for all unicyclic graphs of order \( n-1 \). Let \( G \) be a unicyclic graph of order \( n \) and independence number \( s \) having maximum general sum-connectivity index. By Lemma 2.2 \( \chi_\alpha(C_n) \) cannot be maximum; it follows that \( \Delta(G) \geq 3 \). Denote by \( C \) the unique cycle of \( G \), whose length is at most \( n-1 \). Let \( x_1 \) be a pendant vertex such that the distance \( d(x_1, C) \) is maximum. We shall consider four cases:

- **Case 1.1:** \( d(x_1, C) \geq 2 \) and \( \alpha(G - x_1) = \alpha(G) - 1 \);
- **Case 1.2:** \( d(x_1, C) \geq 2 \) and \( \alpha(G - x_1) = \alpha(G) \);
- **Case 2.1:** \( \max\{d(x, C) \mid d(x) = 1\} = 1 \) and there exists a pendant vertex \( x_1 \) such that \( \alpha(G - x_1) = \alpha(G) - 1 \);
- **Case 2.2:** \( \max\{d(x, C) \mid d(x) = 1\} = 1 \) and for all pendant vertices \( x \) we have \( \alpha(G - x) = \alpha(G) \).

**Case 1.1.** Let \( x_1, x_2, x_3, \ldots \) be the path between \( x_1 \) and \( C \). Since this path has maximum length, it follows that \( x_3 \) is the unique vertex in \( N(x_2) \) such that \( d_3 = d(x_3) \geq 2 \). As in the proof of Theorem 3.1 we deduce \( d_2 = d(x_2) \leq s + 1 \).

We have

\[
\chi_\alpha(G) = \chi_\alpha(G - x_1) + (d_2 + 1)^\alpha + (d_2 - 2)((d_2 + 1)^\alpha - d_2^\alpha) + (d_2 + d_3)^\alpha - (d_2 + d_3 - 1)^\alpha.
\]

\( x_2 \) being adjacent to \( d_2 - 1 \) pendant vertices and in \( G - x_2x_3 \) the degree of \( x_3 \) being \( d_3 - 1 \), it follows that \( d_2 - 1 + d_3 - 2 \leq s \), or \( d_2 + d_3 \leq s + 3 \). We get \( (d_2 + 1)^\alpha \leq (s + 2)^\alpha \) with equality if and only if \( d_2 = s + 1 \) and \( (d_2 + d_3)^\alpha - (d_2 + d_3 - 1)^\alpha \leq (s + 3)^\alpha - (s + 2)^\alpha \) with equality only if \( d_2 + d_3 = s + 3 \). Since by Lemma 2.5 the function \((x - 2)((x + 1)^\alpha - x^\alpha)\) is strictly increasing in \( x \) for \( x \geq 2 \) and \( \alpha \geq 1 \), by the induction hypothesis we obtain

\[
\chi_\alpha(G) \leq \chi_\alpha(S_\Delta(n-1, s-1)) + (s + 2)^\alpha + (s-1)((s + 2)^\alpha - (s + 1)^\alpha) + (s + 3)^\alpha - (s + 2)^\alpha
\]

\[
= (n - s)(s + 2)^\alpha + (2s - n)(s + 1)^\alpha + (n - s - 2)3^\alpha + 4^\alpha + (s - 1)((s + 2)^\alpha - (s + 1)^\alpha) + (s + 3)^\alpha.
\]

By denoting the last expression by \( F(n, s, \alpha) \), we have \( F(n, s, \alpha) \leq \chi_\alpha(S_\Delta(n, s)) \) if and only if

\[
(n - s - 1)(s + 3)^\alpha + (n - s - 1)(s + 1)^\alpha \geq 2(n - s - 1)(s + 2)^\alpha.
\]

(3.2)

Since \( n - s - 1 \geq 1 \), (3.2) is equivalent to \( (s + 3)^\alpha + (s + 1)^\alpha \geq 2(s + 2)^\alpha \), which is true by Jensen inequality, with equality only for \( \alpha = 1 \). If the inequality is strict, \( G \) cannot be extremal, a contradiction. For \( \alpha = 1 \) we have equality only for \( d_2 = s + 1 \) and \( d_2 + d_3 = s + 3 \), which implies \( d_3 = 2 \) and \( G - x_1 = S_\Delta(n-1, s-1) \), \( x_2 \) being the vertex of degree \( s \) in \( S_\Delta(n - 1, s - 1) \). In this case we have \( d(x_1, C) = 1 \), which contradicts the hypothesis.
Case 1.2. As in the proof of Theorem 3.1 we obtain \( x_2 = d(x_2) = 2 \) and \( d_3 = d(x_3) \leq \Delta(G) \leq s + 1 \). By the induction hypothesis we get
\[
\chi_\alpha(G) = \chi_\alpha(G - x_1) + 3\alpha + (d_3 + 2)^\alpha - (d_3 + 1)^\alpha
\leq \chi_\alpha(S_\Delta(n - 1, s)) + 3\alpha + (s + 3)^\alpha - (s + 2)^\alpha
= \chi_\alpha(S_\Delta(n, s)),
\]
with equality if and only if \( G - x_1 = S_\Delta(n - 1, s) \), \( d_2 = 2 \) and \( d_3 = s + 1 \), i.e., \( G = S_\Delta(n, s) \).

Case 2.1. In this case \( x_1 \) is adjacent to \( x_2 \in C \). Let \( x_3 \) and \( x_4 \) be the vertices adjacent to \( x_2 \) on \( C \) and denote \( d(x_2) = d_2 \geq 3 \), \( d(x_3) = d_3 \) and \( d(x_4) = d_4 \). We deduce
\[
\chi_\alpha(G) = \chi_\alpha(G - x_1) + (d_2 + 1)^\alpha + (d_2 - 3)((d_2 + 1)^\alpha - d_2^\alpha) + (d_2 + d_3)^\alpha - (d_2 + 3 - 1)^\alpha + (d_2 + d_4)^\alpha - (d_2 + d_4 + 1)^\alpha.
\]
x_2 is adjacent with \( d_2 - 2 \) pendant vertices and in \( G - x_2x_3 \) the degree of \( x_3 \) is \( d_3 - 1 \). It follows that \( d_2 - 2 + d_3 - 1 \leq s \), or \( d_2 + d_3 \leq s + 3 \). Similarly, \( d_2 + d_4 \leq s + 3 \). One obtains
\[
(d_2 + d_3)^\alpha - (d_2 + d_3 - 1)^\alpha \leq (s + 3)^\alpha - (s + 2)^\alpha;
(d_2 + d_4)^\alpha - (d_2 + d_4 - 1)^\alpha \leq (s + 3)^\alpha - (s + 2)^\alpha.
\]
Since \( d_2 \leq s + 1 \), by Lemma 2.5 we deduce
\[
(d_2 - 3)((d_2 + 1)^\alpha - d_2^\alpha) \leq (s - 2)((s + 2)^\alpha - (s + 1)^\alpha).
\]
By the induction hypothesis we get
\[
\chi_\alpha(G) \leq \chi_\alpha(S_\Delta(n - 1, s - 1)) + (s + 2)^\alpha + (s - 2)((s + 2)^\alpha - (s + 1)^\alpha)
+ 2(s + 3)^\alpha - 2(s + 2)^\alpha
= (n - s)(s + 2)^\alpha + (2s - n)(s + 1)^\alpha + (n - s - 2)3^\alpha + 4^\alpha
- (s + 2)^\alpha + (s - 2)((s + 2)^\alpha - (s + 1)^\alpha) + 2(s + 3)^\alpha.
\]
This upper bound is less than or equal to \( \chi_\alpha(S_\Delta(n, s)) \) if and only if
\[
(n - s - 2)(s + 3)^\alpha + (n - s - 2)(s + 1)^\alpha \geq 2(n - s - 2)(s + 2)^\alpha. \tag{3.3}
\]
If \( s = n - 2 \) then (3.3) is an equality, \( S_\Delta(n - 1, s - 1) \) has no pendant path of length 2, it coincides with \( K_{1,n-2} + e \), \( d_2 = s + 1 \), \( d_3 = d_4 = 2 \) and all inequalities become equalities. In this case \( G = S_\Delta(n, s) \). If \( s < n - 2 \) then \( \chi_\alpha(G - x_1) < \chi_\alpha(S_\Delta(n - 1, s - 1)) \) since \( S_\Delta(n - 1, s - 1) \) has pendant paths of length 2 and \( G - x_1 \) does not have by hypothesis. If \( s < n - 2 \) then (3.3) is valid by Jensen inequality (for \( \alpha = 1 \) (3.3) is an equality), but in this case we have \( \chi_\alpha(G) < \chi_\alpha(S_\Delta(n, s)) \), a contradiction.

Case 2.2. As in the proof of Theorem 3.1 we deduce that \( G \) consists of \( C \) and some pendant vertices adjacent to vertices of \( C \) such that each vertex \( y \in C \) has its degree \( d(y) \in \{2, 3\} \). We shall prove that in this case \( \chi_\alpha(G) < \chi_\alpha(S_\Delta(n, s)) \) unless \( \alpha = 1 \) and \( G = H_6 \), a contradiction.
Suppose that on $C$ there exist four consecutive vertices $x, u, v, y$ such that $d(u) = d(v) = 2$. In this case we shall define a new unicyclic graph $G_1$ of order $n$ by $G_1 = G - vy + wy$. We deduce

$$
\chi_{\alpha}(G_1) - \chi_{\alpha}(G) = (d(x) + 3^{\alpha} + (d(y) + 3^{\alpha} - (d(x) + 2)^{\alpha} - (d(y) + 2)^{\alpha} > 0.
$$

If on $C$ there exist six vertices $x, r, y, p, s, q$ ($y$ may coincide with $p$) such that $d(x) = d(y) = d(p) = d(q) = 3$ and $d(r) = d(s) = 2$, we define a new unicyclic graph $G_2$ with the same vertex set as follows: $G_2 = G - \{xr, ry\} + \{xy, rs\}$. We obtain

$$
\chi_{\alpha}(G_2) - \chi_{\alpha}(G) = 3 \cdot 6^{\alpha} + 4^{\alpha} - 4 \cdot 5^{\alpha} > 0
$$

since $6^{\alpha} + 4^{\alpha} \geq 2 \cdot 5^{\alpha}$ and $2 \cdot 6^{\alpha} > 2 \cdot 5^{\alpha}$. If $G \neq H_n$, by applying step by step this type of transformations we get $H_n$, such that $\chi_{\alpha}(H_n) > \chi_{\alpha}(G)$.

We have $\chi_{\alpha}(H_n) = k6^{\alpha} + k4^{\alpha}$ for $n = 2k$ and $(k - 1)6^{\alpha} + k4^{\alpha} + 2 \cdot 5^{\alpha}$ for $n = 2k + 1$. We get

$$
\chi_{\alpha}(S_{\Delta}(2k, k)) = (k + 3)^{\alpha} + (k + 2)^{\alpha} + (k - 2)^{\alpha} + 4^{\alpha} \quad \text{and}
$$

$$
\chi_{\alpha}(S_{\Delta}(2k + 1, k)) = (k + 1)(k + 3)^{\alpha} + (k - 1)^{\alpha} + 4^{\alpha}.
$$

We shall prove that $\chi_{\alpha}(S_{\Delta}(2k, k)) \geq \chi_{\alpha}(H_n)$ for $n = 2k$ and $k \geq 3$ (equality holds only for $k = 3$ and $\alpha = 1$) and $\chi_{\alpha}(S_{\Delta}(2k + 1, k)) > \chi_{\alpha}(H_n)$ for $n = 2k + 1$ and $k \geq 2$. Since for $n = 5$ and $n = 7$ it can be easily verified that there is no unicyclic graph of order $n$ in Case 2.2, it follows that for $n = 2k + 1$ we may consider that $k \geq 4$. It follows that it is necessary to show that (3.4) holds for $k \geq 3$ (with equality only for $k = 3$ and $\alpha = 1$) and (3.5) is true for $k \geq 4$.

$$
k(k + 3)^{\alpha} + (k + 2)^{\alpha} + (k - 2)^{\alpha} + 4^{\alpha} \geq k6^{\alpha} + k4^{\alpha} \quad (3.4)
$$

$$
(k + 1)(k + 3)^{\alpha} + (k - 1)^{\alpha} + 4^{\alpha} > (k - 1)6^{\alpha} + k4^{\alpha} + 2 \cdot 5^{\alpha} \quad (3.5)
$$

For $\alpha = 1$ (3.4) is equivalent to $k^2 - 3k \geq 0$ with equality only for $k = 3$. Suppose that $\alpha > 1$ and let

$$
\rho(x) = x(x + 3)^{\alpha} + (x + 2)^{\alpha} + (x - 2)^{3^{\alpha}} - (x - 1)4^{\alpha} - x6^{\alpha}.
$$

Since $\rho'(x)$ is strictly increasing for $x \geq 3$, we get

$$
\rho'(x) \geq \rho'(3) = 3\alpha 6^{\alpha-1} + \alpha 5^{\alpha-1} + 3^{\alpha} - 4^{\alpha} > 0
$$

for $\alpha > 1$ [17], which implies $\rho(x) \geq \rho(3) = 5^{\alpha} + 3^{\alpha} - 2 \cdot 4^{\alpha} > 0$ for $\alpha > 1$ by Jensen inequality. This proves (3.4).

Similarly, let

$$
\varphi(x) = (x + 1)(x + 3)^{\alpha} + (x - 1)3^{\alpha} - (x - 1)6^{\alpha} - (x - 1)4^{\alpha} - 2 \cdot 5^{\alpha}.
$$

Since $\varphi'(x)$ is strictly increasing in $x \geq 4$ for $\alpha \geq 1$ and

$$
\varphi'(4) = 7^{\alpha} + 5\alpha 7^{\alpha-1} - 6^{\alpha} - 4^{\alpha} + 3^{\alpha} > 0
$$

for $\alpha \geq 1$ [17], it follows that for $x \geq 4$ we have

$$
\varphi(x) \geq \varphi(4) = 5 \cdot 7^{\alpha} + 3 \cdot 3^{\alpha} - 3 \cdot 6^{\alpha} - 3 \cdot 4^{\alpha} - 2 \cdot 5^{\alpha} > 0
$$
for \( \alpha \geq 1 \) \cite{17} and (3.5) is justified.

Consequently, if \( G \neq H_6 \) we can write

\[
\chi_\alpha(G) \leq \chi_\alpha(H_n) < \chi_\alpha(S_{\Delta}(n, \lfloor n/2 \rfloor)) \leq \chi_\alpha(S_{\Delta}(n, s))
\]

since by Lemma 2.3 the last term is strictly increasing in \( s \), a contradiction. \( \square \)

References


