MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 535-548

ISSN 0340 - 6253

Ordering Trees Having Small General Sum-Connectivity Index [1]

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(Received March 12, 2012)

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 α 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 χ_α.

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

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

[1] This research is partially supported by Higher Education Commission, Pakistan.

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_α, of G is defined as [1]:

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

where α is a real number. Then $R_{-1/2}$ is the classical Randić connectivity index.
The sum-connectivity index was proposed in [15] and both sum-connectivity index and Randić index correlate well with the π - 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 α 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 χ_α 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 $diam(G)$ of a graph G is the maximum distance between the vertices of G, i.e., $diam(G) = \max_{u,v\in V(G)} d(u,v)$. A shortest path of length $diam(G)$ 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 $\frac{f^{(n)}(x)}{(\alpha)_{n-1}} > (x(\alpha+1)+n)(x+3)^{\alpha-n} - ((\alpha+1)x+\alpha+n+1)(x+4)^{\alpha-n}$. Since $\alpha+1 \geq 0$, $\frac{f^{(n)}(x)}{(\alpha)_{n-1}} > 0$ 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 $\lim_{n\to\infty}(\frac{x+3}{x+4})^{\alpha-n} = \infty$ 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. ■

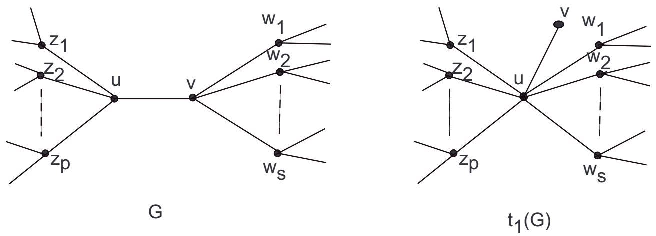

Figure 1: t_1- transform applied to G at vertex v

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 $G'(q) =$

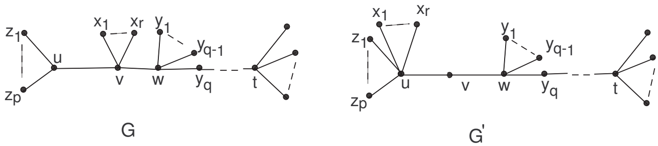

Figure 2: Swaping pendant edges at one end of a diametral path of G

$\alpha[(r+q+3)^{\alpha-1}-(q+3)^{\alpha-1}]>0$ 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^α 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 $\alpha\geq -1$. ∎

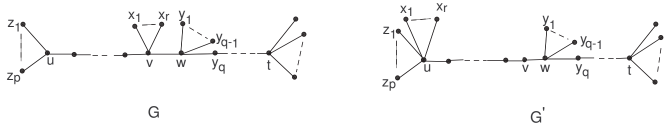

Figure 3: Swaping pendant edges at one end of a diametral path of G

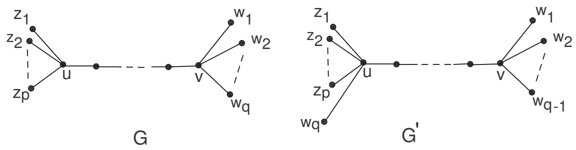

Figure 4: Swaping a pendant edge between ends of a diametral path.

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 $d_{G'}(u) + d_{G'}(v) = d_G(u) + d_G(v) = p+q+2$, 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

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

or $g(q) > g(q+r+1)$, where $g(q) = q(q+2)^\alpha - (q-1)(q+1)^\alpha$.
We deduce $g'(q) = (q+2+\alpha q)(q+2)^{\alpha-1} - (q+1+\alpha(q-1))(q+1)^{\alpha-1} = h(q) - h(q-1)$, 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 $\chi_\alpha\,(-1 \le \alpha < 0)$ FOR TREES OF GIVEN DIAMETER

Let $d \ge 3$. We shall denote by $MS(n_1,\, n_2,\, \ldots,\, n_{d-1})$ where $n_1, n_{d-1} \ge 1$ and $n_i \ge 0$ for $2 \le i \le d-2$, 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 $1 \le i \le d-1$. 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 $n_1,\, n_2 \ge 1$ 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 $2 \le p \le n-1$, $S_{n,p}$ 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 $-1 \le \alpha < 0$ in the set of trees T having order $n \ge 3$ and $diam(T) = d$ $(2 \le d \le n-1)$, $\chi_\alpha(T)$ 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 $-1 \le \alpha < 0$. (a) In the set of trees T of order n we have

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

if $2 \le i < j \le n-1$.
(b) In the set of trees T of order n and diameter d with $3 \le d \le n-2$ 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.

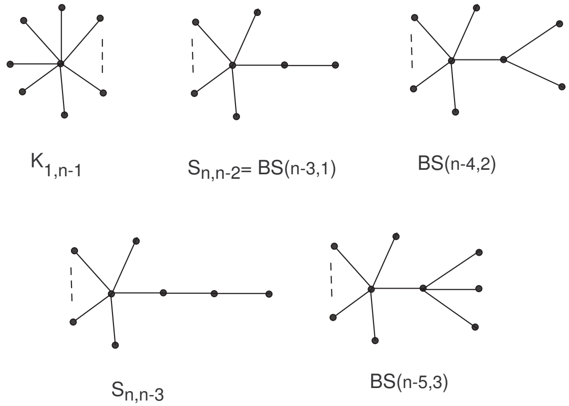

Figure 5: Five trees T having smallest $\chi_\alpha(T)$ for $-1 \le \alpha < 0$.

(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 $-1 \le \alpha < 0$ there exists $n_0(\alpha) > 0$ such that for every $n \ge n_0(\alpha)$ 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 χ_α. The second minimum value of χ_α 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 χ_α 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 $n \ge 6$ the trees having minimum values of χ_α 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 $\lim\limits_{n\to\infty}((n-5)(n-3)^\alpha + n^\alpha - (n-4)(n-2)^\alpha - (n-1)^\alpha) = 0$ since $\alpha < 0$. 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

$$\varphi^{(n)}(x) = (\ln 5)^n \left[3 \cdot 5^x - 4^x \left(\frac{\ln 4}{\ln 5} \right)^n - 3^x \left(\frac{\ln 3}{\ln 5} \right)^n \right],$$

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 χ_α 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 χ_α 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 χ_α 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 pendant 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 pendant 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 $\chi_\alpha(T) - \chi_\alpha(T-u) = (d(w)+2)^\alpha + 3^\alpha - (d(w)+1)^\alpha \geq 4^\alpha$ since the function $(x+2)^\alpha - (x+1)^\alpha$ is strictly increasing for $x \geq 0$.
Equality holds if and only if $d(w) = 2$. In this case $T - u$ has p pendant vertices. By the 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., $T = S_{n,p}$. ■

4. MINIMUM VALUE OF χ_α $(-3 \leq \alpha < 0)$ FOR MULTIGRAPHS

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

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.

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

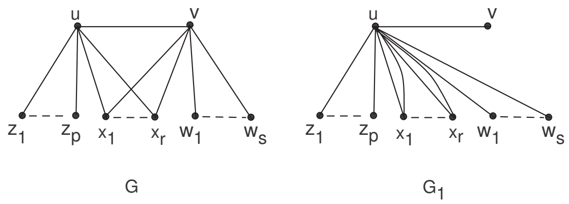

Figure 6: $G_1 = t_2(G)$

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 $uv \in E(G)$. 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 φ 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

$$\chi_\alpha(G) = (n-2)(m+1)^\alpha + (m-n+2)(2m-n+2)^\alpha \ . \qquad \blacksquare$$

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 $(m-n-k+3, \underbrace{2, \ldots, 2}_{k-1}, \underbrace{1, \ldots, 1}_{n-k-1})$.

Also

$$\min_{G \in M_{k,m}(K_{1,n-1})} \chi_\alpha(G) < \min_{G \in M_{k+1,m}(K_{1,n-1})} \chi_\alpha(G) \tag{4}$$

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 χ_α 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. $\blacksquare$

Acknowledgement. The authors are indebted to the referee for his/her careful reading of the manuscript and valuable comments. This work has been done while the first author was invited at Abdus Salam School of Mathematical Sciences, GC University, Lahore.

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