

# General Sum–Connectivity Index with $\alpha \geq 1$ for Bicyclic Graphs<sup>1</sup>

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## Abstract

The general sum–connectivity index of a graph  $G$  is a molecular descriptor 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 to obtain the graph with the maximum general sum–connectivity index among the connected bicyclic graphs of order  $n$  for  $\alpha \geq 1$ .

## 1 Introduction

Following standard notations in graph theory [2], let  $G = (V(G), E(G))$  be a simple, undirected and connected graph with  $V(G)$  the set of its vertices and  $E(G)$  the set of its edges. For a vertex  $u \in V(G)$  let  $d_G(u)$  denote the degree and  $N_G(u)$  the set of its neighbors. Where there is no danger of confusion, we shall give the simplified notation  $d(u)$  for the degree of  $u$ . We will use the notations  $P_r$  and  $C_r$  respectively for a path and a cycle with  $r$  edges. The distance between two vertices  $u$  and  $v$  of a connected graph, denoted by  $d(u, v)$ , is the length of a shortest path between them.

One important molecular descriptor is the Randić index defined in [8] with its generalization proposed in [1]:

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

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The classical Randić index is given by  $\alpha = -1/2$  and it is one of the most used molecular descriptors in the QSAR and QSPR models. Like these descriptors, the sum-connectivity index [12] and the general sum-connectivity index introduced by Zu and Trinastić in [13] and given by

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

were also proposed. Here  $\chi_{-1/2}$  gives the classical sum-connectivity index, which is also studied and applied in QSAR, QSPR modeling.

Several extremal properties of the general sum-connectivity index have already been established for general graphs [13], multigraphs [9], trees [7, 9, 12] and unicyclic graphs [6, 10]. In this paper we want to extend the extremal study of the general sum-connectivity index to bicyclic graphs (connected graphs with  $n$  vertices and  $n+1$  edges). More precisely, we will find the graph with the largest value of  $\chi_\alpha(G)$  among the bicyclic graphs of order  $n$  for  $\alpha \geq 1$ .

## 2 Some initial transformations

For  $n \leq 6$  we can easily see which are the connected bicyclic graphs of order  $n$  with maximum general sum-connectivity index for  $\alpha \geq 1$ . If  $n = 4$  we have a unique bicyclic graph and for  $n = 5$ ,  $n = 6$  the graphs with the largest value of the general sum-connectivity index are given in Fig. 1.



Figure 1: Bicyclic graphs with maximum  $\chi_\alpha$ : (a)  $n = 5$ ; (b)  $n = 6$ .

Thus, we will consider in this paper that  $|V(G)| = n \geq 7$ .

Let  $u$  and  $v$  be two adjacent vertices with  $d(v) \geq 2$  such that  $N_G(u) \cap N_G(v) = \emptyset$  and the neighbors of the vertex  $u$  except  $v$ , denoted  $u_1, \dots, u_r$  are pendent vertices. We

begin with a particular case of the  $t_1$ -transform [9] through which all the pendent edges of vertex  $u$  become incident edges of vertex  $v$ , as below:

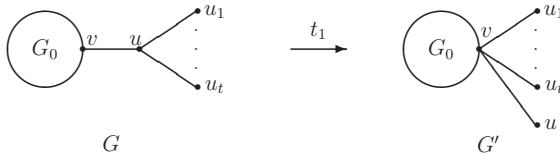


Figure 2:  $t_1$ -transform for pendent edges

Thus the transformation described above built the graph  $t_1(G) = G - \{uu_1, \dots, uu_t\} + \{vu_1, \dots, vu_t\}$  obtained by removing  $uu_1, \dots, uu_t$  and adding  $vu_1, \dots, vu_t$ ,  $t \geq 1$ . We need the following result:

**Lemma 1.** [9] *Let  $G$  and  $G' = t_1(G)$  be the graphs from Fig. 2. Then, for  $\alpha \geq 1$ , we have  $\chi_\alpha(G') > \chi_\alpha(G)$ .*

Since a bicyclic graph has  $n + 1$  edges it can be obtained from a tree to which we add two other edges and thus forming some cycles. Then every bicyclic graph can be viewed as a (possibly empty) set of subtrees, each of them attached to one of the graph's cycles. Applying the  $t_1$ -transform for a finite number of times we easily see that we can reduce any of the above subtrees to a bunch of pendent edges incident to the subtree's cycle vertex of attachment.

As above, we define our next general sum-connectivity enhancing  $t_2^i$ -transform, with the purpose of further reducing our bicyclic graph to an even simpler case.

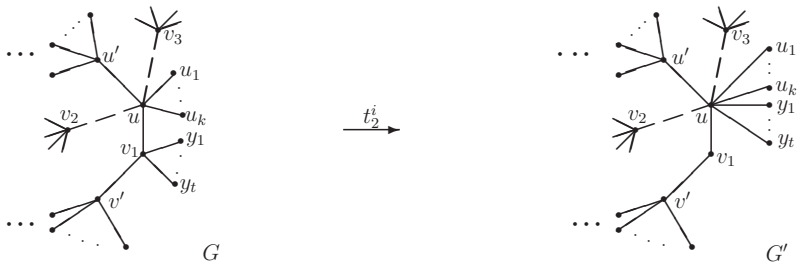


Figure 3:  $t_2^i$ -transform

Let  $G$  be a graph as in Fig. 3 and we denote  $d_G(u) - k = i \geq 2$ . Suppose that the vertex  $u$  has, besides its  $k$  pendent neighbors, at least two (denoted by  $u'$ ,  $v_1$ ) and at most four non-pendent neighbors. Then, if  $i = 3$  we denote by  $v_2$  the third non-pendent neighbor of the vertex  $u$  and for  $i = 4$  we also have the vertex  $v_3$ . Thus we define the transformation  $t_2^i(G) = G - \{v_1y_1, \dots, v_1y_t\} + \{uy_1, \dots, uy_t\}$ . We prove that modifying in this manner the graph, the value of the general sum-connectivity index  $\chi_\alpha$  strictly increases. But first we give a simple result that we will need several times throughout this paper.

**Lemma 2.** *The real function  $f : [0, \infty) \rightarrow \mathbb{R}$  defined by  $f_{\alpha,a}(x) = (x+a)^\alpha - x^\alpha$  is strictly increasing for all  $\alpha > 1$ ,  $a > 0$ .*

**Lemma 3.** *Let  $G$ ,  $G' = t_2^i(G)$  as in Fig. 3 such that  $uv_1 \in E(G)$ ,  $t \geq 1$ ,  $k \geq 0$ ,  $d_G(v_1) - t = 2$  and  $d(u') \geq d(v')$ . Then  $\chi_\alpha(G') > \chi_\alpha(G)$  for all  $\alpha \geq 1$ .*

*Proof.* We can write  $i = 2 + \beta + \gamma$ , where  $\beta = 1$  indicates the existence of the vertex  $v_2$  (otherwise  $\beta = 0$ ) and likewise,  $\gamma = 1$  indicates the existence of the vertex  $v_3$  (otherwise  $\gamma = 0$ ). With the established notations from the above figure, we have:

$\chi_\alpha(G') - \chi_\alpha(G) = [(d(u') + k + t + i)^\alpha - (d(u') + k + i)^\alpha] + [(d(v') + 2)^\alpha - (d(v') + t + 2)^\alpha] + k[(t + k + i + 1)^\alpha - (k + i + 1)^\alpha] + t[(t + k + i + 1)^\alpha - (t + 3)^\alpha] + \beta[(d(v_2) + t + k + i)^\alpha - (d(v_2) + k + i)^\alpha] + \gamma[(d(v_3) + t + k + i)^\alpha - (d(v_3) + k + i)^\alpha]$ . Obviously the sum of the last four square parentheses in this expression is strictly positive. Now for the first two we need the above lemma and if  $i \geq 2$ ,  $d(u') \geq d(v')$  then  $f_{\alpha,t}(d(u') + k + i) \geq f_{\alpha,t}(d(v') + 2)$ , from which we conclude that the  $t_2^i$ -transform strictly increases  $\chi_\alpha$ . ■

### 3 Three particular types of bicyclic graphs

With the notations from [3] and ignoring the possible pendent subtrees that may appear, we have the following three types of bicyclic graphs:

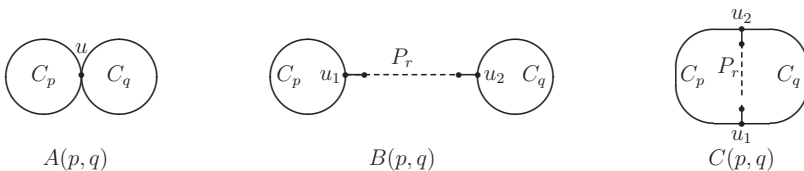


Figure 4: Types of bicyclic graphs

Thus, for the connected bicyclic graphs of order  $n$  we denote by  $A(p, q)$  the set of the graphs that have two cycles  $C_p$  and  $C_q$  with a single vertex  $u$  in common. For the graphs in which these cycles are distinct and connected by a path (of length at least one) we use the notation  $B(p, q)$ . If  $C_p$  and  $C_q$  have in common a path  $P_r$  ( $r \geq 1$ ) we have a  $C(p, q)$ -graph.

In what follows we treat these three cases separately, with the purpose of determining the graph with maximum  $\chi_\alpha$  in each category.

First we examine  $A(p, q)$ . To this category of graphs we apply the  $t_2^2$ -transform to all cycle edges which are not incident to the vertex  $u$  and which have bunches of pendent edges at both ends. Thus, all remaining bunches of pendent edges to  $C_p \cup C_q - \{u\}$  will be situated at distances of at least two one from another.

We now show that moving the remaining bunches of pendent edges in the vertex  $u$ , the index  $\chi_\alpha$  continues to strictly increase. Thus we define a new transformation given by  $t_3(G) = G - \{vy_1, \dots, vy_t\} + \{uy_1, \dots, uy_t\}$ , where  $v \in C_p \cup C_q - \{u\}$  is a vertex that has attached to it the set of the pendent edges  $\{vy_1, \dots, vy_t\}$ ,  $t \geq 1$ . Thus we have:

**Lemma 4.** Denoting by  $G' = t_3(G)$  we have  $\chi_\alpha(G') > \chi_\alpha(G)$  for all  $\alpha \geq 1$ .

*Proof.* Let  $G \in A(p, q)$  be a graph as in Fig. 4 and let  $\{uu_1, \dots, uu_k\}$  be the (possibly empty) set of the pendent edges in the vertex  $\{u\} = C_p \cap C_q$ . The vertex  $v$  with its pendent edges can be adjacent to vertex  $u$  or  $d(u, v) \geq 2$ .

Case I:  $uv \in E(G)$ .

Suppose, for simplicity that  $v \in C_p$  and let  $N_{C_p}(v) = \{u, w\}$ . Then, since all remaining bunches of pendent edges to  $C_p \cup C_q - \{u\}$  are situated at distances of at least two one from another, we have  $d_G(w) = 2 < d_G(u)$ . Finally, since  $d_G(u) - k = 4$ , we can apply the  $t_2^4$ -transform to move in the vertex  $u$  the edges pendent to  $v$ . We repeat this transformation whenever possible for the adjacent vertices of  $u$  situated on the cycles.

Case II:  $d(u, v) > 1$ .

First observe that, since we already applied the  $t_2^2$ -transform whenever possible, both of  $v$ 's cycle neighbors have degree exactly 2 in  $G$ . Moreover, from the previous case we have that all the neighbors of  $u$  situated on the cycles  $C_p$  and  $C_q$  have degree 2 in  $G$  also.

Thus, we have:

$\chi_\alpha(G') - \chi_\alpha(G) = 2[4^\alpha - (t+4)^\alpha] + 4[(k+t+6)^\alpha - (k+6)^\alpha] + k[(t+k+5)^\alpha - (k+5)^\alpha] + t[(k+t+5)^\alpha - (t+3)^\alpha]$ . Applying lemma 2 for the sum of the first two square

parentheses, we have  $f_{\alpha,t}(4) < f_{\alpha,t}(k+6)$  for every  $k \geq 0, t \geq 1$  and the conclusion easily follows. ■

Applying the  $t_3$ -transform for all the bunches of pendent edges to  $C_p \cup C_q - \{u\}$  we obtain the graph  $G_1$  from Fig. 5. We observe now that - through all the transformations used so far - by bringing as many edges as possible in the well chosen vertex  $u$ , the general sum-connectivity index strictly increases. Based on this observation, it appears naturally to extract edges from the two cycles and attach them to the vertex  $u$ . We construct thus the transformation:

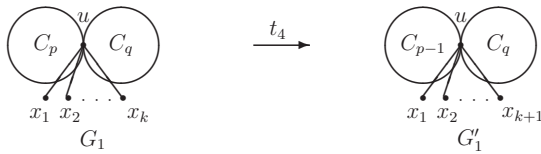


Figure 5: Decreasing of cycles of  $A(p, q)$ -graphs

**Lemma 5.** Denoting by  $A_n(p, q, k)$  the graph  $G_1$  from Fig. 5 we have  $\chi_\alpha(A_n(p, q, k)) < \chi_\alpha(A_n(p-1, q, k+1))$ , for  $p > 3$ .

*Proof.* A simple computation gives us  $\chi_\alpha(A_n(p-1, q, k+1)) - \chi_\alpha(A_n(p, q, k)) = 4[(k+7)^\alpha - (k+6)^\alpha] + k[(k+6)^\alpha - (k+5)^\alpha] + (k+6)^\alpha - 4^\alpha > 0$ . ■

**Theorem 1.** If  $\alpha \geq 1$  then  $A_n(3, 3, n-5)$  is the unique graph with the largest general sum-connectivity index among the graphs of order  $n$  in  $A(p, q)$ .

*Proof.* This result follows from the previous lemmas. If  $G$  is not isomorphic to  $A(3, 3, n-5)$ , then by one of the transformations described above we can find another bicyclic graph of order  $n$  having a greater general sum-connectivity index. Hence  $A(3, 3, n-5)$  maximizes the general sum-connectivity index in the  $A(p, q)$  family of graphs (see Fig. 10(a)). ■

We will analyse now the family of graphs denoted by  $B(p, q)$  (see Fig. 4). We first successively apply the  $t_1$ -transform until we obtain a graph with bunches of pendent edges attached to the cycles  $C_p, C_q$  and to the path  $P_r$ . With the notations from Fig. 6(a) we apply the  $t_2^2$ -transform on the paths  $C_p - \{u_1\}$ ,  $C_q - \{u_2\}$  and  $P_r - \{u_1, u_2\}$ . Thus, on these paths the remaining bunches of pendent edges will be situated at a distance

greater or equal to 2. Apart from these there will eventually remain some bunches of pendent edges in the vertices  $v_1, v_2, v_3, v_4, w_1, w_2$  (see Fig. 6, where  $w_1, w_2$  may coincide or disappear altogether if  $r = 1$ ). Next, we gather all those remaining edges in the vertex  $u_1$  or all in the vertex  $u_2$  to strictly increase the index  $\chi_\alpha$ . For this purpose, we will apply a new transformation which will be handled in a certain manner. Let  $y \in V(G)$  and  $\{yy_1, \dots, yy_t\}$  be the set of the pendent edges in vertex  $y$ ,  $t \geq 1$  and we define the new transformation as  $t_5(G) = G - \{yy_1, \dots, yy_t\} + \{u_iy_1, \dots, u_iy_t\}, i \in \{1, 2\}$ .

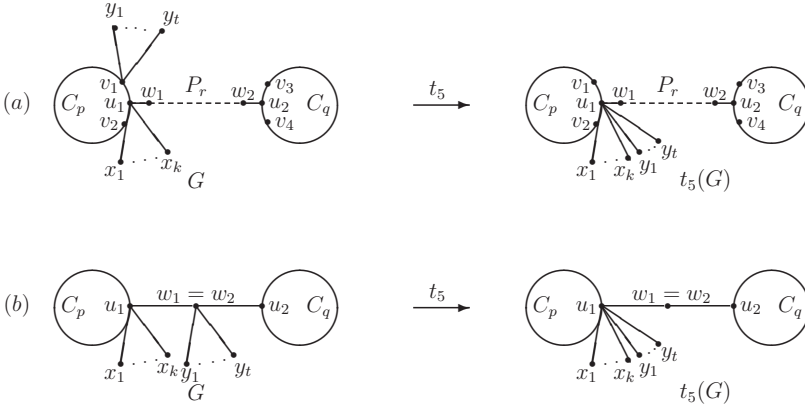


Figure 6: Different cases for shifting the pendent edges for a vertex  $y \in N_G(u_1) \cup N_G(u_2)$

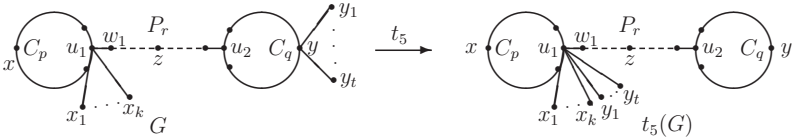


Figure 7: Shifting the pendent edges for vertex  $y \in V(G)$ ,  $d(y, u_i) > 1$ ,  $i \in \{1, 2\}$

**Lemma 6.** Let  $G$  be a  $B(p, q)$ -graph as in Fig. 6 or 7. There exists a sequence of  $t_5$ -transforms, that strictly increase the value of the general sum-connectivity index after which all the pendent edges will be incident to the vertex  $u_1$  or all will be incident to the vertex  $u_2$ .

*Proof.* We construct the sequence in the following order:

Step 1. Let us consider  $y \in N_G(u_i)$ ,  $i \in \{1, 2\}$ . In this case we move all the pendent edges from  $y$  to its adjacent vertex  $u_i$ .

Since we first already applied the  $t_2^2$ -transform whenever possible, for every  $x$  in  $N_G(y) - \{u_1, u_2, y_1, \dots, y_t\}$  we have  $d(x) = 2$ . We will first treat the case when  $y$  is a cycle vertex.

Case 1.1. Let  $y$  be in  $N_G(u_i) \cap (C_p \cup C_q)$ . With the notations from Fig. 6(a),  $y$  is one of the vertices  $v_1, v_2, v_3, v_4$ . For these vertices all conditions in lemma 3 are fulfilled, so we can apply the  $t_2^3$ -transform to bring all the pendent edges from  $v_1$  and  $v_2$  in  $u_1$  and from  $v_3$  and  $v_4$  in  $u_2$ .

Case 1.2. Let  $y$  be in  $N_G(u_i) \cap P_r$ . With the notations in the figure,  $y$  is one of the vertices  $w_1, w_2$ .

Let  $k$  be the number of pendent edges attached to  $u_1$ , i. e.,  $k = d(u_1) - 3$ .

(a) Suppose  $r = 1$ .

If  $k > 0$  we will move to  $u_1$  all the pendent edges attached to  $u_2$ , otherwise we keep these pendent edges in the vertex  $u_2$ .

From case I we have  $d(v_i) = 2$ , for every  $1 \leq i \leq 4$ . So:

$\chi_\alpha(G') - \chi_\alpha(G) = 2[(k+t+5)^\alpha - (k+5)^\alpha] + 2[5^\alpha - (t+5)^\alpha] + t[(k+t+4)^\alpha - (t+4)^\alpha] + k[(k+t+4)^\alpha - (k+4)^\alpha]$ . Here the last two parentheses are clearly positive and for the first two we apply lemma 2.

(b) If  $r = 2$  it follows that  $y = w_1 = w_2$  (Fig. 6(b)).

We observe that we cannot use  $t_2^3$  in this case. Thus we compare directly the values of  $\chi_\alpha$  for  $G$  and  $G' = t_5(G)$ . If  $d(u_1) \geq d(u_2)$  we attach the pendent edges from  $y$  to  $u_1$ . We denote by  $c$  the number of pendent vertices adjacent to  $u_2$  and using the notations from Fig. 6(b) we have:

$\chi_\alpha(G') - \chi_\alpha(G) = 2[(k+t+5)^\alpha - (k+5)^\alpha] + [(c+5)^\alpha - (t+c+5)^\alpha] + t[(k+t+4)^\alpha - (t+3)^\alpha] + k[(k+t+4)^\alpha - (k+4)^\alpha]$ . Since  $d(u_1) \geq d(u_2)$  ( $k+3 \geq c+3$ ), then from lemma 2 we have  $f_{\alpha,t}(c+5) \leq f_{\alpha,t}(k+5)$ , hence  $\chi_\alpha$  strictly increases.

For  $d(u_1) < d(u_2)$  we move the pendent edges from  $y$  to vertex  $u_2$  (the computations are the same as above).

(c) For  $r \geq 3$ , first note that since we already applied the  $t_2^2$ -transform whenever possible, the neighbor of  $y$  on  $P_r - \{u_1, u_2\}$  has degree exactly 2. Thus we can apply the  $t_2^3$ -transform to bring the pendent edges from  $y = w_1$  to  $u_1$  and from  $y = w_2$  to  $u_2$ .

Step 2. Suppose the distance  $d(y, u_i) > 1$ ,  $i \in \{1, 2\}$ , where  $y$  is a vertex situated on  $C_p$ ,  $C_q$  or  $P_r$ .



Observe that, after applying all the transformations from step 1, every non-pendent neighbor of  $y$  has degree exactly 2.

Case 2.1.  $y \neq u_2$  (Fig. 7).

Supposing that  $k > 0$ , we will move all the pendent edges from  $y$  to  $u_1$ . In the case of a null value of  $k$  we move all in the vertex  $u_2$ , with similar computations (even if the vertex  $u_2$  also has no pendent edges attached to it, i.e.  $d(u_2) = 3$ ).

Let us denote  $d(w_1) = c$  and it is easy to observe that if  $r = 1$ , then  $w_1 = u_2$  and  $c = d(u_2)$ , else we have  $c = 2$ . Thus:

$\chi_\alpha(G') - \chi_\alpha(G) = 2[(k+t+5)^\alpha - (k+5)^\alpha] + 2[4^\alpha - (t+4)^\alpha] + t[(k+t+4)^\alpha - (t+3)^\alpha] + k[(k+t+4)^\alpha - (k+4)^\alpha] + (k+t+c+3)^\alpha - (k+c+3)^\alpha$ . Using lemma 2 the conclusion easily follows.

Case 2.2.  $y = u_2$ .

We apply whenever possible the  $t_5$ -transform from the previous step, thus, if  $k = 0$ , all the pendent edges are already attached to the vertex  $u_2$ , then we are done. Otherwise, we have some pendent edges attached to the vertex  $u_1$ , as to the vertex  $u_2$ . In this case, we collect all the pendent edges to the vertex  $u_1$  by moving the pendent edges from  $u_2$ . We get:

$\chi_\alpha(G') - \chi_\alpha(G) = 3[(k+t+5)^\alpha - (k+5)^\alpha] + 3[5^\alpha - (t+5)^\alpha] + t[(k+t+4)^\alpha - (t+4)^\alpha] + k[(k+t+4)^\alpha - (k+4)^\alpha]$ . Using lemma 2 this case is also resolved. ■

Now we modify the obtained graph by deleting edges from the two cycles and from the path joining them and reattaching them to the vertex  $u_1$ , by the transformations  $t_6$  and  $t'_6$ , as below:

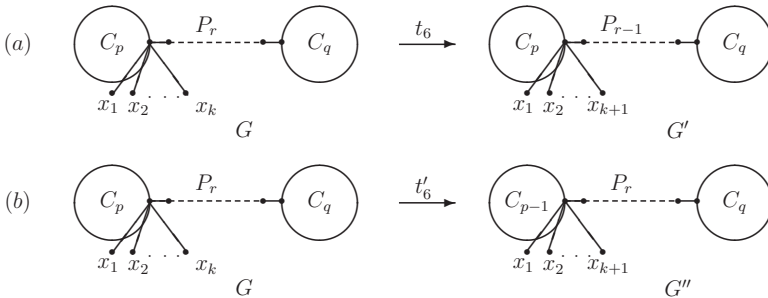


Figure 8: Transformations for  $B(p, q)$ -graphs that strictly increase  $\chi_\alpha$

**Lemma 7.** *Let us denote by  $B_n(p, q, r, k)$  the graph  $G$  in Fig. 8. Then the transformations  $t_6$  and  $t'_6$  strictly increase the general sum-connectivity index for  $\alpha \geq 1$ :*

$$(a) \chi_\alpha(B_n(p, q, r, k)) < \chi_\alpha(B_n(p, q, r-1, k+1)) \text{ for } r > 2;$$

$$(b) \chi_\alpha(B_n(p, q, r, k)) < \chi_\alpha(B_n(p-1, q, r, k+1)) \text{ for } p > 3.$$

*Proof.* We can see that

$$\chi_\alpha(B_n(p, q, r-1, k+1)) - \chi_\alpha(B_n(p, q, r, k)) = (k+5)^\alpha - 4^\alpha + k[(k+5)^\alpha - (k+4)^\alpha] + 3[(k+6)^\alpha - (k+5)^\alpha] > 0 \text{ for all } \alpha \geq 1, k \geq 0.$$

Since  $\chi_\alpha(B_n(p, q, r-1, k+1)) = \chi_\alpha(B_n(p-1, q, r, k+1)) = \chi_\alpha(B_n(p, q-1, r, k+1))$ , then (b) is also true. ■

From the above proof we easily see that the  $t'_6$ -transform can be used to shrink the  $C_p$  cycle as well as the  $C_q$  cycle. Keeping in mind the requirements of this lemma, we can repeat the above transformations successively to obtain graphs with greater  $\chi_\alpha$  until  $r = 2$ ,  $p = 3$  and  $q = 3$ , which gives us the graph  $B_n(3, 3, 2, n-7)$ .

**Theorem 2.**  *$B_n(3, 3, 1, n-6)$  from Fig. 10(b) is the graph of order  $n$  that maximizes the general sum-connectivity index for  $\alpha \geq 1$  in the set  $B(p, q)$ .*

*Proof.* Using the above remark, all that remains is to compare the general sum-connectivity values for  $B_n(3, 3, 2, n-7)$  and  $B_n(3, 3, 1, n-6)$ . Thus:

$$\begin{aligned} \chi_\alpha(B_n(3, 3, 1, n-6)) - \chi_\alpha(B_n(3, 3, 2, n-7)) &= 2(n-1)^\alpha + n^\alpha + (n-6)(n-2)^\alpha - 5^\alpha - \\ &- 3(n-2)^\alpha - (n-7)(n-3)^\alpha = 2[(n-1)^\alpha - (n-2)^\alpha] + (n-7)[(n-2)^\alpha - (n-3)^\alpha] + n^\alpha - 5^\alpha, \end{aligned}$$

which is surely positive for  $\alpha \geq 1, n \geq 7$ . ■

We continue now by finding the maximal graph in the category  $C(p, q)$ . We observe that the procedure of increasing the index  $\chi_\alpha$  through transformations used for the  $B(p, q)$  family of graphs, that bring as many edges as possible in a well selected vertex, can be also applied in this case. Thus we have:

**Lemma 8.** *Let  $G$  be a graph such as in Fig. 9. There exists a sequence of  $t_5$ -transforms, that strictly increases the value of the general sum-connectivity index after which all the pendent edges will be incident to the vertex  $u_1$  or all will be incident to the vertex  $u_2$ .*

*Proof.* The proof is identical to the case of the  $B(p, q)$ -graphs. We only need to use the cycles  $C_p$  and  $C_q$  excluding the common path  $P_r$ . Thus, if in the proof of lemma 6 we use the paths  $C_p - P_r$  and  $C_q - P_r$  instead of  $C_p$  and  $C_q$ , then we get the conclusion. ■

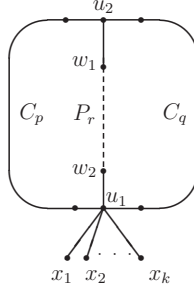


Figure 9: Graph in  $C(p, q)$

From here we will further proceed as in the case of the  $B(p, q)$  family by removing edges from the cycles and reattaching them to the vertex  $u_1$ . Denoting by  $C_n(p, q, r, k)$  the graph in Fig. 9, we define the transformations  $t_7$ ,  $t'_7$ ,  $t''_7$  by  $t_7(C_n(p, q, r, k)) = C_n(p-1, q, r, k+1)$ ,  $t'_7(C_n(p, q, r, k)) = C_n(p, q-1, r, k+1)$ ,  $t''_7(C_n(p, q, r, k)) = C_n(p-1, q-1, r-1, k+1)$ . Noting that by the transformations  $t_7$  and  $t'_7$  we remove edges from the paths  $C_p - P_r$ ,  $C_q - P_r$  (not from the entire cycle) and by  $t''_7$ -transform we remove only an edge from the path  $P_r$  (so, implicitly,  $p$  and  $q$  decrease by one unit).

**Lemma 9.** For  $\alpha \geq 1$  we have:

- (a)  $\chi_\alpha(C_n(p, q, r, k)) < \chi_\alpha(C_n(p-1, q, r, k+1))$  for  $p-r > 2$ ;
- (b)  $\chi_\alpha(C_n(p, q, r, k)) < \chi_\alpha(C_n(p-1, q-1, r-1, k+1))$  for  $r > 2$ .

*Proof.* These inequalities are proved in the same way as in Lemma 7. ■

With these preparations we have the following result:

**Theorem 3.** The graph of order  $n$  that maximizes the general sum connectivity index for  $\alpha \geq 1$  in the family  $C(p, q)$  is  $C_n(3, 3, 1, n-4)$  (Fig. 10(c)).

*Proof.* By the previous lemma, we strictly increase the value of  $\chi_\alpha$  by repeated use of the transformations  $t_7$ ,  $t'_7$  and  $t''_7$ , that gives us the graph  $C_n(4, 4, 2, n-5)$ . Since lemma 9

cannot be applied for  $r = 2$ , we have to show that in this case the  $t_7''$ -transform also strictly increases  $\chi_\alpha$ . For this we see that  $\chi_\alpha(C_n(3, 3, 1, n-4)) - \chi_\alpha(C_n(4, 4, 2, n-5)) = 2[(n+1)^\alpha - n^\alpha] + (n-5)[n^\alpha - (n-1)^\alpha] + (n+2)^\alpha - 5^\alpha$ , which is obviously positive for  $\alpha \geq 1$ . ■

## 4 Maximum value of $\chi_\alpha$ for bicyclic graphs ( $\alpha \geq 1$ )

We have obtained so far, for each of the families  $A(p, q)$ ,  $B(p, q)$  and  $C(p, q)$ , the graph which maximizes the general sum-connectivity index  $\chi_\alpha$  for  $\alpha \geq 1$  (see Fig. 10).

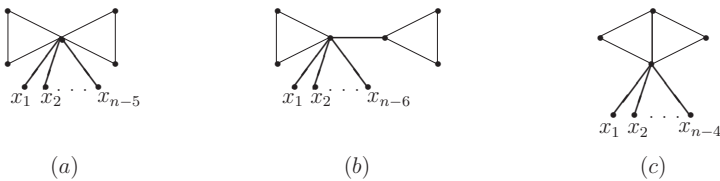


Figure 10: (a)  $A_n(3, 3, n-5)$ ; (b)  $B_n(3, 3, 1, n-6)$ ; (c)  $C_n(3, 3, 1, n-4)$ .

We shall now find which is the graph with the greatest  $\chi_\alpha$  index in the category of bicyclic graphs. Thus we have the following:

**Theorem 4.**  $C_n(3, 3, 1, n-4)$  is the unique graph with the largest general sum-connectivity index for  $\alpha \geq 1$  among all the connected bicyclic graphs of order  $n \geq 4$ .

*Proof.* Using the three theorems above all that remains is to compare the graphs from Fig. 10. Thus:

$$\chi_\alpha(A(3, 3, n-5)) = 2 \cdot 4^\alpha + 4(n+1)^\alpha + (n-5)n^\alpha;$$

$$\chi_\alpha(B(3, 3, 1, n-6)) = 2 \cdot 4^\alpha + 2 \cdot 5^\alpha + 2(n-1)^\alpha + n^\alpha + (n-6)(n-2)^\alpha;$$

$$\chi_\alpha(C(3, 3, 1, n-4)) = 2 \cdot 5^\alpha + 2(n+1)^\alpha + (n+2)^\alpha + (n-4)n^\alpha.$$

Now we have that:

$$\chi_\alpha(C(3, 3, 1, n-4)) - \chi_\alpha(B(3, 3, 1, n-6)) = 2(n+1)^\alpha + (n+2)^\alpha + (n-4)n^\alpha - 2 \cdot 4^\alpha - 2(n-1)^\alpha - n^\alpha - (n-6)(n-2)^\alpha = 2[(n+1)^\alpha - (n-1)^\alpha] + (n-6)[n^\alpha - (n-2)^\alpha] + (n+2)^\alpha + n^\alpha - 2 \cdot 4^\alpha.$$

Since  $\alpha \geq 1$  and  $n \geq 7$ , the expression above is strictly positive.

$\chi_\alpha(C(3, 3, 1, n-4)) - \chi_\alpha(A(3, 3, n-5)) = 2[5^\alpha - 4^\alpha] + (n+2)^\alpha + n^\alpha - 2(n+1)^\alpha$ . The square parenthesis is obviously positive and for the last three terms of the sum we shall

consider the function  $f : [0, \infty) \rightarrow \mathbb{R}$  defined by  $f_\alpha(n) = n^\alpha$ . Since  $f$  is convex for  $\alpha \geq 1$  then by Jensen's inequality we deduce the positivity of the last part of the sum. ■

**Remark 1.** We note that in the category of connected bicyclic graphs, the graph that maximizes the general sum-connectivity index for  $\alpha \geq 1$  is the same that maximizes the Zagreb indices [3], the Merrifield–Simmons index [5] and minimizes the Hosoya index [4]. Moreover it is one of the two graphs that maximizes the Harary index [11].

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