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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 ${}^0R_\alpha(G)$ 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

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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_α, was defined by Bollobás and Erdős [1] as

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

where α 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 α 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 α 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 ${}^0R_\alpha(T)$ 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 ${}^0R_\alpha(G)$ 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:

$$\begin{aligned} {}^0R_\alpha(S_\Delta(n,s)) &= (s+1)^\alpha + s(1-2^\alpha) + 2^\alpha n - 1; \\ \chi_\alpha(S_\Delta(n,s)) &= (n-s)(s+3)^\alpha + (2s-n+1)(s+2)^\alpha + (n-s-2)3^\alpha + 4^\alpha. \end{aligned}$$

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 $\alpha \geq 1$:*

$$ {}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > {}^0R_\alpha(C_n) \tag{2.1}$$

$$ \chi_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > \chi_\alpha(C_n). \tag{2.2}$$

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

$$(k+1)^\alpha - 2^\alpha k + k - 1 > 0, \tag{2.3}$$

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 $\varphi'(x) = \alpha(x+1)^{\alpha-1} - 2^\alpha + 1 \geq \alpha 4^{\alpha-1} - 2^\alpha + 1$. 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

$$4^\alpha - 3 \cdot 2^\alpha + 2 > 0, \tag{2.4}$$

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^α 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 $\xi'(x) = (x+3)^\alpha + \alpha x(x+3)^{\alpha-1} + \alpha(x+2)^{\alpha-1} + 3^\alpha - 2 \cdot 4^\alpha$. 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. □

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 $f'(x) = (x+3)^{\alpha-1}E(n,x,\alpha)$, 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 $\frac{\alpha(\alpha-1)(n+3)}{x+2} \geq \alpha(\alpha - 1)$ and from (2.6) we obtain

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

If $\alpha \geq 2$ then $\max_{x\geq 2} \frac{3^\alpha}{(x+3)^{\alpha-1}} = 5(\frac{3}{5})^\alpha \leq \frac{9}{5}$, 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 $v_1, \dots, v_r$. If $r \geq 2$ then any maximum independent subset of $V(G)$ contains $v_1, \dots, v_r$.*

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 $\alpha \geq 1$. □

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: $d(x_1, C) \geq 2$ and
- Case 2: $d(x_1, C) = 1$.

Case 1. Let $x_1, x_2, \dots, x_p$, 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:

- Subcase 1.1: $\alpha(G - x_1) = \alpha(G) - 1$ and
- Subcase 1.2: $\alpha(G - x_1) = \alpha(G)$.

Subcase 1.1. By the induction hypothesis we can write

$$\begin{aligned} {}^0R_\alpha(G) &= {}^0R_\alpha(G - x_1) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\ &\leq {}^0R_\alpha(S_\Delta(n-1, s-1)) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\ &= s^\alpha + 2^\alpha(n - s) + s - 2 + 1 + d_2^\alpha - (d_2 - 1)^\alpha. \end{aligned}$$

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 ${}^0R_\alpha(G) \leq {}^0R_\alpha(S_\Delta(n, s))$, 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, ${}^0R_\alpha(G) < (s + 1)^\alpha + 2^\alpha(n - s) + s - 1 = {}^0R_\alpha(S_\Delta(n, s))$, 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 $x_1, \dots, x_p$ 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

$$\begin{aligned} {}^0R_\alpha(G) &= {}^0R_\alpha(G - x_1) + 2^\alpha \\ &\leq {}^0R_\alpha(S_\Delta(n-1, s)) + 2^\alpha \\ &= (s + 1)^\alpha + 2^\alpha(n - 1 - s) + s - 1 + 2^\alpha \\ &= {}^0R_\alpha(S_\Delta(n, s)). \end{aligned}$$

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:

- 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
- Subcase 2.2: For all pendant vertices x we have $d(x, C) = 1$ and $\alpha(G - x) = \alpha(G)$.

Subcase 2.1. As for Subcase 1.1 we get $d_2 = d(x_2) \le s+1$ and by the same arguments ${}^0R_\alpha(G) \le (s+1)^\alpha + 2^\alpha(n-s)+s-1 = {}^0R_\alpha(S_\Delta(n,s))$ 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 $s = n-2$.

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 ${}^0R_\alpha(G) < {}^0R_\alpha(S_\Delta(n,s))$, 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 ${}^0R_\alpha(G_1) - {}^0R_\alpha(G) = 3^\alpha + 1^\alpha - 2\cdot 2^\alpha > 0$ 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: $G_2 = G - \{xr, ry\} + \{xy, rs\}$. By the same argument we obtain ${}^0R_\alpha(G_2) > {}^0R_\alpha(G)$. If $G \ne H_n$, by applying step by step this type of transformations we get H_n, such that ${}^0R_\alpha(H_n) > {}^0R_\alpha(G)$.

We have ${}^0R_\alpha(H_n) = k\cdot 3^\alpha + k$ for $n = 2k$ and $k \cdot 3^\alpha + 2^\alpha + k$ for $n = 2k+1$ and

$$ {}^0R_\alpha(S_\Delta(2k,k)) = (k+1)^\alpha + k2^\alpha + k - 1 \text{ and} $$
$$ {}^0R_\alpha(S_\Delta(2k+1,k) = (k+1)^\alpha + (k+1)2^\alpha + k - 1. $$

In both cases, $n = 2k$ or $n = 2k+1$ the inequalities ${}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) > {}^0R_\alpha(H_n)$ coincide with

$$ (k+1)^\alpha - k(3^\alpha - 2^\alpha) - 1 > 0 \tag{3.1} $$

for every $k \ge 4$ and $\alpha > 1$. Let $g(x) = (x+1)^\alpha - x(3^\alpha - 2^\alpha) - 1$. We have

$$ g(4) = 5^\alpha - 4\cdot 3^\alpha + 4 \cdot 2^\alpha - 1 > 0 \text{ for } \alpha > 1 \text{ [17] and} $$
$$ g'(x) = \alpha(x+1)^{\alpha-1} - 3^\alpha + 2^\alpha. $$

$g'(x)$ 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 $x \ge 4$ and $\alpha > 1$ and (3.1) is proved. Consequently, we can write ${}^0R_\alpha(G) \le {}^0R_\alpha(H_n) < {}^0R_\alpha(S_\Delta(n, \lfloor n/2 \rfloor)) \le {}^0R_\alpha(S_\Delta(n,s))$ since the last term is strictly increasing in s, a contradiction. □

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

Corollary 3.2 ([8, 18]). *Let G be a unicyclic graph of order $n \ge 7$. Then for every $\alpha > 1$, ${}^0R_\alpha(G)$ 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 $n \ge 3$, $\lfloor n/2 \rfloor \le s \le n-2$ and G be a unicyclic graph of order n with independence number s. Then for every $\alpha \ge 1$, $\chi_\alpha(G)$ 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

$$\begin{aligned}\chi_\alpha(G) &\leq \chi_\alpha(S_\Delta(n - 1, s - 1)) + (s + 2)^\alpha + (s - 1)((s + 2)^\alpha - (s + 1)^\alpha) \\ &\quad + (s + 3)^\alpha - (s + 2)^\alpha \\ &= (n - s)(s + 2)^\alpha + (2s - n)(s + 1)^\alpha + (n - s - 2)3^\alpha + 4^\alpha \\ &\quad + (s - 1)((s + 2)^\alpha - (s + 1)^\alpha) + (s + 3)^\alpha.\end{aligned}$$

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

$$(n - s - 1)(s + 3)^\alpha + (n - s - 1)(s + 1)^\alpha \geq 2(n - s - 1)(s + 2)^\alpha. \tag{3.2}$$

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

$$\begin{aligned}\chi_\alpha(G) &= \chi_\alpha(G - x_1) + 3^\alpha + (d_3+2)^\alpha - (d_3+1)^\alpha \\ &\leq \chi_\alpha(S_\Delta(n-1,s)) + 3^\alpha + (s+3)^\alpha - (s+2)^\alpha \\ &= \chi_\alpha(S_\Delta(n,s)),\end{aligned}$$

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

$$\begin{aligned}\chi_\alpha(G) = \chi_\alpha(G - x_1) + (d_2+1)^\alpha + (d_2-3)((d_2+1)^\alpha - d_2^\alpha) + (d_2+d_3)^\alpha \\ - (d_2+d_3-1)^\alpha + (d_2+d_4)^\alpha - (d_2+d_4-1)^\alpha.\end{aligned}$$

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

$$\begin{aligned}(d_2+d_3)^\alpha - (d_2+d_3-1)^\alpha &\leq (s+3)^\alpha - (s+2)^\alpha; \\ (d_2+d_4)^\alpha - (d_2+d_4-1)^\alpha &\leq (s+3)^\alpha - (s+2)^\alpha.\end{aligned}$$

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

$$\begin{aligned}\chi_\alpha(G) &\leq \chi_\alpha(S_\Delta(n-1,s-1)) + (s+2)^\alpha + (s-2)((s+2)^\alpha - (s+1)^\alpha) \\ &\quad + 2(s+3)^\alpha - 2(s+2)^\alpha \\ &= (n-s)(s+2)^\alpha + (2s-n)(s+1)^\alpha + (n-s-2)3^\alpha + 4^\alpha \\ &\quad - (s+2)^\alpha + (s-2)((s+2)^\alpha - (s+1)^\alpha) + 2(s+3)^\alpha.\end{aligned}$$

This upper bound is less than or equal to $\chi_\alpha(S_\Delta(n,s))$ if and only if

$$(n-s-2)(s+3)^\alpha + (n-s-2)(s+1)^\alpha \geq 2(n-s-2)(s+2)^\alpha. \qquad (3.3)$$

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 $G_1 = G - vy + uy$. 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 $\chi_\alpha(H_n) = k\,6^\alpha + k\,4^\alpha$ for $n = 2k$ and $(k-1)6^\alpha + k\,4^\alpha + 2 \cdot 5^\alpha$ for $n = 2k+1$. We get

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

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 $k \geq 4$.

$$k(k+3)^\alpha + (k+2)^\alpha + (k-2)3^\alpha + 4^\alpha \geq k\,6^\alpha + k\,4^\alpha \tag{3.4}$$
$$(k+1)(k+3)^\alpha + (k-1)3^\alpha + 4^\alpha > (k-1)6^\alpha + k\,4^\alpha + 2 \cdot 5^\alpha \tag{3.5}$$

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 $\alpha \geq 1$ [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. □

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