

## GENERAL SUM-CONNECTIVITY INDEX OF TREES AND UNICYCLIC GRAPHS WITH FIXED MAXIMUM DEGREE

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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  $d(v)$  denotes the degree of the vertex  $v$  in  $G$  and  $\alpha$  is a real

number. In this paper it is deduced the maximum value for the general sum-connectivity index of  $n$ -vertex trees for  $-1.7036 \leq \alpha < 0$  and of  $n$ -vertex unicyclic graphs for  $-1 \leq \alpha < 0$  respectively, with fixed maximum degree  $\Delta$ . The corresponding extremal graphs, as well as the  $n$ -vertex unicyclic graphs with the second maximum general sum-connectivity index for  $n \geq 4$  are characterized. This extends the corresponding results by Du, Zhou and Trinajstić [arXiv.org/1210.5043] about sum-connectivity index.

**Key words:** Vertex degree, tree, unicyclic graphs, maximum degree, general sum-connectivity index.

### 1. INTRODUCTION

Let  $G(V(G), E(G))$  be a simple graph, where  $V(G)$  and  $E(G)$  are the sets of vertices and of edges, respectively. For a vertex  $v \in V(G)$ ,  $d(v)$  denotes the degree of vertex  $v$ ,  $N(v)$  is the set of vertices adjacent to  $v$  and the maximum vertex degree of the graph  $G$  is denoted by  $\Delta(G)$ . If  $uv \in E(G)$ ,  $G - uv$  denotes the subgraph of  $G$  obtained by deleting the edge  $uv$ ; similarly is defined the graph  $G + uv$  if  $uv \notin E(G)$ . For  $n \geq 3$  let  $T(n, \Delta)$  be the set of trees with  $n$  vertices and maximum degree  $\Delta$  and  $U(n, \Delta)$  be the set of unicyclic graphs with  $n$  vertices and maximum degree  $\Delta$  ( $2 \leq \Delta \leq n - 1$ ). Let  $P_n$  and  $C_n$  be the path and the cycle, respectively, on  $n \geq 3$  vertices. For  $\Delta = 2$ ,  $T(n, \Delta) = \{P_n\}$  and  $U(n, \Delta) = \{C_n\}$ . Attaching a path  $P_r$  to a vertex  $v$  of a graph means adding an edge between  $v$  and a terminal vertex of the path. If  $r = 1$ , then we attach a pendant vertex.

The Randić index  $R(G)$  was proposed by Randić [10]. This is one of the most used molecular descriptors in structure-property and structure-activity relationship studies [2, 6, 7, 8]. The Randić index is also called product-connectivity index and it is defined as

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

Bollobás and Erdős [1] generalized the idea of Randić index and proposed the general Randić index, denoted as  $R_\alpha$ . It is defined as

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

where  $\alpha$  is a real number.

The sum-connectivity index was proposed by Trinajstić et al. [13] and it was observed that sum-connectivity index and product-connectivity index correlate well among themselves and with the  $\Pi$ -electronic energy of benzenoid hydrocarbons [9]. This concept was extended to the general sum-connectivity index in [14] and defined as

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

Then  $\chi_{-1/2}$  is the sum-connectivity index [13].

Several extremal properties of the sum-connectivity and general sum-connectivity indices for trees, unicyclic graphs and general graphs were given in [3, 4, 11, 12, 13, 14].

In [5] Zhou et al. obtained the maximum sum-connectivity index of graphs in the set of trees and in the set of unicyclic graphs respectively, with a given number of vertices and maximum degree and determined the corresponding extremal graphs. They also found the  $n$ -vertex unicyclic graphs with the first two maximum sum-connectivity indices for  $n \geq 4$ . In this paper we extend these results for the general sum-connectivity index.

## 2. MAIN RESULTS

First we will discuss two lemmas that will be used in the proofs.

LEMMA 2.1 [4]. *Let  $Q$  be a connected graph with at least two vertices. For  $a \geq b \geq 1$ , let  $G_1$  be the graph obtained from  $Q$  by attaching two paths  $P_a$  and  $P_b$  to  $u \in V(Q)$  and  $G_2$  the graph obtained from  $Q$  by attaching a path  $P_{a+b}$  to  $u$ . Then  $\chi_\alpha(G_2) > \chi_\alpha(G_1)$ , for  $\alpha_1 \leq \alpha < 0$ , where  $\alpha_1 \approx -1.7036$  is the unique root of the equation  $\frac{3^\alpha - 4^\alpha}{4^\alpha - 5^\alpha} = 2$ .*

The following property is an extension of a transformation defined in [5].

LEMMA 2.2 [5]. *Let  $M$  be a connected graph with  $|V(M)| \geq 3$  and  $u$  be a vertex of degree two of  $M$ . Let  $H$  be the graph obtained from  $M$  by attaching a path  $P_a$  to  $u$ . Denote by  $u_1$  and  $u_2$  the two neighbors of  $u$  in  $M$ , and by  $u'$  the pendant vertex of the path attached to  $u$  in  $H$ . If  $d_H(u_2) \leq 3$ , then for  $H' = H - \{uu_2\} + \{u'u_2\}$  we have  $\chi_\alpha(H') > \chi_\alpha(H)$ , where  $-1 \leq \alpha < 0$ .*

*Proof.* If  $d_H(u, u') = 1$ , then for  $\alpha < 0$  we have:

$$\chi_\alpha(H') - \chi_\alpha(H) = (d_H(u_1) + 2)^\alpha + (d_H(u_2) + 2)^\alpha - (d_H(u_1) + 3)^\alpha - (d_H(u_2) + 3)^\alpha > 0.$$

If  $d_H(u, u') \geq 2$ , then

$$\begin{aligned} \chi_\alpha(H') - \chi_\alpha(H) &= (d_H(u_1) + 2)^\alpha - (d_H(u_1) + 3)^\alpha + (d_H(u_2) + 2)^\alpha - (d_H(u_2) + 3)^\alpha + 2 \cdot 4^\alpha - 3^\alpha - 5^\alpha \\ &> (d_H(u_2) + 2)^\alpha - (d_H(u_2) + 3)^\alpha + 2 \cdot 4^\alpha - 3^\alpha - 5^\alpha. \end{aligned}$$

Since  $(x+2)^\alpha - (x+3)^\alpha$  is decreasing for  $x \geq 0$ , we have  $(d_H(u_2) + 2)^\alpha - (d_H(u_2) + 3)^\alpha \geq 5^\alpha - 6^\alpha$ .

Therefore

$$\chi_\alpha(H') - \chi_\alpha(H) > 2 \cdot 4^\alpha - 3^\alpha - 6^\alpha.$$

The function  $\eta(x) = 2 \cdot 4^x - 3^x - 6^x$  has roots  $x_1 = -1$  and  $x_2 = 0$  and  $\eta(x) > 0$  for  $x \in (-1, 0)$  [15]. It follows that  $\chi_\alpha(H') > \chi_\alpha(H)$  for every  $-1 \leq \alpha < 0$ . For  $\frac{n}{2} \leq \Delta \leq n-1$ , let  $T_{n,\Delta}$  be the tree

obtained by attaching  $2\Delta+1-n$  pendant vertices and  $n-\Delta-1$  paths of length two to a vertex. For  $\frac{n+2}{2} \leq \Delta \leq n-1$ , let  $U_{n,\Delta}$  be the unicyclic graph obtained by attaching  $2\Delta-n-1$  pendant vertices and  $n-\Delta-1$  paths of length two to the same vertex of a triangle.

For  $\frac{n}{2} \leq \Delta \leq n-1$ , let  $T_{n,\Delta}$  be the tree obtained by attaching  $2\Delta+1-n$  pendant vertices and  $n-\Delta-1$  paths of length two to a vertex. For  $\frac{n+2}{2} \leq \Delta \leq n-1$ , let  $U_{n,\Delta}$  be the unicyclic graph obtained by attaching  $2\Delta-n-1$  pendant vertices and  $n-\Delta-1$  paths of length two to the same vertex of a triangle.

**THEOREM 2.3.** *Let  $G \in T(n, \Delta)$ , where  $2 \leq \Delta \leq n-1$  and  $\alpha_1 \leq \alpha < 0$ , where  $\alpha_1 \approx -1.7036$  is the unique root of the equation  $\frac{3^\alpha - 4^\alpha}{4^\alpha - 5^\alpha} = 2$ . Then*

$$\chi_\alpha(G) \leq \begin{cases} ((\Delta+2)^\alpha - (\Delta+1)^\alpha + 3^\alpha)(n-\Delta-1) + \Delta(\Delta+1)^\alpha & \text{if } \frac{n}{2} \leq \Delta \leq n-1 \\ ((\Delta+2)^\alpha + 3^\alpha - 4^\alpha)\Delta + (n-\Delta-1)4^\alpha & \text{if } 2 \leq \Delta \leq \frac{n-1}{2} \end{cases}$$

and equality holds if and only if  $G = T_{n,\Delta}$  for  $\frac{n}{2} \leq \Delta \leq n-1$ , and  $G$  is a tree obtained by attaching  $\Delta$  paths of length at least two to a unique vertex for  $2 \leq \Delta \leq \frac{n-1}{2}$ .

*Proof.* The case  $\Delta = 2$  is clear since in this case  $G = P_n$ . Suppose that  $\Delta \geq 3$  and let  $G$  be a tree in  $T(n, \Delta)$  having maximum general sum-connectivity index. Let  $v$  be a vertex of degree  $\Delta$  in  $G$ . If there exists some vertex of degree greater than two in  $G$  different from  $v$ , then by Lemma 2.1, we may get a tree in  $T(n, \Delta)$  with greater general sum-connectivity index, a contradiction. It follows that  $v$  is the unique vertex of degree greater than two in  $G$ . Let  $k$  be the number of neighbors of  $v$  with degree two. Since in  $V(G) \setminus (\{v\} \cup N(v))$  there are  $n-\Delta-1$  vertices, it follows that  $k \leq \min\{n-\Delta-1, \Delta\}$ . If  $n-\Delta-1 \geq \Delta$ , i.e.,  $\Delta \leq \frac{n-1}{2}$ , then  $1 \leq k \leq \Delta$ . If  $n-\Delta-1 < \Delta$ , i.e.,  $\Delta \geq \frac{n}{2}$ , then  $0 \leq k \leq n-\Delta-1$ . We get

$$\begin{aligned} \chi_\alpha(G) &= (\Delta-k)(\Delta+1)^\alpha + k(\Delta+2)^\alpha + k \cdot 3^\alpha + (n-\Delta-k-1)4^\alpha \\ &= k((\Delta+2)^\alpha - (\Delta+1)^\alpha + 3^\alpha - 4^\alpha) + \Delta(\Delta+1)^\alpha + (n-\Delta-1)4^\alpha. \end{aligned}$$

Since  $(\Delta+2)^\alpha - (\Delta+1)^\alpha$  is increasing for  $\Delta \geq 3$  we obtain

$(\Delta+2)^\alpha - (\Delta+1)^\alpha + 3^\alpha - 4^\alpha \geq 5^\alpha + 3^\alpha - 2 \cdot 4^\alpha > 0$ , the last inequality holding by Jensen's inequality.

Consequently,

$$\chi_\alpha(G) \leq \begin{cases} ((\Delta+2)^\alpha - (\Delta+1)^\alpha + 3^\alpha)(n-\Delta-1) + \Delta(\Delta+1)^\alpha & \text{if } \frac{n}{2} \leq \Delta \leq n-1 \\ ((\Delta+2)^\alpha + 3^\alpha - 4^\alpha)\Delta + (n-\Delta-1)4^\alpha & \text{if } 2 \leq \Delta \leq \frac{n-1}{2}. \end{cases}$$

For  $\frac{n}{2} \leq \Delta \leq n-1$ , the equality holds if and only if  $k = n - \Delta - 1$ , i.e., each of the  $n - \Delta - 1$  neighbors of degree two of the vertex  $v$  is adjacent to exactly a pendant vertex, i.e.,  $G = T_{n,\Delta}$ . For  $2 \leq \Delta \leq \frac{n-1}{2}$  the equality holds for  $k = \Delta$ , i.e.,  $G$  is a tree obtained by attaching  $\Delta$  paths of length at least two to a unique vertex.

Now we obtain the maximum general sum-connectivity index of graphs in  $U(n, \Delta)$  and deduce the extremal graphs. As a consequence, we deduce the  $n$ -vertex unicyclic graphs with the first and second maximum general sum-connectivity indices for  $n \geq 4$ .

**THEOREM 2.4.** *Let  $G \in U(n, \Delta)$ , where  $2 \leq \Delta \leq n-1$  and  $-1 \leq \alpha < 0$ . Then*

$$\chi_\alpha(G) \leq \begin{cases} (n - \Delta - 1)3^\alpha + (n - \Delta + 1)(\Delta + 2)^\alpha + (2\Delta - n - 1)(\Delta + 1)^\alpha + 4^\alpha & \text{if } \frac{n+2}{2} \leq \Delta \leq n-1 \\ (\Delta - 2)3^\alpha + \Delta(\Delta + 2)^\alpha + (n - 2\Delta + 2)4^\alpha & \text{if } 2 \leq \Delta \leq \frac{n+1}{2}. \end{cases}$$

For  $\frac{n+2}{2} \leq \Delta \leq n-1$  the equality holds if and only if  $G = U_{n,\Delta}$ . If  $2 \leq \Delta \leq \frac{n+1}{2}$  the equality holds if and only if  $G$  is a unicyclic graph obtained by attaching  $\Delta - 2$  paths of length at least two to a fixed vertex of a cycle.

*Proof.* The case  $\Delta = 2$  is trivial since in this case  $G = C_n$ . Suppose that  $\Delta \geq 3$ ,  $G$  is a graph in  $U(n, \Delta)$  with maximum general sum-connectivity index, and  $C$  is the unique cycle of  $G$ . Let  $v$  be a vertex of degree  $\Delta$  in  $G$ .

If  $\Delta = 3$  and there exists some vertex outside  $C$  with degree three, then by Lemma 2.1, we may get a graph in  $U(n, 3)$  with greater general sum-connectivity index, a contradiction. If there are at least two vertices on  $C$  with degree three, then by Lemma 2.2, we may deduce the same conclusion. Thus,  $v \in V(C)$  and  $v$  is the unique vertex in  $G$  with degree three. Then either  $\chi_\alpha(G) = (n-2)4^\alpha + 2 \cdot 5^\alpha$  when  $v$  is adjacent to a vertex of degree one and two vertices of degree two for  $n \geq 4$ , or  $\chi_\alpha(G) = (n-4)4^\alpha + 3 \cdot 5^\alpha + 3^\alpha$  when  $v$  is adjacent to three vertices of degree two for  $n \geq 5$ . The difference of these two numbers equals  $(n-2)4^\alpha + 2 \cdot 5^\alpha - (n-4)4^\alpha - 3 \cdot 5^\alpha - 3^\alpha = 2 \cdot 4^\alpha - 5^\alpha - 3^\alpha < 0$  by Jensen's inequality. Hence,  $G$  is the graph obtained by attaching a pendant vertex to a triangle for  $n = 4$ , i.e.,  $G = U_{4,3}$ , and a graph obtained by attaching a path of length at least two to a cycle for  $n \geq 5$ .

Now suppose that  $\Delta \geq 4$ . As for the case  $\Delta = 3$  we deduce that the vertex of maximum degree is unique, otherwise  $G$  has not a maximum general sum-connectivity index in  $U(n, \Delta)$ . We will show that the vertex of maximum degree  $v$  lies on  $C$ . Suppose that  $v$  is not on  $C$ . Let  $w$  be the vertex on  $C$  such that  $d_G(v, w) = \min\{d_G(v, x) : x \in V(C)\}$ . If there is some vertex outside  $C$  with degree greater than two different from  $v$ , or if there is some vertex on  $C$  with degree greater than two different from  $w$ , then by Lemmas 2.1 and 2.2, we may get a graph in  $U(n, \Delta)$  with greater general sum-connectivity index, a contradiction. Thus,  $v$  and  $w$  are the only vertices of degree greater than two in  $G$ , and  $d_G(v) = \Delta$  and  $d_G(w) = 3$ . Let  $Q$  be the path connecting  $v$  and  $w$ . Suppose that  $v_1, v_2, \dots, v_{\Delta-1}$  are the neighbors of  $v$  outside  $Q$ . Let  $d_i = d_G(v_i)$  for  $i = 1, \dots, \Delta-1$ . Note that since  $G$  has maximum general sum-connectivity index, then  $d_1, \dots, d_{\Delta-1} \in \{1, 2\}$ , since otherwise we can apply Lemma 2.1 and obtain a graph having a

greater general sum-connectivity index. Consider  $G_1 = G - \{v_3, \dots, v_{\Delta-1}\} + \{w_3, \dots, w_{\Delta-1}\} \in U(n, \Delta)$ . Note that  $d_{G_1}(w) = \Delta$  and  $d_{G_1}(v) = 3$ . Then

$$\begin{aligned} \chi_\alpha(G_1) - \chi_\alpha(G) &= (d_1 + 3)^\alpha - (d_1 + \Delta)^\alpha + (d_2 + 3)^\alpha - (d_2 + \Delta)^\alpha + 2(\Delta + 2)^\alpha - 2 \cdot 5^\alpha \\ &> 5^\alpha - (2 + \Delta)^\alpha + 5^\alpha - (2 + \Delta)^\alpha + 2(\Delta + 2)^\alpha - 2 \cdot 5^\alpha = 0, \end{aligned}$$

since the function  $(x + 3)^\alpha - (x + \Delta)^\alpha$  is strictly decreasing in  $x \geq 0$  for  $\Delta \geq 4$ . Because  $d_{G_1}(v) = 3$ , then by Lemma 2.1, we may get a graph  $G'$  in  $U(n, \Delta)$  such that  $\chi_\alpha(G') > \chi_\alpha(G_1) \geq \chi_\alpha(G)$ , a contradiction. Hence, we have shown that  $v$  lies on  $C$ .

If there is some vertex outside  $C$  with degree greater than two, then by Lemma 2.1 we may obtain a graph in  $U(n, \Delta)$  with greater general sum-connectivity index, a contradiction. If there is some vertex on  $C$  with degree three, then by Lemma 2.2, we may get a graph in  $U(n, \Delta)$  with greater general sum-connectivity index, a contradiction. Thus,  $G$  is a graph obtained from  $C$  by attaching  $\Delta - 2$  paths to  $v$ . Let  $k$  be the number of neighbors of  $v$  with degree two. Then as above we get  $k \leq \min\{n - \Delta - 1, \Delta - 2\}$ . If  $n - \Delta - 1 \geq \Delta - 2$ , i.e.,  $\Delta \leq \frac{n+1}{2}$ , then  $0 \leq k \leq \Delta - 2$ . If  $n - \Delta - 1 < \Delta - 2$ , i.e.,  $\Delta \geq \frac{n+2}{2}$ , then  $0 \leq k \leq n - \Delta - 1$ . We get

$$\begin{aligned} \chi_\alpha(G) &= k3^\alpha + (k+2)(\Delta+2)^\alpha + (\Delta-k-2)(\Delta+1)^\alpha + (n-\Delta-k)4^\alpha \\ &= (3^\alpha + (\Delta+2)^\alpha - (\Delta+1)^\alpha - 4^\alpha)k + (\Delta-2)(\Delta+1)^\alpha + 2(\Delta+2)^\alpha + 4^\alpha(n-\Delta). \end{aligned}$$

We have

$$3^\alpha - 4^\alpha + (\Delta+2)^\alpha - (\Delta+1)^\alpha \geq 3^\alpha - 4^\alpha + 6^\alpha - 5^\alpha > 0$$

since the function  $f(x) = (x+2)^\alpha - (x+1)^\alpha$  is strictly increasing for  $\alpha < 0$ , hence  $f(\Delta) \geq f(4)$  and  $f(4) > f(2)$ . It follows that  $\chi_\alpha(G)$  is bounded above by

$$\begin{aligned} &\begin{cases} (3^\alpha + (\Delta+2)^\alpha - (\Delta+1)^\alpha - 4^\alpha)(n-\Delta-1) + (\Delta-2)(\Delta+1)^\alpha + 2(\Delta+2)^\alpha + 4^\alpha(n-\Delta) & \text{if } \frac{n+2}{2} \leq \Delta \leq n-1 \\ (3^\alpha + (\Delta+2)^\alpha - (\Delta+1)^\alpha - 4^\alpha)(\Delta-2) + (\Delta-2)(\Delta+1)^\alpha + 2(\Delta+2)^\alpha + 4^\alpha(n-\Delta) & \text{if } 2 \leq \Delta \leq \frac{n+1}{2} \end{cases} \\ &= \begin{cases} (n-\Delta-1)3^\alpha + (n-\Delta+1)(\Delta+2)^\alpha + (2\Delta-n-1)(\Delta+1)^\alpha + 4^\alpha & \text{if } \frac{n+2}{2} \leq \Delta \leq n-1 \\ (\Delta-2)3^\alpha + \Delta(\Delta+2)^\alpha + (n-2\Delta+2)4^\alpha & \text{if } 2 \leq \Delta \leq \frac{n+1}{2} \end{cases} \end{aligned}$$

Equality holds for  $\frac{n+2}{2} \leq \Delta \leq n-1$  if and only if  $k = n - \Delta - 1$ , i.e.,  $G = U_{n,\Delta}$ ; if  $2 \leq \Delta \leq \frac{n+1}{2}$  then equality is reached if and only if  $k = \Delta - 2$ , i.e.,  $G$  is a unicyclic graph obtained by attaching  $\Delta - 2$  paths of length at least two to a unique vertex of a cycle.

**THEOREM 2.5.** *If  $-1 \leq \alpha < 0$ , among the unicyclic graphs on  $n \geq 4$  vertices,  $C_n$  is the unique graph with maximum general sum-connectivity index, which is equal to  $n4^\alpha$ . For  $n = 4$ ,  $U_{4,3}$  is the unique graph with the second maximum general sum-connectivity index, which is equal to  $2 \cdot 4^\alpha + 2 \cdot 5^\alpha$ . For  $n \geq 5$ ,*

the graphs obtained by attaching a path of length at least two to a vertex of a cycle are the unique graphs with the second maximum general sum-connectivity index, which is equal to  $(n-4)4^\alpha + 3 \cdot 5^\alpha + 3^\alpha$ .

*Proof.* For  $n=4$  we get

$$\chi_\alpha(U_{4,3}) - \chi_\alpha(C_4) = 2 \cdot 5^\alpha - 2 \cdot 4^\alpha < 0.$$

Now, suppose that  $n \geq 5$  and  $G$  is a unicyclic graph on  $n$  vertices. Let  $\Delta$  be the maximum degree of  $G$ , where  $2 \leq \Delta \leq n-1$ . Let  $f(x) = (x-2)3^\alpha + x(x+2)^\alpha + (n-2x+2)4^\alpha$  for  $x \geq 2$ . If  $\frac{n+2}{2} \leq \Delta \leq n-1$ , then by Theorem 2.4,

$$\begin{aligned} \chi_\alpha(G) &\leq (n-\Delta-1)3^\alpha + (n-\Delta+1)(\Delta+2)^\alpha + (2\Delta-n-1)(\Delta+1)^\alpha + 4^\alpha \\ &= f(\Delta) + (n-2\Delta+1)(3^\alpha - 4^\alpha + (\Delta+2)^\alpha - (\Delta+1)^\alpha) < f(\Delta) \end{aligned}$$

since the function  $x^\alpha - (x+1)^\alpha$  is strictly decreasing for  $x \geq 0$  and  $\Delta \geq 4$ .

If  $2 \leq \Delta \leq \frac{n+1}{2}$ , then by Theorem 2.4,  $\chi_\alpha \leq f(\Delta)$  and equality can be reached. We shall prove that  $f'(x) < 0$ , which implies that  $f(x)$  is strictly decreasing for  $x \geq 2$ . One deduces

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

Let

$$g(x) = (x+2)^\alpha + \alpha x(x+2)^{\alpha-1}.$$

We get

$$g'(x) = \alpha(x+2)^{\alpha-2}(x(\alpha+1)+4) < 0.$$

So,  $g(x)$  is strictly decreasing for  $x \geq 2$ , thus implying  $g(x) \leq 4^\alpha + 2\alpha 4^{\alpha-1}$ . Consequently,

$$f'(x) \leq 3^\alpha - 4^\alpha + 2\alpha 4^{\alpha-1} = 4^\alpha \left( \left( \frac{3}{4} \right)^\alpha + \frac{\alpha}{2} - 1 \right).$$

Considering the function  $h(x) = \frac{x}{2} + \left(\frac{3}{4}\right)^x$ , we get  $h''(x) = \left(\ln\left(\frac{3}{4}\right)\right)^2 \left(\frac{3}{4}\right)^x > 0$ , hence  $h(x)$  is strictly convex. Since  $h(-1) = 5/6 < 1$  and  $h(0) = 1$ ,  $h(x)$  being strictly convex on  $[-1, 0)$ , it follows that  $h(x) < 1$  on this interval, or  $f'(x) < 0$  for every  $-1 \leq \alpha < 0$ , hence  $f(x)$  is strictly decreasing for  $x \geq 2$ .

It follows that for  $3 < \frac{n+2}{2} \leq \Delta \leq n-1$  we have  $\chi_\alpha(G) < f(\Delta) < f(3) < f(2)$  and for  $3 \leq \Delta \leq \frac{n+1}{2}$  we obtain  $\chi_\alpha(G) \leq f(\Delta) \leq f(3) < f(2)$ . It follows that  $C_n$  is the unique  $n$ -vertex unicyclic graph with maximum general sum-connectivity index, equal to  $f(2)$ . Also the  $n$ -vertex unicyclic graphs with maximum degree  $\Delta = 3$  and general sum-connectivity index  $f(3)$  are the  $n$ -vertex graphs with the second maximum general sum-connectivity index. By Theorem 2.4, these graphs consist from a cycle  $C_l$  of an arbitrary length  $l$ ,  $3 \leq l \leq n-2$  and a path of length at least two attached to a vertex of  $C_l$ .

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