General Sum–Connectivity Index with $\alpha \geq 1$ for Bicyclic Graphs

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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]:

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

\[1\]

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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 Trinajstić 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 $u_1, \ldots, u_r$ 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:

\[
\begin{array}{c}
G_0 \quad v \quad u_1 \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
G \\
\end{array}
\quad \xleftarrow{t_1} \quad 
\begin{array}{c}
G_0 \quad v \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
\end{array}
\]

Figure 2: \( t_1 \)-transform for pendent edges

Thus the transformation described above built the graph \( t_1(G) = G - \{uu_1, \ldots, uu_t\} + \{vu_1, \ldots, vu_t\} \) obtained by removing \( uu_1, \ldots, uu_t \) and adding \( vu_1, \ldots, vu_t, t \geq 1 \). 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 \( t_2 \)-transform, with the purpose of further reducing our bicyclic graph to an even simpler case.

\[
\begin{array}{c}
\ldots \quad v \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
G \\
\end{array}
\quad \xleftarrow{t_2} \quad 
\begin{array}{c}
\ldots \quad v \\
\vdots \\
\vdots \\
\vdots \\
\vdots \\
G' \\
\end{array}
\]

Figure 3: \( t_2 \)-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 $t_2^i(G) = G - \{v_1y_1, \ldots, v_1y_t\} + \{uy_1, \ldots, uy_t\}$. 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 $f: [0, \infty) \to \mathbb{R}$ 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:

- **A(p, q)**
- **B(p, q)**
- **C(p, q)**

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 $t_3(G) = G - \{vy_1, \ldots, vy_t\} + \{uy_1, \ldots, uy_t\}$, where $v \in C_p \cup C_q - \{u\}$ is a vertex that has attached to it the set of the pendent edges $\{vy_1, \ldots, vy_t\}$, $t \geq 1$. 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 $\{uu_1, \ldots, uu_k\}$ 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 $t_2^2$-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:

\[
C_p \cup C_q \xrightarrow{t_4} C_{p-1} \cup C_q
\]

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)).
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 \( \{yy_1, \ldots, yy_t\} \) be the set of the pendent edges in vertex \( y \), \( t \geq 1 \) and we define the new transformation as \( t_5(G) = G - \{yy_1, \ldots, yy_t\} + \{u_iy_1, \ldots, u_iy_t\}, i \in \{1, 2\} \).

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

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

**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 \( t_2^3 \)-transform whenever possible, for every \( x \) in \( N_G(y) - \{ u_1, u_2, y_1, \ldots, y_t \} \) 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:

\[
\chi(G') - \chi(G) = 2[(k + t + 5)^\alpha - (k + 5)^\alpha] + 2[5^\alpha - (t + 5)^\alpha] + t[(k + t + 4)^\alpha - (t + 4)^\alpha] + k[(k + t + 4)^\alpha - (k + 4)^\alpha].
\]

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 \( \chi \) 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:

\[
\chi(G') - \chi(G) = 2[(k + t + 5)^\alpha - (k + 5)^\alpha] + [(c + 5)^\alpha - (t + c + 5)^\alpha] + t[(k + t + 4)^\alpha - (t + 3)^\alpha] + k[(k + t + 4)^\alpha - (k + 4)^\alpha].
\]

Since \( d(u_1) \geq d(u_2) \) \((k + 3 \geq c + 3)\), then from lemma 2 we have \( f_{a,t}(c + 5) \leq f_{a,t}(k + 5) \), hence \( \chi \) 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 \( t_2^3 \)-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 $\chi_\alpha$.](image-url)
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) $\chi_\alpha(B_n(p, q, r, k)) < \chi_\alpha(B_n(p, q, r - 1, k + 1))$ for $r > 2$;
(b) $\chi_\alpha(B_n(p, q, r, k)) < \chi_\alpha(B_n(p - 1, q, r, k + 1))$ for $p > 3$.

Proof. We can see that

$$\chi_\alpha(B_n(p, q, r - 1, k + 1)) - \chi_\alpha(B_n(p, q, r, k)) = \alpha [k + 5]^\alpha - 4^\alpha + k[(k + 5)^\alpha - (k + 4)^\alpha] + 3[(k + 6)^\alpha - (k + 5)^\alpha] > 0$$

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:

$$\chi_\alpha(B_n(3, 3, 1, n - 6)) - \chi_\alpha(B_n(3, 3, 2, n - 7)) = 2(n - 1)^\alpha + n^\alpha + (n - 6)(n - 2)^\alpha - 5^\alpha - 3(n - 2)^\alpha - (n - 7)(n - 3)^\alpha = 2[(n - 1)^\alpha - (n - 2)^\alpha] + (n - 7)[(n - 2)^\alpha - (n - 3)^\alpha] + n^\alpha - 5^\alpha,$$

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 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 $u_2$. 

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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 \( t'_r \)-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 \( \alpha \geq 1 \).

\[\square\]

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](image)

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:
\[
\chi_\alpha(C(3, 3, 1, n - 4)) - \chi_\alpha(B(3, 3, 1, n - 6)) = 2(n+1)^\alpha+(n+2)^\alpha+(n-4)n^\alpha-2\cdot4^\alpha-2(n-1)^\alpha-n^\alpha-(n-6)(n-2)^\alpha = 2[(n+1)^\alpha-(n-1)^\alpha]+(n-6)[n^\alpha-(n-2)^\alpha]+(n+2)^\alpha+n^\alpha-2\cdot4^\alpha.
\]

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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**References**


1252–1270.

210–218.