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Maximum General Sum–Connectivity Index for Trees with Given Independence Number [1]

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Abstract

Das, Xu and Gutman [MATCH Commun. Math. Comput. Chem. 70(2013) 301-314] 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. In this paper, we show that in the same class of trees T, $S_{n,s}$ is the unique graph maximizing zeroth-order general Randić index ${}^0R_\alpha(T)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(T)$ for $\alpha \geq 1$. This property does not hold for general Randić index $R_\alpha(T)$ if $\alpha \geq 2$.

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 $\Delta(G)$. 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. The diameter of G is the maximum distance between vertices of G. If $x \in V(G)$, $G - x$ denotes the subgraph of G obtained by deleting x and its incident edges. A similar

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notation is $G - xy$, where $xy \in E(G)$. 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 $\alpha(G)$. $K_{1,n-1}$ and P_n will denote, respectively, the star and the path on n vertices. Since a tree on n vertices is a bipartite graph, at least one partite set, which is an independent set, has at least $n/2$ vertices, which implies that for any tree T we have $\alpha(T) \geq \lceil n/2 \rceil$ and this bound is reached for paths. Also, $\alpha(T) \leq n-1$ and the equality holds only for the star graph. For every $n \geq 2$ and $n/2 \leq s \leq n-1$ the spur $S_{n,s}$ [2] is a tree consisting of $2s - n + 1$ edges and $n - s - 1$ paths of length 2 having a common endvertex; in other words, it is obtained from a star $K_{1,s}$ by attaching a pendant edge to $n - s - 1$ pendant vertices of $K_{1,s}$. We have $\alpha(S_{n,s}) = s$. A bistar of order n, denoted by $BS(p, q)$, consists of two vertex disjoint stars, $K_{1,p}$ and $K_{1,q}$, where $p + q = n - 2$, and a new edge joining the centers of these stars.

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

The Randić index $R(G)$, proposed by Randić [12] in 1975, one of the most used molecular descriptors in structure-property and structure-activity relationship studies [5, 6, 9, 10, 11, 13, 14, 15], 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 Erdös [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 [18], 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 [17].

The zeroth-order general Randić index, denoted by ${}^0R_\alpha(G)$ was defined in [8] and [9] as

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

where α is a real number. For $\alpha = 2$ this index is also known as first Zagreb index and denoted by $M_1(G)$. Notice that $\chi_1(G) = {}^0R_2(G) = M_2(G)$.

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 [18].

Several extremal properties of the sum-connectivity and general sum-connectivity indices for trees, unicyclic graphs and general graphs were given in [3, 4, 17, 18].

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. In this paper, we further study the extremal properties of this graph, showing that $S_{n,s}$ is the unique graph maximizing zeroth-order general Randić index ${}^0R_\alpha(T)$ for $\alpha > 1$ and general sum-connectivity index $\chi_\alpha(T)$ for $\alpha \geq 1$ in the set of trees of order n and independence number s. This property is not still valid for general Randić index $R_\alpha(T)$ if $\alpha \geq 2$.

2 Main results

The zeroth-order general Randić index and general sum-connectivity index of $S_{n,s}$ are readily calculated:

$$^0R_\alpha(S_{n,s}) = s^\alpha + s(1-2^\alpha) + 2^\alpha(n-1);$$

$$\chi_\alpha(S_{n,s}) = (2s-n+1)(s+1)^\alpha + (n-s-1)((s+2)^\alpha + 3^\alpha).$$

The path P_n has independence number equal to $\lceil n/2 \rceil$.

Lemma 2.1. *Let $n \geq 5$ and $\alpha > 1$. The following inequalities hold:*

$$^0R_\alpha(S_{n,\lceil n/2\rceil}) > {}^0R_\alpha(P_n) \tag{1}$$

$$\chi_\alpha(S_{n,\lceil n/2\rceil}) > \chi_\alpha(P_n). \tag{2}$$

Proof. We get ${}^0R_\alpha(P_n) = (n-2)2^\alpha + 2$ and $\chi_\alpha(P_n) = (n-3)4^\alpha + 2\cdot 3^\alpha$. If n is even, $n = 2k$, (1) can be written as

$$k^\alpha - 2^\alpha k + k + 2^\alpha - 2 > 0, \tag{3}$$

where $k \geq 3$ and $\alpha > 1$. Consider the function $\varphi(x) = x^\alpha - 2^\alpha x + x$, where $x \geq 3$. We get $\varphi'(x) = \alpha x^{\alpha-1} - 2^\alpha + 1 \geq \alpha 3^{\alpha-1} - 2^\alpha + 1$. By letting $\psi(y) = y3^{y-1} - 2^y + 1$,

where $y > 1$, we have $\psi'(y) = 3^{y-1}(1 + y\ln 3) - \ln 2 \cdot 2^y$. Since $(\frac{3}{2})^y > 1.5$ we deduce $\psi'(y) > 2^y(\frac{1+y\ln 3}{2} - \ln 2) > 2^y(\frac{1+\ln 3}{2} - \ln 2) = 2^{y-1}\ln\frac{3e}{4} > 0$.
Because $\psi(1) = 0$ we have $\psi(y) > 0$, thus $\varphi(x)$ is strictly increasing for $x \geq 3$ and $\alpha > 1$. It follows that it is sufficient to prove (3) for $k = 3$. For $k = 3$ (3) becomes

$$3^\alpha - 2 \cdot 2^\alpha + 1 > 0, \tag{4}$$

where $\alpha > 1$. (4) can be deduced by Jensen inequality written for the function x^α, which is strictly convex for $\alpha > 1$.

If $n = 2k + 1$, where $k \geq 2$, we have $\alpha(P_{2k+1}) = k + 1$ and (1) becomes (3) in which $k \geq 3$ has been replaced by $k + 1 \geq 3$, which is true.

In order to prove (2) consider first the case n even, $n = 2k$. In this case (2) is

$$(k + 1)^\alpha + (k - 1)((k + 2)^\alpha + 3^\alpha) - (2k - 3)4^\alpha - 2 \cdot 3^\alpha > 0, \tag{5}$$

where $k \geq 3$ and $\alpha > 1$. For $k = 3$ (5) becomes $2 \cdot 5^\alpha - 2 \cdot 4^\alpha > 0$, which is true. Consider the function $\xi(x) = (x + 1)^\alpha + (x - 1)((x + 2)^\alpha + 3^\alpha) - 2 \cdot 4^\alpha x$, where $x \geq 3$. We get $\xi'(x) = \alpha(x + 1)^{\alpha-1} + (x + 2)^\alpha + 3^\alpha + \alpha(x + 2)^{\alpha-1}(x - 1) - 2 \cdot 4^\alpha$. We have $(x + 2)^\alpha + 3^\alpha - 2 \cdot 4^\alpha \geq 5^\alpha + 3^\alpha - 2 \cdot 4^\alpha > 0$ by Jensen inequality. This implies that $\xi'(x) > 0$, hence $\xi(x)$ is strictly increasing. Thus (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. ∎

The following observation will be useful.

Lemma 2.2. *Let T be a tree and $x \in V(T)$, which is adjacent to pendant vertices $v_1, \ldots v_r$. If $r \geq 2$ then any maximum independent subset of $V(T)$ contains $v_1, \ldots, v_r$.*

Theorem 2.3. *Let $n \geq 2$, $n/2 \leq s \leq n - 1$ and T be a tree of order n with independence number s. Then for every $\alpha > 1$, ${}^0R_\alpha(T)$ is maximum if and only if $T = S_{n,s}$.*

Proof. The proof is by induction on n. For $n = 2$ we get $s = 1$ and $S_{2,1} = P_2$ and for $n = 3$ we deduce $s = 2$ and $S_{3,2} = P_3$. For $n = 4$ we have two possible values for s: $s = 2$, when $S_{4,2} = P_4$ and $s = 3$, when $S_{4,3} = K_{1,3}$. These trees are unique for respective values of parameters n and s, therefore they are extremal.
Let $n \geq 5$ and suppose that the property is true for all trees of order $n - 1$. By Lemma

2.1 ${}^0R_\alpha(P_n)$ cannot be maximum. Since $n \geq 5$ we deduce $s \geq 3$. Suppose that $s = 3$. It follows that $n = 5$ or $n = 6$. For $n = 5$ we get only two trees of order 5 and independence number 3, namely P_5 and $S_{5,3}$ and for $n = 6$ we get P_6 and $S_{6,3}$. The theorem is verified in this case since P_5 and P_6 are not extremal. It follows that we can consider only the case when $\Delta(T) \geq 3$ and $s \geq 4$.

Let T be a tree of order $n \geq 5$ having $\Delta(T) \geq 3$ and independence number $s \geq 4$. As in [2] we shall consider a path $v_1, v_2, \ldots, v_{d+1}$ of maximum length in T, where d is the diameter of T. We can suppose that $d \geq 3$ since otherwise $T = K_{1,n-1}$, $s = n - 1$ and the theorem is verified. Both vertices v_1 and v_{d+1} are pendant. By letting $d(v_2) = d_2$, we obtain $s \geq \Delta(T) \geq d_2$.

First we consider the case when $\alpha(T - v_1) = \alpha(T) - 1$. By the induction hypothesis we can write

$$
\begin{aligned}
{}^0R_\alpha(T) &= {}^0R_\alpha(T - v_1) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\
&\leq {}^0R_\alpha(S_{n-1,s-1}) + 1 + d_2^\alpha - (d_2 - 1)^\alpha \\
&= (s-1)^\alpha + (s-1)(1 - 2^\alpha) + 2^\alpha(n-2) + 1 + d_2^\alpha - (d_2 - 1)^\alpha .
\end{aligned}
$$

Since the function $x^\alpha - (x-1)^\alpha$ is strictly increasing for $x \geq 1$ and $\alpha > 1$, it follows that $d_2^\alpha - (d_2 - 1)^\alpha \leq s^\alpha - (s-1)^\alpha$, equality holding if and only if $d_2 = s$.

It follows that ${}^0R_\alpha(T) \leq s^\alpha + s(1 - 2^\alpha) + 2^\alpha(n-1) = {}^0R_\alpha(S_{n,s})$ and equality holds if and only if $T - v_1 = S_{n-1,s-1}$ and pendant vertex v_1 is adjacent to a vertex of degree $s - 1$ in $S_{n-1,s-1}$. Since $s - 1 \geq 3$ it follows that for equality v_1 must be adjacent to the central vertex of the star $K_{1,s-1}$ of $S_{n-1,s-1}$. We deduce that $T = S_{n,s}$.

Next we assume that $\alpha(T - v_1) = \alpha(T)$. If v_2 would be adjacent to a vertex $w \neq v_1, v_3$, the degree of w cannot be greater than one, since in this case the path $v_1, \ldots, v_{d+1}$ has not maximum length in T. It follows that $d(w) = 1$ and by Lemma 2.2 every maximum independent set of vertices of T include both v_1 and w. This implies $\alpha(T - v_1) = \alpha(T) - 1$, which contradicts the hypothesis. It follows that $d_2 = 2$. We can write

$$
{}^0R_\alpha(T) = {}^0R_\alpha(T - v_1) + 2^\alpha \leq {}^0R_\alpha(S_{n-1,s}) + 2^\alpha = s^\alpha + s(1 - 2^\alpha) + 2^\alpha(n-1) = {}^0R_\alpha(S_{n,s}).
$$

The equality holds if and only if $T - v_1 = S_{n-1,s}$ and pendant vertex v_1 is adjacent to a pendant vertex of $S_{n-1,s}$. Let x be the vertex of degree s of $S_{n-1,s}$. If v_1 is adjacent to a pendant vertex v_2 of $S_{n-1,s}$ such that $d(v_2, x) = 2$, the resulting tree T has $\alpha(T) =$

$s+1$,which contradicts the hypothesis. We deduce that v_1 is adjacent to a pendant vertex which is adjacent to x, which implies that $T = S_{n,s}$. ■

A similar result holds for general sum-connectivity index.

Theorem 2.4. *Let $n \geq 2$, $n/2 \leq s \leq n-1$ and T be a tree of order n with independence number s. Then for every $\alpha \geq 1$, $\chi_\alpha(T)$ is maximum if and only if $T = S_{n,s}$.*

Proof. For $\alpha = 1$ we have $\chi_1(T) =^0 R_2(T)$ and by Theorem 2.3 the result holds true. Suppose that $\alpha > 1$. We shall use induction on n in the same way as in the proof of Theorem 2.3. By the same arguments and inequality (2) we can consider $n \geq 5$, $s \geq 4$, a tree T of order n and independence number s such that $\Delta(T) \geq 3$, and a path $v_1, v_2, \ldots, v_{d+1}$ of length d in T, where $d \geq 3$ is the diameter of T.
First we consider the case when $\alpha(T - v_1) = \alpha(T)$. As in the proof of Theorem 2.3 we deduce $d(v_2) = 2$ and $d(v_3) = d_3 \leq \Delta(T) \leq s$.
By the induction hypothesis we get

$$\chi_\alpha(T) = \chi_\alpha(T - v_1) + 3^\alpha + (d_3 + 2)^\alpha - (d_3 + 1)^\alpha$$

$$\leq (2s - n + 2)(s + 1)^\alpha + (n - s - 2)(s + 2)^\alpha + (n - s - 2)3^\alpha + 3^\alpha + (d_3 + 2)^\alpha - (d_3 + 1)^\alpha.$$

Since $d_3 \leq s$ we have $(d_3 + 2)^\alpha - (d_3 + 1)^\alpha \leq (s + 2)^\alpha - (s + 1)^\alpha$ and equality holds if and only if $d_3 = s$.

It follows that $\chi_\alpha(T) \leq (2s-n+1)(s+1)^\alpha+(n-s-1)(s+2)^\alpha+(n-s-1)3^\alpha = \chi_\alpha(S_{n,s})$ and equality holds if and only if $T - v_1 = S_{n-1,s}$, $d(v_2) = 2$ and $d_3 = s$, which implies that $T = S_{n,s}$.

Next we assume that $\alpha(T - v_1) = \alpha(T) - 1$. Since $v_1, v_2, v_3, \ldots, v_{d+1}$ is a path of maximum length of T, v_3 is the only vertex in $N(v_2)$ having degree $d_3 \geq 2$. By letting $d(v_2) = d_2 \leq s$ we have

$$\chi_\alpha(T) = \chi_\alpha(T - v_1) + (d_2 + 1)^\alpha + (d_2 - 2)((d_2 + 1)^\alpha - d_2^\alpha) + (d_2 + d_3)^\alpha - (d_2 + d_3 - 1)^\alpha.$$

The function $(x - 2)((x + 1)^\alpha - x^\alpha)$ being strictly increasing in x for $x \geq 2$ and $\alpha \geq 1$, we have $(d_2 - 2)((d_2 + 1)^\alpha - d_2^\alpha) \leq (s - 2)((s + 1)^\alpha - s^\alpha)$; also $(d_2 + 1)^\alpha \leq (s + 1)^\alpha$. v_2 is adjacent to $d_2 - 1$ pendant vertices and in the graph $T - v_2v_3$ the degree of v_3 is equal to $d_3 - 1$. It follows that $d_2 - 1 + d_3 - 1 \leq s$, or $d_2 + d_3 \leq s + 2$ since T has at least $d_2 + d_3 - 2$ pendant vertices. This implies $(d_2 + d_3)^\alpha - (d_2 + d_3 - 1)^\alpha \leq (s + 2)^\alpha - (s + 1)^\alpha$ with equality if and only if $d_2 + d_3 = s + 2$. By the induction hypothesis we have $\chi_\alpha(T - v_1) \leq \chi_\alpha(S_{n-1,s-1})$. Thus we get $\chi_\alpha(T) \leq (2s-n)s^\alpha + (n-s-1)(s+1)^\alpha + (n-s-1)3^\alpha + (s+1)^\alpha + (s-2)((s+1)^\alpha - s^\alpha) + (s+2)^\alpha - (s+1)^\alpha = (s+2)^\alpha + (n-3)(s+1)^\alpha + (s-n+2)s^\alpha + (n-s-1)3^\alpha$. By denoting the last expression by $E(n,s,\alpha)$, the inequality $E(n,s,\alpha) \leq \chi_\alpha(S_{n,s})$ is equivalent to

$$(n-s-2)(s+2)^\alpha + (n-s-2)s^\alpha \geq 2(n-s-2)(s+1)^\alpha. \tag{6}$$

If $s = n-1$ then $T = K_{1,n-1} = S_{n,n-1}$ and the theorem is true. If $s = n-2$ then (6) becomes an equality. Otherwise $n-s-2 \geq 1$ and (6) is equivalent to $(s+2)^\alpha + s^\alpha \geq 2(s+1)^\alpha$. By Jensen inequality this inequality is strict. It follows that if $\alpha(T-v_1) = \alpha(T)-1$ we have $\chi_\alpha(T) \leq \chi_\alpha(S_{n,s})$ and the equality holds only if $s = n-2, T - v_1 = S_{n-1,n-3}, d_2 = s$ and $d_2 + d_3 = s + 2$, i. e., $d_3 = 2$. It follows that the equality holds only if $T = S_{n,n-2}$ and the proof is complete.
Notice that only if $n - s - 1 \in \{0, 1\}$ a pendant vertex adjacent to the center of the star $K_{1,s}$ is the endvertex of a longest path in $S_{n,s}$, and this corresponds to the equality in (6). ■

In the family of trees T of order n and independence number s the second Zagreb index $M_2(G) = R_1(T)$ is maximum if and only if $T = S_{n,s}$ [2]. But this property does not hold for $R_\alpha(T)$ if $\alpha \geq 2$, since in [7] it was shown that for $\alpha \geq 2$ and $n \geq 8$, only the balanced double star $S(p,q)$, where $p + q = n - 2$ and $|p - q| \leq 1$ realizes the maximum value of $R_\alpha(T)$ in the set of trees of order n. The independence number of $S(p,q)$ is $n-2$, but $S_{n,n-2}$ is not a balanced double star.

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