Ordering Trees Having Small General Sum-Connectivity Index

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Abstract

The general sum-connectivity index of a graph $G$ is defined as $\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u)+d(v))^\alpha$, where $d(u)$ denotes the degree of vertex $u$ in $G$, and $\alpha$ is a real number. The aim of this paper is twofold. We determine the minimum value of the general sum-connectivity index:

(i) for trees of order $n \geq 3$ and diameter $d$, $2 \leq d \leq n-1$ and of trees of order $n \geq 5$ having $p$ pendant vertices, $3 \leq p \leq n-2$ and the corresponding extremal trees for $-1 \leq \alpha < 0$ and

(ii) for connected multigraphs of order $n \geq 3$ and size $m$, $m \geq n-1$ and the corresponding extremal multigraphs for $-3 \leq \alpha < 0$. Further, for $n$ sufficiently large and $-1 \leq \alpha < 0$, we characterize five $n$-vertex trees having smallest values of $\chi_\alpha$.

1. INTRODUCTION

Let $G$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, $N(u)$ denotes the set of its neighbors in $G$ and the degree of $u$ is $d(u) = d_G(u) = |N(u)|$. The Randić index $R(G)$, proposed by Randić [11] in 1975, is defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$
It is one of the most used molecular descriptors in structure-property and structure-activity relationship studies [6, 8, 10, 12]. The general Randić connectivity index (or general product-connectivity index), denoted by \( R_\alpha \), of \( G \) is defined as [1]:

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

where \( \alpha \) is a real number. Then \( R_{-1/2} \) is the classical Randić connectivity index.

The sum-connectivity index was proposed in [15] and both sum-connectivity index and Randić index correlate well with the \( \pi \)-electronic energy of benzenoid hydrocarbons [9]. This concept was extended to the general sum-connectivity index \( \chi_\alpha(G) \) in [16], which is defined as

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

where \( \alpha \) is a real number. Then \( \chi_{-1/2}(G) \) is the sum-connectivity index [15]. Several extremal properties of the sum-connectivity and general sum-connectivity index for trees, unicyclic graphs and general graphs were given in [3, 4, 15, 16]. Thus for a tree \( T \) with \( n \geq 4 \) vertices, it was shown in Proposition 3 of [16] that if \( \alpha > 0 \), then \( \chi_\alpha(T) \leq (n-1)n^\alpha \) and if \( \alpha < 0 \) then \( \chi_\alpha(T) \geq (n-1)n^\alpha \). The unique extremal graph is the \( n \)-vertex star \( S_n \) (also denoted by \( K_{1,n-1} \)) in both cases. In [15] the tree minimizing \( \chi_{-1/2} \) in the set of trees with \( n \geq 5 \) vertices and \( p \) pendant vertices was characterized, where \( 3 \leq p \leq n-2 \).

This result will be extended in section 3 for index \( \chi_\alpha \) with \(-1 \leq \alpha < 0\).

Another variant of the Randić index of a graph \( G \) is the harmonic index, denoted by \( H(G) \) and defined as

\[
H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} = 2\chi_{-1}(G).
\]

We have \( H(G) \leq R(G) \) by the inequality between arithmetic and geometric means, with equality if and only if \( G \) is a regular graph. This index first appeared in [5] and was studied for simple connected graphs and trees in [14]. We conclude this section with some notation and terminology.

For a simple connected graph \( G \) the distance between vertices \( u \) and \( v \) is the length of a shortest path between them. The diameter \( \text{diam}(G) \) of a graph \( G \) is the maximum distance between the vertices of \( G \), i.e., \( \text{diam}(G) = \max_{u,v \in V(G)} d(u,v) \). A shortest path of length \( \text{diam}(G) \) is called a diametral path of \( G \). For \( v \in V(G) \), \( G - v \) denotes the graph obtained from \( G \) by deleting \( v \) and the edges incident with \( v \). The path on \( n \) vertices is
denoted as $P_n$. A caterpillar is a tree with the property that deleting all pendant vertices the resulting graph is a path. For other notations in graph theory, we follow [2].

2. GRAPH TRANSFORMATIONS

In this section we shall define some graph transformations which strictly decrease the general sum-connectivity index in the case $-1 \leq \alpha < 0$. First we need a technical lemma.

Lemma 2.1. For every $-1 \leq \alpha < 0$ the function

$$f(x) = x(x + 2)^\alpha - x(x + 3)^\alpha - (x + 4)^\alpha$$

defined on the interval $[0, \infty)$ is strictly increasing.

Proof. It is necessary to show that $f'(x) > 0$ for every $x \in [0, \infty)$. By induction we easily deduce that the $n$-th derivative of $f$ equals

$$f^{(n)}(x) = (\alpha)_{n-1}[(x+2)^{\alpha-n}((\alpha+1)x+2n)-(x+3)^{\alpha-n}((\alpha+1)x+3n)-(\alpha-n+1)(x+4)^{\alpha-n}],$$

where $(\alpha)_n = \alpha(\alpha-1)\ldots(\alpha-n+1)$ and $(\alpha)_0 = 1$.

The function $(x + 2)^\alpha - (x + 3)^\alpha$ defined on $[0, \infty)$ is strictly decreasing for $\alpha < 0$ since its derivative equals $\alpha((x + 2)^{\alpha-1} - (x + 3)^{\alpha-1}) < 0$.

It follows that $(x + 2)^{\alpha-n} - (x + 3)^{\alpha-n} > (x + 3)^{\alpha-n} - (x + 4)^{\alpha-n}$, which implies that

$$f^{(n)}(x) > (\alpha(n)(x+1)+n)(x+3)^{\alpha-n} - ((\alpha+1)x + \alpha + n + 1)(x + 4)^{\alpha-n}. $$

Since $\alpha + 1 \geq 0$,

$$f^{(n)}(x) > 0 $$

is equivalent to

$$\left(\frac{x + 3}{x + 4}\right)^{\alpha-n} > \frac{(\alpha+1)x+\alpha+n+1}{(\alpha+1)x+n}.$$}

There exists an index $n_0$ such that this inequality is true, since for a fixed $x \geq 0$ we have $\lim_{n \to \infty} \frac{x + 3}{x + 4} = \frac{3}{4}$ and the right-hand side tends to 1 as $n \to \infty$. We also deduce $\lim_{n \to \infty} f^{(n)}(x) = 0$ for any $n \in \mathbb{N}$. Suppose that $n_0$ is even. Then $(\alpha)_{n_0-1}$ is negative, which implies that $f^{(n_0)}(x) < 0$ for any $x \in [0, \infty)$. We deduce that $f^{(n_0-1)}(x)$ is strictly decreasing and since $\lim_{n \to \infty} f^{(n_0-1)}(x) = 0$ this implies that $f^{(n_0-1)}(x) > 0$ for $x \in [0, \infty)$. By induction we deduce that for any $n \leq n_0$, $f^{(n)}(x) > 0$ for odd $n$ and $f^{(n)}(x) < 0$ for even $n$ for any $x \in [0, \infty)$. In particular, $f'(x) > 0$. The same conclusion follows if $n_0$ is odd. ■
Let $u$ and $v$ be two adjacent vertices of a graph $G$ such that $N(u) = \{v, z_1, \ldots, z_p\}$, $N(v) = \{u, w_1, \ldots, w_s\}$, where $\{z_1, \ldots, z_p\} \cap \{w_1, \ldots, w_s\} = \emptyset$, $p \geq 0$ and $s \geq 1$. We define a graph denoted by $t_1(G)$ by removing edges $vw_1, vw_2, \ldots, vw_s$ and adding new edges $uw_1, uw_2, \ldots, uw_s$. We say that $t_1(G)$ is a $t_1-$ transform of $G$ (see Fig. 1).

**Lemma 2.2.** [3] For a graph $G$ denote $G' = t_1(G)$. If $\alpha < 0$ then $\chi_\alpha(G') < \chi_\alpha(G)$ and if $\alpha > 0$ then the inequality is reversed.

**Proof.** We have $d_{G'}(u) = d_G(u) + s > d_G(u)$ and $d_{G'}(u) + d_{G'}(v) = d_G(u) + d_G(v) = p + s + 2$. Since $\alpha < 0$ we get

$$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{i=1}^{p} [(d_G(z_i) + d_G(u) + s)^\alpha - (d_G(z_i) + d_G(u))^\alpha] + \sum_{i=1}^{s} [(d_G(w_i) + d_G(u) + s)^\alpha - (d_G(w_i) + s + 1)^\alpha] < 0,$$

since $\alpha < 0$ and the degrees of the vertices $z_1, \ldots, z_p, w_1, \ldots, w_s$ remain unchanged. $

Other transformations are described below.

**Lemma 2.3.** For trees $G$ and $G'$ from Fig. 2, where $d_G(w, t) \geq 1$ we have $\chi_\alpha(G) > \chi_\alpha(G')$ for any $p, q, r \geq 1$ and $-1 \leq \alpha < 0$.

**Proof.** It is easily seen that:

$$\chi_\alpha(G) - \chi_\alpha(G') = p(p + 2)^\alpha + r(r + 3)^\alpha + (r + q + 3)^\alpha - (p + r)(p + r + 2)^\alpha - (q + 3)^\alpha = r(r + 3)^\alpha + F(p) + G(q),$$

where $F(p) = p(p + 2)^\alpha - (p + r)(p + r + 2)^\alpha$ and $G(q) = (r + q + 3)^\alpha - (q + 3)^\alpha$.

We obtain $F'(p) = (p+2+p\alpha)(p+2)^{\alpha-1}-(p+r+\alpha(p+r)+2)(p+r+2)^{\alpha-1} = g(p)-g(p+r)$, by denoting $g(x) = (x+\alpha x + 2)(x+2)^{\alpha-1}$.

Also $g'(x) = \alpha(x+2)^{\alpha-2}(x(\alpha+1)+4) < 0$ for every $x > 0$ and $-1 \leq \alpha < 0$. It follows that $F'(p) > 0$, which implies that $F(p)$ is strictly increasing. Since $G'(q) =$
\[ \alpha[(r + q + 3)^{\alpha - 1} - (q + 3)^{\alpha - 1}] > 0 \] for \( \alpha < 0 \) we get that \( G(q) \) is also strictly increasing.

We can write \( \chi_{\alpha}(G) - \chi_{\alpha}(G') \geq r(r + 3)^{\alpha} + F(1) + G(1) = (r + 4)^{\alpha} - (r + 3)^{\alpha} + 3^\alpha - 4^\alpha. \)

Consider the function \( h(x) = (x + 4)^{\alpha} - (x + 3)^{\alpha} \). We get \( h'(x) = \alpha[(x + 4)^{\alpha - 1} - (x + 3)^{\alpha - 1}] > 0 \), which implies \( h(r) \geq h(1) = 5^\alpha - 4^\alpha \) for \( x \geq 1 \).

It remains to show that \( 5^\alpha + 3^\alpha > 2 \cdot 4^\alpha \). This inequality can be deduced by Jensen’s inequality since the function \( x^\alpha \) is strictly convex for \(-1 \leq \alpha < 0\).

**Lemma 2.4.** Consider two trees \( G \) and \( G' \) from Fig. 3, where \( d_G(u, v) = d_{G'}(u, v) \geq 2 \) and \( d_G(w, t) = d_{G'}(w, t) \geq 0 \). If \( p, q, r \geq 1 \) and \(-1 \leq \alpha < 0\) then \( \chi_{\alpha}(G) > \chi_{\alpha}(G') \).

**Proof.** As for the previous lemma we get:

\[ \chi_{\alpha}(G) - \chi_{\alpha}(G') = p(p + 2)^{\alpha} + (p + 3)^{\alpha} + r(r + 3)^{\alpha} + (r + 4)^{\alpha} + (r + q + 3)^{\alpha} - (p + r)(p + r + 2)^{\alpha} - (p + r + 3)^{\alpha} - (q + 3)^{\alpha} - 4^\alpha. \]

By denoting \( f(p) = (p + 3)^{\alpha} - (p + r + 3)^{\alpha} + p(p + 2)^{\alpha} - (p + r)(p + r + 2)^{\alpha} \) and \( g(q) = (r + q + 3)^{\alpha} - (q + 3)^{\alpha} \), it follows that

\[
\chi_{\alpha}(G) - \chi_{\alpha}(G') = f(p) + g(q) + (r + 4)^{\alpha} + r(r + 3)^{\alpha} - 4^\alpha. \tag{1}
\]

Since \( g'(q) > 0 \) for any \(-1 \leq \alpha < 0\) we can write \( g(q) \geq g(1) = (r + 4)^{\alpha} - 4^\alpha \). For \( f(p) \) we get \( f'(p) = h(p) - h(p + r) \) by denoting \( h(p) = \alpha(p + 3)^{\alpha - 1} + (p + 2)^{\alpha} + \alpha p + (p + 2)^{\alpha - 1} \).

We obtain \( h'(p) = \alpha[(\alpha - 1)(p + 3)^{\alpha - 2} + (4 + (\alpha + 1)p)(p + 2)^{\alpha - 2}] \).

The expression \((\alpha - 1)(p + 3)^{\alpha - 2} + (4 + (\alpha + 1)p)(p + 2)^{\alpha - 2} \geq (\alpha - 1)(p + 3)^{\alpha - 2} + 4(p + 3)^{\alpha - 2} = (\alpha + 3)(p + 3)^{\alpha - 2} > 0\), thus implying \( h'(p) < 0 \). We have deduced \( f'(p) > 0 \), hence \( f(p) \geq f(1) = 4^\alpha - (r + 4)^{\alpha} + 3^\alpha - (r + 1)(r + 3)^\alpha \).

From (1) we can write

\[ \chi_{\alpha}(G) - \chi_{\alpha}(G') \geq (r + 4)^{\alpha} - (r + 3)^{\alpha} + 3^\alpha - 4^\alpha > 0 \]

since \( r \geq 1 \), function \((r + 4)^{\alpha} - (r + 3)^{\alpha}\) is strictly increasing for \( r \geq 0 \) and \( \alpha \geq -1 \).
Lemma 2.5. Let $G$ and $G'$ be trees from Fig. 4, where $d_G(u,v) \geq 1$. If $-1 \leq \alpha < 0$ and $p \geq q \geq 2$ then $\chi_\alpha(G) > \chi_\alpha(G')$.

Proof. If $d_G(u,v) = 1$ then $d_G(u) + d_G(v) = p + q + 2$, and

$$\chi_\alpha(G) - \chi_\alpha(G') = p(p + 2)\alpha + q(q + 2)\alpha - (p + 1)(p + 3)\alpha - (q - 1)(q + 1)\alpha.$$ 

By denoting $p = q + r$, where $r \geq 0$, it is necessary to prove that

$$(q + r)(q + r + 2)\alpha - (q + r + 1)(q + r + 3)\alpha + q(q + 2)\alpha - (q - 1)(q + 1)\alpha > 0, \quad (2)$$

or $g(q) > g(q + r + 1)$, where $g(q) = q(q + 2)\alpha - (q - 1)(q + 1)\alpha$.

We deduce $g'(q) = (4\alpha + \alpha(q + 1)\alpha)q(2)\alpha - 1 - (q + 1 + \alpha(q - 1))(q + 1)\alpha - 1 = h(q) - h(q - 1)$, where $h(q) = (q + 2 + \alpha q)(q + 2)\alpha - 1$.

Finally, $h'(q) = (4\alpha + \alpha(1 + \alpha)q)(q + 2)\alpha - 2 < 0$ since $-1 \leq \alpha < 0$.

Consequently, $h(q) - h(q - 1) < 0$, which implies $g'(q) < 0$. Since $g'$ is strictly decreasing we have $g(q) > g(q + r + 1)$ and (2) is proved.

If $d_G(u,v) \geq 2$ then $\chi_\alpha(G) - \chi_\alpha(G') = p(p + 2)\alpha - p(p + 3)\alpha - (p + 4)\alpha - (q - 1)(q + 1)\alpha + (q - 1)(q + 2)\alpha + (q + 3)\alpha = f(p) - f(q - 1)$, where $f(x) = x(x + 2)\alpha - x(x + 3)\alpha - (x + 4)\alpha$.

By Lemma 2.1 $f(x)$ is strictly increasing for $x \geq 0$, which implies $f(p) > f(q - 1)$.
3. MINIMUM VALUE OF $\chi_\alpha$ ($-1 \leq \alpha < 0$) FOR TREES OF GIVEN DIAMETER

Let $d \geq 3$. We shall denote by $MS(n_1, n_2, \ldots, n_{d-1})$ where $n_1, n_{d-1} \geq 1$ and $n_i \geq 0$ for $2 \leq i \leq d - 2$, the caterpillar consisting of a path $v_1, v_2, \ldots, v_{d-1}$ of length $d - 2$ with $n_i$ pendant vertices attached at $v_i$ for $1 \leq i \leq d - 1$. It has diameter equal to $d$. This multistar may also be obtained by joining by edges the centers of stars $K_{1,n_1}, K_{1,n_2}, \ldots, K_{1,n_{d-1}}$. Note that every tree of order $n$ and diameter three is a bistar $MS(n_1, n_2)$ (denoted by $BS(n_1, n_2)$ in [13]), where $n_1, n_2 \geq 1$ and $n_1 + n_2 = n - 2$. Observe that $MS(n_1, n_2, \ldots, n_{d-1})$ is isomorphic to $MS(n_{d-1}, n_{d-2}, \ldots, n_1)$. The multistar with $d = n - p + 1$, $n_1 = p - 1$, $n_2 = \ldots = n_{d-2} = 0$ and $n_{d-1} = 1$ has $p$ pendant vertices and order $n$ and was denoted by $S_{n,p}$ in [15]. Equivalently, for every integers $n, p$ with $2 \leq p \leq n - 1$, $S_{n,p}$ is the tree formed by attaching $p - 1$ pendant vertices to an end vertex of the path $P_{n-p+1}$. We have $S_{n,2} = P_n$ and $S_{n,n-1}$ is the star $K_{1,n-1}$. $S_{n,p}$ has diameter equal to $n - p + 1$.

**Theorem 3.1.** For every $-1 \leq \alpha < 0$ in the set of trees $T$ having order $n \geq 3$ and $\text{diam}(T) = d$ ($2 \leq d \leq n - 1$), $\chi_\alpha(T)$ is minimum if and only if $T = S_{n,n-d+1}$.

**Proof.** Using the $t_1-$ transform in Lemma 2.2 at vertices not belonging to a diametral path of $T$, we can deduce that among $n$-vertex trees $T$ with diameter $d$, the minimum of $\chi_\alpha(T)$ is achieved exactly in the set of multistars $MS(n_1, n_2, \ldots, n_{d-1})$.

Applying transformations described in Lemmas 2.3 – 2.5 it follows that minimum of $\chi_\alpha(T)$ is achieved only for $n_1 = n - d$, $n_2 = n_3 = \ldots = n_{d-2} = 0$ and $n_{d-1} = 1$, i.e., for $S_{n,n-d+1}$.

**Corollary 3.2.** Let $-1 \leq \alpha < 0$. (a) In the set of trees $T$ of order $n$ we have

$$\min_{\text{diam}(T) = i} \chi_\alpha(T) < \min_{\text{diam}(T) = j} \chi_\alpha(T)$$

if $2 \leq i < j \leq n - 1$.

(b) In the set of trees $T$ of order $n$ and diameter $d$ with $3 \leq d \leq n - 2$ the trees having smallest general sum-connectivity index $\chi_\alpha(T)$ are (in this order):

$MS(n-d, 0, \ldots, 0, 1), MS(n-d-1, 0, \ldots, 0, 2), \ldots, MS(\lceil \frac{n-d+1}{2} \rceil, 0, \ldots, 0, \lfloor \frac{n-d+1}{2} \rfloor)$.

**Proof.** (a) This inequality follows from Lemma 2.2 since $MS(n-i, 0, \ldots, 0, 1)$ can be obtained from $MS(n-j, 0, \ldots, 0, 1)$ applying several times the $t_1-$ transform.
Figure 5: Five trees \( T \) having smallest \( \chi_\alpha(T) \) for \(-1 \leq \alpha < 0\).

(b) This ordering can be deduced using Lemmas 2.2 – 2.4 and then making use of Lemma 2.5 to multistars of order \( n \) \( MS(p, 0, \ldots, 0, q) \) with \( p + q = n - d + 1 \).

**Theorem 3.3.** For every \(-1 \leq \alpha < 0\) there exists \( n_0(\alpha) > 0 \) such that for every \( n \geq n_0(\alpha) \) the trees \( T \) having the smallest \( \chi_\alpha(T) \) are \( K_{1,n-1}, BS(n-3, 1), BS(n-4, 2), S_{n,n-3} \) and \( BS(n-5, 3) \) (in this order). Also we have \( n_0(-1) = 16 \).

**Proof.** The unique tree having diameter two is the star \( K_{1,n-1} \) and by Corollary 3.2 it reaches the minimum of \( \chi_\alpha \). The second minimum value of \( \chi_\alpha \) is achieved for \( S_{n,n-2} = BS(n-3, 1) \), which minimizes this index in the set of trees of diameter three.

The next minimum values in the set of trees of diameter three are reached by \( BS(n-4, 2) \) (which coincides to \( BS(n-3, 1) \) for \( n = 5 \)) and \( BS(n-5, 3) \) and the minimum value of \( \chi_\alpha \) in the set of trees of diameter four by \( S_{n,n-3} \).

We get \( \chi_\alpha(BS(n-4, 2)) < \chi_\alpha(S_{n,n-3}) \) since \( BS(n-4, 2) \) can be obtained from \( S_{n,n-3} \) by a \( t_1 \)- transform. It follows that for every \( n \geq 6 \) the trees having minimum values of \( \chi_\alpha \) are \( K_{1,n-1}, BS(n-3, 1) \) and \( BS(n-4, 2) \).

In order to obtain the fourth term in this sequence it is necessary to compare \( \chi_\alpha(BS(n-5, 3)) \) with \( \chi_\alpha(S_{n,n-3}) \). We get

\[
\chi_\alpha(BS(n-5, 3)) - \chi_\alpha(S_{n,n-3}) = (n-5)(n-3)^\alpha + n^\alpha - (n-4)(n-2)^\alpha - (n-1)^\alpha + 3 \cdot 5^\alpha - 4^\alpha - 3^\alpha
\]

and

\[
\lim_{n \to \infty} ((n-5)(n-3)^\alpha + n^\alpha - (n-4)(n-2)^\alpha - (n-1)^\alpha) = 0 \quad \text{since} \quad \alpha < 0.
\]

We shall
prove that $3 \cdot 5^\alpha - 4^\alpha - 3^\alpha \geq \frac{1}{60}$.

For this consider the function $\varphi(x) = 3 \cdot 5^x - 4^x - 3^x$ defined for $-1 \leq x < 0$. Since
\[
\varphi^{(m)}(x) = (\ln 5)^n \left[ 3 \cdot 5^x - 4^x \left( \frac{\ln 4}{\ln 5} \right)^n - 3^x \left( \frac{\ln 3}{\ln 5} \right)^n \right],
\]
there exists an index $m$ such that $\varphi^{(m)}(x) > 0$.

This means that $\varphi^{(m-1)}(x)$ is strictly increasing on $[-1, 0)$, hence $\varphi^{(m-1)}(x) > \varphi^{(m-1)}(-1) = \frac{3}{5}(\ln 5)^{m-1} - \frac{1}{4}(\ln 4)^{m-1} - \frac{1}{3}(\ln 3)^{m-1} > (\ln 5)^{m-1}(\frac{3}{5} - \frac{1}{4} - \frac{1}{3}) > 0$. By induction it follows that $\varphi(x)$ is strictly increasing for $x \in [-1, 0)$ and we deduce that $\varphi(x) \geq \varphi(-1) = \frac{3}{5} - \frac{1}{4} - \frac{1}{3} = \frac{1}{60}$.

It follows that $\lim_{n \to \infty} (\chi(\alpha)(BS(n-5, 3)) - \chi(\alpha)(S_{n,n-3})) = 3 \cdot 5^\alpha - 4^\alpha - 3^\alpha \geq \frac{1}{60}$, which means that there exists $n_0(\alpha)$ such that $\chi(\alpha)(BS(n-5, 3)) > \chi(\alpha)(S_{n,n-3})$ for every $n \geq n_0(\alpha)$.

If $\alpha = -1$ (corresponding to the harmonic index), the difference
\[
\chi_{-1}(BS(n-5, 3)) - \chi_{-1}(S_{n,n-3}) = \frac{n - 5}{n - 3} - \frac{n - 4}{n - 2} - \frac{1}{n(n - 1)} + \frac{1}{60}
\]
is negative for $n \leq 15$ but becomes positive for $n \geq 16$.

We also have
\[
\chi(\alpha)(BS(n-5, 3)) - \chi(\alpha)(MS(n-5, 0, 2)) = n^\alpha - (n - 2)^\alpha + 2(5^\alpha - 4^\alpha) < 0
\]
for every $n \geq 3$ and $\alpha < 0$, where $MS(n-5, 0, 2)$ realizes the second minimum value of $\chi(\alpha)$ in the set of trees of diameter four after $S_{n,n-3}$. Using a $t_1$- transform it can be easily seen that the tree $MS(n-5, 0, 0, 1)$, reaching minimum of $\chi(\alpha)$ in the set of trees of diameter five obeys $\chi(\alpha)(MS(n-5, 0, 0, 1)) > \chi(\alpha)(MS(n-5, 0, 2))$, which concludes the proof.

Note that for $\alpha = -1/2$ first three trees from Fig. 5 having smallest $\chi(\alpha)$ index were found in [15]. Another extremal property of the tree $S_{n,p}$ is the following, which extends the corresponding property given in [15] from $\alpha = -1/2$ to $-1 \leq \alpha < 0$.

**Theorem 3.4.** Let $T$ be a tree with $n \geq 5$ vertices and $p$ pendent vertices, where $3 \leq p \leq n - 2$ and $-1 \leq \alpha < 0$. Then
\[
\chi(\alpha)(T) \geq (p - 1)(p + 1)^\alpha + (p + 2)^\alpha + 3^\alpha + (n - p - 2)4^\alpha
\]
with equality if and only if $T = S_{n,p}$.

**Proof.** First we shall prove that under the assumption of the theorem, if $u$ is a pendent vertex being adjacent to $v$, then
\[
\chi(\alpha)(T) - \chi(\alpha)(T - u) \geq (p - 2)(p + 1)^\alpha + (p + 2)^\alpha - (p - 2)p^\alpha
\]
with equality if and only if $T = S_{n,p}$ and $d(v) = p$.
Note that $N(v) \setminus \{u\}$ contains some vertex $w_0$ of degree $d(w_0) \geq 2$ since otherwise $T$ is a star with center $v$ having $p = n - 1$ pendant vertices, which contradicts the hypothesis. We obtain
\[
\chi_\alpha(T) - \chi_\alpha(T - u) = (d(v) + 1)^\alpha - \sum_{w \in N(v) \setminus \{u\}} [(d(v) + d(w) - 1)^\alpha - (d(v) + d(w))^\alpha].
\]
Since the function $f(x) = (x - 1)^\alpha - x^\alpha$ is strictly decreasing for $x \geq 1$ and $\alpha < 0$ we have $(d(v) + d(w_0) - 1)^\alpha - (d(v) + d(w_0))^\alpha \leq (d(v) + 1)^\alpha - (d(v) + 2)^\alpha$ and for all other $d(v) - 2$ vertices $w \in N(v) \setminus \{u, w_0\}$ we deduce $(d(v) + d(w) - 1)^\alpha - (d(v) + d(w))^\alpha \leq (d(v))^\alpha - (d(v) + 1)^\alpha$ because $d(w) \geq 1$. It follows that
\[
\chi_\alpha(T) - \chi_\alpha(T - u) \geq (d(v) + 1)^\alpha - [(d(v) + 1)^\alpha - (d(v) + 2)^\alpha] - (d(v) - 2)[d(v)^\alpha - (d(v) + 1)^\alpha] = (d(v) + 2)^\alpha + (d(v) - 2)(d(v) + 1)^\alpha - (d(v) - 2)d(v)^\alpha.
\]
We also have $d(v) \leq p$ since $T - v$ consists of $d(v)$ trees. Making use of Lemma 2.1 the function $g(x) = (x + 2)^\alpha + (x - 2)(x + 1)^\alpha - (x - 2)x^\alpha$ is strictly decreasing for $-1 \leq \alpha < 0$ and $x \geq 2$ since $-g(x)$ is strictly increasing. Since $2 \leq d(v) \leq p$ this implies
\[
\chi_\alpha(T) - \chi_\alpha(T - u) \geq (p - 2)(p + 1)^\alpha + (p + 2)^\alpha - (p - 2)p^\alpha.
\]
Equality holds if and only if we have $d(v) = p$, one neighbor of $v$ has degree two, and others are pendant vertices, i.e., $T = S_{n,p}$ and $u$ is adjacent to the vertex of degree $p$ of $S_{n,p}$.

Now the proof of the theorem follows by induction on $n$. For $n = 5$ we get $p = 3$ and $S_{5,3} = BS(1,2)$ from Fig. 5 is a single tree of order five having three pendant vertices.

Let $n \geq 6$ and suppose that the theorem is true for all trees of order $n - 1$ having $p$ pendant vertices, where $3 \leq p \leq n - 3$. Let $u$ be a pendant vertex adjacent to the vertex $v$. We shall consider two subcases: $A. d(v) = 2$ and $B. d(v) \geq 3$.

$A$. In this case the unique vertex $w$ adjacent to $v$ has $d(w) \geq 2$, which implies
\[
\chi_\alpha(T) - \chi_\alpha(T - u) = (d(w) + 2)^\alpha + 3^\alpha - (d(w) + 1)^\alpha \geq 4^\alpha
\]
which follows by induction hypothesis, for $p \leq n - 3$ we have $\chi_\alpha(T - u) \geq \chi_\alpha(S_{n-1,p})$ with equality if and only if $T - u = S_{n-1,p}$. In this case
\[
\chi_\alpha(T) \geq \chi_\alpha(T - u) + 4^\alpha \geq \chi_\alpha(S_{n-1,p}) + 4^\alpha = \chi_\alpha(S_{n,p})
\]
and equality holds if and only if $T - u = S_{n-1,p}$ and $d(v) = d(w) = 2$, i.e., $T = S_{n,p}$.
If \( p = n - 2 \), \( T - u \) has \( n - 1 \) vertices, and \( n - 2 \) pendant vertices, i.e., \( T - u = K_{1,n-1} \) and \( T = S_{n,n-2} = S_{n,p} \).

B. If \( d(v) \geq 3 \) then \( T - u \) has \( n - 1 \) vertices and \( p - 1 \) pendant vertices. Using the induction hypothesis for \( T - u \) and the above property we get \( \chi_\alpha(T) \geq \chi_\alpha(T - u) + (p - 2)(p + 1)^\alpha + (p + 2)^\alpha - (p - 2)p^\alpha \geq \chi_\alpha(S_{n-1,p-1}) + (p - 2)(p + 1)^\alpha + (p + 2)^\alpha - (p - 2)p^\alpha = \chi_\alpha(S_{n,p}) \).

Equality holds if and only if \( T - u = S_{n-1,p-1} \) and \( d(v) = p \), i.e., \( T = S_{n,p} \).

\section{4. Minimum Value of \( \chi_\alpha (\alpha \leq -3 < 0) \) for Multigraphs}

The index \( \chi_\alpha(G) \) may be defined in the same way when \( G \) is a multigraph containing parallel edges.

\textbf{Theorem 4.1.} Let \( m, n \in \mathbb{N} \) such that \( n \geq 3, m \geq n - 1 \) and \( -3 \leq \alpha < 0 \). If \( G \) is a connected multigraph with \( n \) vertices and \( m \) edges, then

\[ \chi_\alpha(G) \geq (n - 2)(m + 1)^\alpha + (m - n + 2)(2m - n + 2)^\alpha \]

with equality if and only if \( G \) is \( K_{1,n-1} \) having one edge of multiplicity \( m - n + 2 \) and \( n - 2 \) edges of multiplicity 1.

\textbf{Proof.} For any multigraph \( G \) we shall define the \( t_2 \)-transform relatively to the pair \( \{u, v\} \) of adjacent vertices from \( V(G) \) such that \( N(u) \neq \{v\} \) and \( N(v) \neq \{u\} \). Suppose that \( N(u) \setminus N(v) = \{v\} \cup \{z_1, \ldots, z_p\}; N(v) \setminus N(u) = \{u\} \cup \{w_1, \ldots, w_s\} \) and \( N(u) \cap N(v) = \{x_1, \ldots, x_r\} \), where \( p, r, s \geq 0 \) and \( p + r \geq 1, s + r \geq 1 \).

We swap all edges \( x_1v, \ldots, x_rv, w_1v, \ldots, w_sv \) incident to \( v \) from \( v \) to \( u \), making them incident to \( u \) and preserving their multiplicities. If \( m_{G}(xy) \) denotes the multiplicity of an edge \( xy \) in \( G \), this means that in the graph \( G_1 = t_2(G) \) thus obtained \( v \) is adjacent only to \( u \) and \( m_{G_1}(uw_i) = m_{G}(vw_i) \) for every \( 1 \leq i \leq s \), \( m_{G_1}(ux_i) = m_{G}(ux_i) + m_{G}(vx_i) \) for every \( 1 \leq i \leq r \).

We have \( d_{G_1}(v) = m_{G}(uv), m_{G_1}(uv) = m_{G}(uv) \), hence \( d_{G_1}(u) + d_{G_1}(v) = d_{G}(u) + d_{G}(v) \).

This transformation is illustrated in Fig. 6 when \( G \) does not contain parallel edges.

By this transformation only degrees of vertices \( u \) and \( v \) are changed. We can write

\[ d_{G}(u) \geq m_{G}(uv) + p + r \geq m_{G}(uv) + 1. \]

We deduce \( d_{G_1}(u) = d_{G}(u) + d_{G}(v) - m_{G}(uv) \geq d_{G}(v) + 1 \) and also \( d_{G_1}(u) \geq d_{G}(u) \).

It follows that for all edges \( xy \), invariant or transformed, the sum of degrees increases
or remains constant in $G_1$ and for at least one edge the increment is positive. We get $\chi_{\alpha}(G) > \chi_{\alpha}(G_1)$.

Let $G$ be a connected multigraph of order $n$ and size $m \geq n - 1$ such that $\chi_{\alpha}(G)$ is minimum and let $uw \in E(G)$. If $N(u) \neq \{v\}$ and $N(v) \neq \{u\}$ we have seen that $\chi_{\alpha}(G)$ cannot be minimum, thus yielding $N(u) = \{v\}$ or $N(v) = \{u\}$. Suppose that $N(v) = \{u\}$; for any edge $uz$ of $G$ incident to $u$ we also have $N(z) = \{u\}$. Since $G$ is connected we obtain that $G$ is $K_{1,n-1}$ containing some parallel edges, such that the size of $G$ is $m$. Let $w$ be the center of $K_{1,n-1}$. If there exist two vertices $u, v \neq w$ such that $m(uw) = p$, $m(vw) = q$ and $p \geq q \geq 2$, we shall prove that $\chi_{\alpha}(G)$ cannot be minimum. For this we shall define another graph $G_2$ which is obtained by transforming one parallel edge between $w$ and $v$ into a parallel edge between $w$ and $u$, such that $d_{G_2}(u) = p + 1$, $d_{G_2}(v) = q - 1$ and other degrees remain unchanged. If $d(w) = p + q + s$ and $s \geq 0$ we get

$$\chi_{\alpha}(G_2) - \chi_{\alpha}(G) = (p+1)(2p+q+s+1)^{\alpha} - (q-1)(p+2q+s-1)^{\alpha} - p(2p+q+s)^{\alpha} - q(p+2q+s)^{\alpha}.$$ 

We shall prove that if $-3 \leq \alpha < 0$ then $\chi_{\alpha}(G_2) - \chi_{\alpha}(G) < 0$, which is equivalent to

$$(p+1)(2p+q+s+1)^{\alpha} - p(2p+q+s)^{\alpha} < q(p+2q+s)^{\alpha} - (q-1)(p+2q+s-1)^{\alpha}. \quad (3)$$

Consider the function $f(x) = (x+1)(x+a+1)^{\alpha} - x(x+a)^{\alpha}$, where $x > 0$ and $a > x$. We have $f'(x) = \varphi(x+1) - \varphi(x)$, where $\varphi(x) = (x+a+\alpha x)(x+a)^{\alpha-1}$. Since $-3 \leq \alpha < 0$ and $a > x$ one obtains $\varphi'(x) = \alpha(x+a)^{\alpha-2}(2a + x + \alpha x) < 0$, thus implying that $\varphi$ is strictly decreasing on $(0, \infty)$, hence $f'(x) < 0$, or $f(x)$ is strictly decreasing on $(0, \infty)$.

Consequently, $f(p) < f(q-1)$ for any $a > p$ since $p > q - 1$ and we can write $(p+1)(p+a+1)^{\alpha} - p(p+a)^{\alpha} < q(q+a)^{\alpha} - (q-1)(q-1+a)^{\alpha}$. Letting $a = p + q + s > p$ this inequality becomes (3).

Consequently, if $\chi_{\alpha}(G)$ is minimum then only one vertex different from $w$ has degree equal
to \( m - n + 2 \) and other non-central vertices have degree equal to 1, whenever

\[
\chi_\alpha(G) = (n - 2)(m + 1)^\alpha + (m - n + 2)(2m - n + 2)^\alpha.
\]

If \( m = n - 1 \) then \( G \) is a tree and \( \min \chi_\alpha(G) \) is reached if and only if \( G \) is \( K_{1,n - 1} \), which does not contain parallel edges. This result holds for trees in a more general setting when \( \alpha < 0 \) [16].

Denote by \( M_{k,m}(K_{1,n - 1}) \) the set of multigraphs of size \( m \geq n + k - 1 \) deduced from \( K_{1,n - 1} \) by considering \( k \) multiple edges and \( n - 1 - k \) simple edges for \( 1 \leq k \leq n - 1 \). Denote also by \( (d_1, \ldots, d_k, 1, \ldots, 1) \) with \( d_1 \geq d_2 \geq \ldots \geq d_k \geq 2 \) the vector of degrees of non-central vertices, where \( \sum_{i=1}^{k} d_i = m - n + k + 1 \).

From this proof it follows that if \( m \geq n + k - 1 \) then the multigraph \( G \) of order \( n \) and size \( m \) having \( k \) multiple edges and minimum general sum-connectivity index belongs to \( M_{k,m}(K_{1,n - 1}) \), it is unique and has the vector of degrees \( (m - n - k + 3, 2, \ldots, 2, 1, \ldots, 1) \).

Also

\[
\min_{G \in M_{k,m}(K_{1,n - 1})} \chi_\alpha(G) < \min_{G \in M_{k+1,m}(K_{1,n - 1})} \chi_\alpha(G)
\]

(4)

holds for any \( 1 \leq k \leq n - 2 \) provided \( m \geq n + k \).

**Corollary 4.2.** Suppose that \(-3 \leq \alpha < 0\). For fixed \( n \geq 3 \) and \( m \geq n + 3 \), among the connected multigraphs of order \( n \) and size \( m \) the multigraphs having the minimum, the second and the third minimum general sum-connectivity index are deduced from \( K_{1,n - 1} \) having the vectors of degrees of non-central vertices equal to \((m - n + 2, 1, \ldots, 1), (m - n + 1, 2, 1, \ldots, 1) \) and \((m - n, 3, 1, \ldots, 1)\), respectively.

**Proof.** We have seen that \((m - n + 2, 1, \ldots, 1)\) corresponds to the multigraph reaching \(\min \chi_\alpha(G)\); in this case \( k = 1 \).

If \( k = 2 \) the minimum is reached for \((m - n + 1, 2, 1, \ldots, 1)\) and the second minimum is achieved for \((m - n, 3, 1, \ldots, 1)\).

For \( k = 3 \) the minimum is reached for \((m - n, 2, 2, 1, \ldots, 1)\). The value of \( \chi_\alpha \) corresponding to this vector is greater than the value corresponding to \((m - n, 3, 1, \ldots, 1)\), as we have seen in the proof of Theorem 4.1. Since (4) holds, the conclusion follows. ■

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