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On Degree–Based Topological Indices for Bicyclic Graphs[1]

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Abstract

Given a graph $G = (E(G), V(G))$, a degree-based topological index is defined as $TI(G) = \sum_{uv \in E(G)} F(d(u), d(v))$, where $F(x, y)$ is a particular function. In this paper we determine extremal bicyclic graphs with fixed number of pendants or fixed girth, for a group of degree-based topological indices such as the first Zagreb index, the general zeroth-order Randić index, the multiplicative Zagreb indices, the Narumi-Katayama index and the general sum-connectivity index with $\alpha > 1$.

1 Introduction

One of the most investigated categories of topological indices used in mathematical chemistry is that of the so-called degree-based topological indices, which are defined in terms of the degrees of the vertices of a graph. Thus, we can write the definition of such a topological index in the form given in [7] as

$$TI(G) = \sum_{uv \in E(G)} F(d(u), d(v)), \tag{1}$$

where $G = (V(G), E(G))$ is a simple, undirected, connected graph and $d(u)$ denotes the degree of the vertex u.

The aim of this paper is to determine extremal bicyclic graphs with given number of pendants or girth for certain degree-based topological indices which are representative in mathematical chemistry.

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First, considering $F(d(u),d(v)) = d(u)^{\alpha-1}+d(v)^{\alpha-1}$ we obtain the *general zeroth-order Randić index* given by

$$^0R_\alpha(G) = \sum_{u\in V(G)} d(u)^\alpha\,,$$

which for $\alpha = 2$ further gives *the first Zagreb index* (also named *the Gutman index* in [16]). This invariant introduced together with the second Zagreb index [9] arose from the desire to examine the dependence of the total π-electron energy on the molecular structure (see also [10]). Subsequently, both indices proved to have considerable applications in chemistry ([12], [18]). Moreover, $\alpha = -1/2$ gives the known *zeroth-order Randić index* $^0R_{-1/2}(G)$, usually denoted by $^0R(G)$.

Another generalization of the first Zagreb index is the general sum-connectivity index given by

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

and defined in [19] with the purpose of extending the classical sum-connectivity index, $\chi_{-1/2}(G)$.

We also consider two fairly new indices [15], [17] with higher prediction ability then their classical versions, named the *multiplicative Zagreb indices* [8], which are given by

$$PM_1(G) = \textstyle\prod_{u\in V(G)} d(u)^2 \qquad \text{and} \qquad PM_2(G) = \prod_{u\in V(G)} d(u)^{d(u)}.$$

The logarithms of these indices can also be represented in the form of equation (1) by choosing $F(d(u),d(v)) = 2\left(\frac{\ln d(u)}{d(u)} + \frac{\ln d(v)}{d(v)}\right)$ and $F(d(u),d(v)) = \ln d(u) + \ln d(v)$, respectively.

Remark 1. We recall here the relations between the multiplicative Zagreb indices and *the Narumi-Katayama index* [11] with its modified version [6], namely $PM_1(G) = NK(G)^2$ and $PM_2(G) = NK(G)^*$.

Remark 2. We note that there exists in the literature other directions of research in the problem of finding extremal graphs for degree-based topological indices. One of them is based on the fomula $TI(G) = \sum_{1\le i\le j\le n-1} m_{ij}(G)\varphi_{ij}$, where $m_{ij}(G)$ represents the number of edges in G between vertices of degree i and degree j (see [1], [3], [4], [13]).

In what follows, we shall split the above mentioned degree-based topological indices in two categories. The first category is made of those indices in whose definition we have a sum or a product after the graph's vertices, whereas the second is formed by those indices for which the sum or the product in their definition is taken after the graph's edges. In this paper, we shall call the first category *topological indices based on vertices* and the second *topological indices based on edges.*

2 Main transformations and lemmas

Following standard notations in graph theory [2], let $u \in V(G)$ be a vertex and $N_G(u)$ the set of its neighbors. If a vertex has degree one we say that it is a pendant. We will also use the notations P_r and C_r respectively for a path and a cycle with r edges. Moreover, (P_r) will represent the path obtained by deleting the end vertices of the path P_r.

Let $\mathcal{B}_n$ be the set of bicyclic graphs of order n, $\mathcal{B}_n^g$ the set of bicyclic graphs of order n with given girth $g \geq 3$ and $\mathcal{B}_{n,k}$ the set of bicyclic graphs having k pendant vertices, with $0 \leq k \leq n-5$. Let us consider further the three standard subsets of such bicyclic graphs: we use the notation $\mathcal{A}_{p,q}$ for the set of graphs that have two cycles C_p and C'_q with a single vertex x in common; if the graph G has two disjoint cycles C_p and C'_q connected by a path of length $r \geq 1$ we use the notation $G \in \mathcal{B}_{p,q,r}$. For the graphs in which the two cycles have a common path P_r ($r \geq 1$) we say that we have a $\mathcal{C}_{p,q,r}$-graph.

We will further need some technical lemmas.

Lemma 1. *Let $\psi_\alpha(a,b,c) = a^\alpha(b+c)^\alpha - (a+c)^\alpha b^\alpha$, with $a,b,c > 0$ integers and α a real nonzero number. Then we have $sgn(\psi_\alpha(a,b,c)) = sgn(\alpha(a-b))$.*

Proof. Dividing by $b^\alpha(b+c)^\alpha$, the conclusion easily follows. ■

Lemma 2. *Let $\varphi(a,b,c) = (a+c)^{a+c}b^b - a^a(b+c)^{b+c}$, with $a,b,c > 0$ integers, such that $a > b$. Then we have $\varphi(a,b,c) > 0$.*

Proof. Case 1: $c = 1$. We see that $\varphi(a,b,1) > 0$ is equivalent with $\frac{(a+1)^{(a+1)}}{a^a} > \frac{(b+1)^{(b+1)}}{b^b}$. To show this, consider the function $f : [1,\infty) \to \mathbb{R}$ defined by $f(x) = \frac{(x+1)^{x+1}}{x^x}$. By writing $f(x) = (x+1)\left(1+\frac{1}{x}\right)^x$, we see that f is a strictly increasing function if the function $x \to \left(1+\frac{1}{x}\right)^x$ is. But this is a well known function in real analysis, which is increasing indeed.

Case 2: $c > 1$. Since $\varphi(a,b,c) > 0$ is equivalent with $\frac{(a+c)^{(a+c)}}{a^a} > \frac{(b+c)^{(b+c)}}{b^b}$, we consider $g : [1,\infty) \to \mathbb{R}$ defined by $g(x) = \frac{(x+c)^{x+c}}{x^x}$. A simple computation gives $g(cx) = c^c f(x)^c$, showing that g is a strictly increasing function also. ■

Lemma 3. *The real function* $f : [-2, \infty) \to \mathbb{R}$ *defined by* $f_{\alpha,a,b}(x) = (x+a)^\alpha - (x+b)^\alpha$, $a > b \geq -2$ *is strictly increasing for all* $\alpha \in (-\infty, 0) \cup (1, \infty)$ *and strictly decreasing for all* $\alpha \in (0, 1)$.

Proof. By considering f', the conclusion easily follows. ■

Lemma 4. *Consider* $g_\alpha : (0, \infty) \to \mathbb{R}$ *defined by* $g_\alpha(x) = x - 2^\alpha(x+1) + (x+2)^\alpha$. *Then* g_α *is strictly negative for* $\alpha \in (0, 1)$ *and strictly positive for* $\alpha \in (-\infty, 0) \cup (1, \infty)$.

Proof. We have $g'_\alpha(x) = 1 - 2^\alpha + \alpha(x+2)^{\alpha-1}$ and $g''_\alpha(x) = \alpha(\alpha-1)(x+2)^{\alpha-2}$, thus g''_α is strictly negative for $\alpha \in (0, 1)$ and strictly positive for $\alpha \in (-\infty, 0) \cup (1, \infty)$.

Suppose $\alpha \in (0, 1)$. Then $g'_\alpha(x)$ is strictly decreasing, thus $g'_\alpha(x) < g'_\alpha(+0)$ for $x \in (0, \infty)$. But, by the mean value theorem, $g'_\alpha(+0) = \alpha 2^{\alpha-1} - \frac{2^\alpha - 1}{2-1} = \alpha(2^{\alpha-1} - c^{\alpha-1}) < 0$ for some $c \in (1, 2)$, so g'_α is strictly negative for all $x \in (0, \infty)$. Thus g_α is also strictly decreasing, so $g_\alpha(x) < g_\alpha(+0) = 0$ for all $x \in (0, \infty)$.

The case $\alpha \in (-\infty, 0) \cup (1, \infty)$ is treated similarly. ■

Let $G \in \mathcal{B}_{n,k}$ and we further choose $x \in V(G)$ such that $\{x\} = C_p \cap C'_q$ for a $\mathcal{A}_{p,q}$-graph, $\{x\} = C_p \cap P_r$ for a $\mathcal{B}_{p,q,r}$-graph and $x \in (C_p - (P_r)) \cap (C'_q - (P_r))$ for a $\mathcal{C}_{p,q,r}$-graph.

We first define a transformation that takes any subtree $T \subset G$ attached in a vertex of degree greater than two and moves it incident to the vertex x. Let $y \in V(G)$ with $d(y) > 2$ such that $G = G_0 \cup T$ with $G_0 \cap T = \{y\}$ and $x \in G_0$. We denote $N_G(y) = \{y_1, y_2, \ldots, y_{d(y)}\}$ and, after a possible renumbering, we may assume $N_G(y) \cap T = \{y_1, \ldots, y_s\}$ and $N_G(y) \cap G_0 = \{y_{s+1}, \ldots, y_{d(y)}\}$. Then, we define the transformation $t_1(G) = G - \{yy_1, yy_2, \ldots, yy_s\} + \{xy_1, xy_2, \ldots, xy_s\}$.

Lemma 5. *Let* $G \in \mathcal{B}_{n,k}$ *and* $G' = t_1(G) \in \mathcal{B}_{n,k}$. *Then we have:*

(a) ${}^0R_\alpha(G') >^0 R_\alpha(G)$ *for* $\alpha \in (-\infty, 0) \cup (1, \infty)$ *and* ${}^0R_\alpha(G') <^0 R_\alpha(G)$ *for* $\alpha \in (0, 1)$;

(b) $PM_1(G') < PM_1(G)$;

(c) $PM_2(G') > PM_2(G)$.

Proof. Following the notations above we have $d(y) = s + \beta$ with $\beta \in \{2, 3\}$, where $\beta = 3$ iff G is a $\mathcal{C}_{p,q,r}$-graph and $y \in (C_p - (P_r)) \cap (C'_q - (P_r))$, $y \neq x$.

A direct computation gives us:

(a) $${}^0R_\alpha(G') -^0 R_\alpha(G) = (d(x)+s)^\alpha + \beta^\alpha - (\beta+s)^\alpha - d(x)^\alpha$$
$$= \Big[(d(x)+s)^\alpha - d(x)^\alpha\Big] + \Big[\beta^\alpha - (\beta+s)^\alpha\Big] = f_{\alpha,s,0}(d(x)) - f_{\alpha,s,0}(\beta).$$

From the way vertex x was chosen, we see that $d(x) \geq \beta$, which gives us the conclusion using Lemma 3.

(b) $PM_1(G') - PM_1(G) = \Big[(d(x)+s)^2\beta^2 - d(x)^2(\beta+s)^2\Big] \prod_{z\in V(G)-\{x,y\}} d(z)^2$
$= -\psi_2(d(x),\beta,s) \prod_{z\in V(G)-\{x,y\}} d(z)^2 < 0$ by Lemma 1.

(c) Similarly, $PM_2(G') - PM_2(G) = \varphi(d(x),\beta,s) \prod_{z\in V(G)-\{x,y\}} d(z)^{d(z)} > 0$ by Lemma 2. ■

We remark that for a topological index based on edges (such as the χ_α index) we can not move a subgraph $G_0 \subset G$ attached to a vertex to any another vertex in order to strictly increase or decrease the value of the index. Thus, a new transformation is needed for this purpose. Such a transformation, which will push step by step all the subtrees into the vertex x, is given in [14]. We recall it here, with the necessary changes for it to work on bicyclic graphs. Let $P_r = [v,\ldots,w] \subset G$, $r \geq 1$ such that $d(z) = 2$ for every vertex $z \in (P_r)$. We denote $G_0 \cap P_r = \{v\}$, $N_G(v) - P_r = \{u, v_1, \ldots, v_s\}$ and $N_G(w) - P_r = \{w_1,\ldots,w_t\}$, with $s \geq 1$, $t \geq 2$ and $N_G(v) \cap G_0 = \{v_1,\ldots,v_s\}$. Using these notations, we define the transformation which moves the subgraph G_0 attached in the vertex v to the vertex w: $t_1^r(G) = G - \{vv_1,\ldots,vv_s\} + \{wv_1,\ldots,wv_s\}$. It is necessary to observe that, in the case of bicyclic graphs, if there exists a vertex $z \in \{v_1,\ldots,v_s\} \cap \{w_1,\ldots,w_t\}$ and $z \neq u$, then moving the subgraph G_0 to the vertex w, the edge $wz \in E(G)$ would become a double edge. Taking this into account, we modify Lemmas 2 and 3 from [14] accordingly. The proof is ommited, due to the similarity of results.

Lemma 6. *Let $G \in \mathcal{B}_n$ and $G' = t_1^r(G)$ be two graphs, such that $d(v) > 2$, $d(w) > 2$, $d(z) = 2$ for every vertex $z \in (P_r)$ and $\{v_1,\ldots,v_s\} \cap \{w_1,\ldots,w_t\} \subseteq \{u\}$. If there exists $y \in N_G(w) - P_r$ with $d(y) \geq d(u)$, then $\chi_\alpha(G') > \chi_\alpha(G)$ for $\alpha > 1$.*

3 Topological indices based on vertices

3.1 Bicyclic graphs with k pendants

Let $G \in \mathcal{B}_{n,k}$ be a graph. We apply the t_1-transform for any subtree T of G, and note that after finishing this process all pendant paths will be attached in the chosen vertex x.

We shall establish some necessary notations in what follows. Let $\mathcal{T}_{n,k}$ denote the set of trees of order n having k pendant vertices and, moreover:

$\mathcal{T}^*_{n,k} = \{T \in \mathcal{T}_{n,k} | T$ has k pendant paths joined in a single endvertex $x\}$. We call $T \in \mathcal{T}^*_{n,k}$ a *star-like tree*;

$\mathcal{A}^*_{p,q,k} = \{G \in \mathcal{A}_{p,q} | G = C_p \cup C'_q \cup T, T \cap C_p \cap C'_q = \{x\}, T \in \mathcal{T}^*_{n,k}\}$;

$\mathcal{B}^*_{p,q,r,k} = \{G \in \mathcal{B}_{p,q,r} | G = C_p \cup C'_q \cup P_r \cup T, T \cap C_p \cap P_r = \{x\}, T \in \mathcal{T}^*_{n,k}\}$;

$\mathcal{C}^*_{p,q,r,k} = \{G \in \mathcal{C}_{p,q,r} | G = C_p \cup C'_q \cup T, T \cap (C_p - (P_r)) \cap (C'_q - (P_r)) = \{x\}, T \in \mathcal{T}^*_{n,k}\}$.

We note that for $k = n-4$ we have a unique graph $G \in \mathcal{B}_{n,k}$, namely $\mathcal{C}^*_{3,3,1,n-4}$, so we consider further $0 \leq k < n-4$. Then we can give our first result.

Theorem 1. *Let G^* be a bicyclic graph of order n with $0 \leq k < n-4$ pendant vertices. Then G^* minimizes the indices PM_1, ${}^0R_\alpha$ for $\alpha \in (0,1)$ and maximizes the indices PM_2, ${}^0R_\alpha$ for $\alpha \in (-\infty, 0) \cup (1, \infty)$ iff $G^* \in \mathcal{A}^*_{p,q,k}$.*

Proof. We need to observe that all graphs in $\mathcal{B}^*_{p,q,r,k} \cup \mathcal{C}^*_{p',q',r',k}$ have the same vertex-degree multiset $(k+3, 3, 2, \ldots, 2, 1, \ldots, 1)$, where the number 1 appears k times. Thus each of the indices ${}^0R_\alpha$, PM_1 and PM_2 has a unique value on the set $\mathcal{B}^*_{p,q,r,k} \cup \mathcal{C}^*_{p',q',r',k}$. From Lemma 5 it follows that any graphs $G^*_1 \in \mathcal{A}^*_{p,q,k}$ and $G^*_2 \in \mathcal{B}^*_{p,q,r,k} \cup \mathcal{C}^*_{p',q',r',k}$ are extremal in their categories w.r.t. the mentioned topological indices. Now, by direct computation we have

$${}^0R_\alpha(G^*_1) -{}^0 R_\alpha(G^*_2) = (k+4)^\alpha - (k+3)^\alpha - (3^\alpha - 2^\alpha) = f_{\alpha,1,0}(k+3) - f_{\alpha,1,0}(2),$$

which is strictly negative for $\alpha \in (0,1)$ and strictly positive for $\alpha \in (-\infty, 0) \cup (1, \infty)$, and following Lemma 5 we have the conclusion;

$PM_1(G^*_1) - PM_1(G^*_2) = (k+4)^2 4^{n-k-1} - (k+3)^2 4^{n-k-2} 3^2 < 0$ iff $\frac{k+3}{k+4} > \frac{2}{3}$, which is true for $k \geq 0$;

$$\begin{aligned} PM_2(G') - PM_2(G) &= (k+4)^{k+4} 4^{n-k-1} - (k+3)^{k+3} 4^{n-k-2} 3^3 \\ &= 4^{n-k-2} \Big[2^2 (k+4)^{k+4} - 3^3 (k+3)^{k+3} \Big] = 4^{n-k-2} \varphi(k+3, 2, 1) > 0, \end{aligned}$$

from Lemma 2. ∎

3.2 Bicyclic graphs with given girth g

First, we remark that the transformations described above keep unchanged the number of pendants but also the girth. Thus we continue the process to increase or decrease the values of the indices using the already established extremal categories $\mathcal{A}^*_{p,q,k}$ and $\mathcal{B}^*_{p,q,r,k} \cup \mathcal{C}^*_{p,q,r,k}$ obtained before. So, let $G \in \mathcal{A}^*_{p,q,k} \cup \mathcal{B}^*_{p,q,r,k} \cup \mathcal{C}^*_{p,q,r,k}$ be such a graph.

We define further a transformation which extracts an internal edge $uv \in E(G)$ from a cycle of length $p > g$ or from a pendant path of length $r > 1$ and reattaches it as a pendant edge incident to the chosen vertex x. Let $uv \in E(G)$ such that $u \neq x$, $d(u) = 2$ and $d(v) \in \{1, 2\}$. Then $t_2(G) = G - uv - vv' + uv' + xv$, where $v' \in N_G(v) - \{u\}$. We note that if there doesn't exist an internal edge $uv \in E(G)$ such that $d(u) = 2$ and $d(v) \in \{1, 2\}$ it follows that G is a graph with girth 4, namely $G \in \mathcal{C}^*_{4,4,2,n-5}$. But this is just a special case of Lemma 8 below. Thus, whenever $G \notin \mathcal{C}^*_{4,4,2,n-5}$, there exists an edge $uv \in E(G)$ such that the t_2-transform can be applied to G.

Lemma 7. *Let $G \in \mathcal{A}^*_{p,q,k} \cup B^*_{p,q,r,k} \cup C^*_{p,q,r,k}$ and $G' = t_2(G)$ be two graphs. Then we have:*

(a) ${}^0R_\alpha(G') >{}^0 R_\alpha(G)$ *for* $\alpha \in (-\infty, 0) \cup (1, \infty)$ *and* ${}^0R_\alpha(G') <{}^0 R_\alpha(G)$ *for* $\alpha \in (0, 1)$;

(b) $PM_1(G') < PM_1(G)$;

(c) $PM_2(G') > PM_2(G)$;

Proof. Performing similar computations as for Lemma 5, the conclusion immediately follows. ■

We continue the above process by applying the t_2-transform on these graphs for any $uv \in E(G)$ which is not a part of a cycle of length g. It follows that as many pendant edges as possible will become incident to the chosen vertex x, without changing the graph's girth. Hence, the path P_r of the $\mathcal{B}^*_{p,q,r,k}$-graphs will be transformed into a bunch of r pendant edges incident to x. Moreover, any $\mathcal{B}^*_{p,q,r,k}$-graph will be reduced to a $\mathcal{A}^*_{p,q,k}$-graph. We next introduce simplified notations for the $\mathcal{A}_{p,q}$ and $\mathcal{C}_{p,q,r}$-graphs in which any vertex $y \in V(G) - V(C_p \cup C'_q)$ is pendant and incident to the chosen vertex x: $A^*_{p,q}$ and $C^*_{p,q,r}$, respectively. Since the first set contains only one graph and the second set contains just two isomorphic graphs, $A^*_{p,q}$ will actually denote the graph itself, and $C^*_{p,q,r}$ will denote any of the two above mentioned isomorphic graphs.

Following this notations we have the next lemma.

Lemma 8. *Let $C^*_{p,q,r} \in \mathcal{B}^g_n$ be a graph such that ${}^0R_\alpha(C^*_{p,q,r}) \geq{}^0 R_\alpha(C^*_{p',q',r'})$ for any $C^*_{p',q',r'} \in \mathcal{B}^g_n$, where $\alpha \in (-\infty, 0) \cup (1, \infty)$. Then $C^*_{p,q,r} = C^*_{g,g,\frac{g}{2}}$ for g an even number and $C^*_{p,q,r} \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.*

Proof. Let $C^*_{p,q,r} \in \mathcal{B}^g_n$ be a graph as in the hypothesis and let us suppose that $r \neq \frac{g-\beta}{2}$, where $\beta = 0$ if g is even and $\beta = 1$ if g is odd.

We note that $C^*_{p,q,r} \simeq C^*_{p,p+q-2r,p-r} \simeq C^*_{p+q-2r,q,q-r}$ because we can change the path P_r to be one of the paths $C_p - P_r$ or $C'_q - P_r$, by simply redrawing the graph. Thus we consider further that $r = \min\{r, p-r, q-r\}$.

Suppose $r < \frac{g-\beta}{2}$. Since $C^*_{p,q,r} \in \mathcal{B}^g_n$, we have $p - r > \frac{g+\beta}{2}$ and also $q - r > \frac{g+\beta}{2}$, so $|(C_p - P_r) \cup (C'_q - P_r)| = p + q - 2r > g + \beta$. Here we give the transformation from Fig. 1 defined as $t_3(G) = G - zz'' + z'z'' - x'x'' + xx''$. The result is a new graph $C^*_{p,q,r+1} \in \mathcal{B}^g_n$ and by a simple computation we have ${}^0R_\alpha(C^*_{p,q,r+1}) >^0 R_\alpha(C^*_{p,q,r})$ for $\alpha \in (-\infty, 0) \cup (1, \infty)$, a contradiction with the hypothesis.

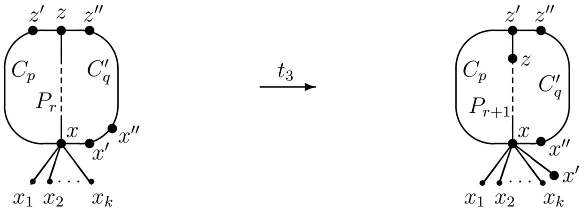

Figure 1: t_3-transform

If $r > \frac{g-\beta}{2}$ it follows that $r \geq \frac{g+1}{2}$ and since $r = \min\{r, p-r, q-r\}$ we obtain $p + q - 2r \geq g - 1 > g$ and $p > g, q > g$. Under these conditions we can apply the t_2-transform to an edge $uv \in P_r$. Thus we obtain a new graph $C^*_{p-1,q-1,r-1}$ of girth g also, but with a greater value for the ${}^0R_\alpha$-index, also a contradiction.

Both assumptions are false, thus $r = \frac{g-\beta}{2}$. If g is an even number it follows that $r = p - r = q - r = \frac{g}{2}$, so $C^*_{p,q,r} = C^*_{p,p+q-2r,p-r} = C^*_{p+q-2r,q,q-r} = C^*_{g,g,\frac{g}{2}}$, hence a unique graph maximizes the index ${}^0R_\alpha$. Otherwise, if g is an odd number, we have $r = \frac{g-1}{2}$ and $C^*_{p,q,r} = C^*_{g,g,\frac{g-1}{2}} \simeq C^*_{g+1,g,\frac{g+1}{2}} \simeq C^*_{g,g+1,\frac{g+1}{2}}$. ■

We have a similar result for $\alpha \in (0,1)$:

Lemma 9. *Let $C^*_{p,q,r} \in \mathcal{B}^g_n$ be a graph such that ${}^0R_\alpha(C^*_{p,q,r}) \leq^0 R_\alpha(C^*_{p',q',r'})$ for any $C^*_{p',q',r'} \in \mathcal{B}^g_n$, where $\alpha \in (0,1)$. Then $C^*_{p,q,r} = C^*_{g,g,\frac{g}{2}}$ for g an even number and $C^*_{p,q,r} \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.*

Analogous results also hold for the multiplicative Zagreb indices:

Lemma 10. *Let $C^*_{p,q,r} \in \mathcal{B}^g_n$ be a graph such that $PM_1(C^*_{p,q,r}) \leq PM_1(C^*_{p',q',r'})$ for any $C^*_{p',q',r'} \in \mathcal{B}^g_n$ (or $PM_2(C^*_{p,q,r}) \geq PM_2(C^*_{p',q',r'})$ for any $C^*_{p',q',r'} \in \mathcal{B}^g_n$). Then $C^*_{p,q,r} = C^*_{g,g,\frac{g}{2}}$ for g an even number and $C^*_{p,q,r} \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.*

Now, we can sum up all previously stated facts in the following results.

Theorem 2. *Let G^* be a bicyclic graph of order n and girth $g \geq 3$. Then we have:*

(a) $A^*_{g,g}$ is the unique graph which minimizes the index ${}^0R_\alpha$ for $\alpha \in (0,1)$;

(b) If G^* maximizes any of the indices PM_2 or ${}^0R_\alpha$ for $\alpha \in (-\infty,0) \cup (1,\infty)$ or minimizes the index PM_1 then G^* is the graph $C^*_{g,g,\frac{g}{2}}$ for g an even number and $G^* \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.

Proof. We first treat the zeroth-order general Randić index. From Lemmas 5 and 7 we conclude that $A^*_{g,g}$ is the minimal graph among all graphs of type $(\mathcal{A}_{p,q} \cup \mathcal{B}_{p,q,r}) \cap \mathcal{B}^g_n$ for $\alpha \in (0,1)$ and at the same time, the maximal graph for $\alpha \in (-\infty,0) \cup (1,\infty)$. For the class $\mathcal{C}_{p,q,r} \cap \mathcal{B}^g_n$, following Lemma 10 it results that the corresponding extremal graph is $C^*_{g,g,\frac{g}{2}}$ for even g or isomorphic with $C^*_{g,g,\frac{g-1}{2}}$ for odd g. Hence we must compare the values of the indices for these two graphs to obtain the extremal graph among the bicyclic graphs of given girth g.

Following all previous notations we have:

$${}^0R_\alpha(A^*_{g,g}) = (4r+2\beta-2)2^\alpha + (n-4r-2\beta+1) + (n-4r-2\beta+5)^\alpha,$$

$${}^0R_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) = (3r+2\beta-3)2^\alpha + 3^\alpha + (n-3r-2\beta+1) + (n-3r-2\beta+4)^\alpha,$$

so

$${}^0R_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) -{}^0 R_\alpha(A^*_{g,g}) = r - 2^\alpha(r+1) + (n-3r-2\beta+4)^\alpha - (n-4r-2\beta+5)^\alpha + 3^\alpha.$$

Case (a): $\alpha \in (0,1)$. Applying Lemma 3 with $x = n-4r-2\beta$, $a = r+4$ and $b = 5$, we have $f_{\alpha,r+4,5}(x) < f_{\alpha,r+4,5}(-2)$ for $x > -2$, so

$${}^0R_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) -{}^0 R_\alpha(A^*_{g,g}) < r - 2^\alpha(r+1) + (r+2)^\alpha$$

for all $r \geq 0$. But ${}^0R_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) -{}^0 R_\alpha(A^*_{g,g}) < 0$ by Lemma 4.

Case (b): $\alpha \in (-\infty,0) \cup (1,\infty)$. We proceed in a similar way.

For the PM_1-index we have

$$PM_1(C^*_{g,g,\frac{g-\beta}{2}}) - PM_1(A^*_{g,g}) = (n-3r-2\beta+4)^2 4^{3r+2\beta-3} 3^2 - (n-4r-2\beta+5)^2 4^{4r+2\beta-2}$$

$$= 4^{3r+2\beta-3}\Big\{\Big[(n-4r-2\beta+5)+(r-1)\Big]^2 3^2 - (n-4r-2\beta+5)^2 4^{r+1}\Big\}.$$

Consider now the real function $g : [0,\infty) \to \mathbb{R}$ defined by $g_k(x) = (k+x)^2 3^2 - k^2 4^{x+2}$ with $k \geq 2$. Since $g'_k(x) = 2(k+x)3^2 - k^2 4^{x+2} \ln 4$ and $g''_k(x) = 18 - k^2 4^{x+2} \ln^2 4 < 0$, we get that g' is strictly decreasing and $g'_k(x) < g'_k(0) < 0$ for all $x \geq 0$ and $k \geq 2$. It follows that g is also a strictly decreasing function and $g_k(x) < g_k(0) < 0$ for $x \geq 0$ and $k \geq 2$. Now, considering $k = n - 4r - 2\beta + 5$ and $x = r - 1$, it follows that the expression in the braces is strictly negative. Hence the graph $C^*_{g,g,\frac{g-\beta}{2}}$ minimizes the PM_1-index.

For the PM_2-index we obtain that

$$\begin{aligned} &PM_2(C^*_{g,g,\frac{g-\beta}{2}}) - PM_2(A^*_{g,g}) \\ &\quad = 3^3 4^{3r+2\beta-3}(n-3r-2\beta+4)^{n-3r-2\beta+4} - 4^{4r+2\beta-2}(n-4r-2\beta+5)^{n-4r-2\beta+5} \\ &\quad > 3^3 4^{3r+2\beta-3}(n-4r-2\beta+5)^{n-4r-2\beta+5+(r-1)} - 4^{4r+2\beta-2}(n-4r-2\beta+5)^{n-4r-2\beta+5} \\ &\quad = 4^{3r+2\beta-3}(n-4r-2\beta+5)^{n-4r-2\beta+5}\Big[3^3(n-4r-2\beta+5)^{r-1} - 4^{r+1}\Big]. \end{aligned}$$

Since the number of pendants for the graph $A^*_{g,g}$ is $n - 4r - 2\beta + 1 \geq 0$, it follows that the square paranthesis is strictly positive, so the $C^*_{g,g,\frac{g-\beta}{2}}$ graph also maximizes the PM_2-index. ■

Theorem 3. *(a) The bicyclic graph G^* of order n and girth $g \geq 3$ minimizes the NK-index iff G^* minimizes the index PM_1.*

(b) The bicyclic graph G^* of order n and girth g maximizes the NK^*-index iff G^* maximizes the index PM_2.

Proof. Obvious, using Remark 1. ■

4 General sum–connectivity index

We will keep all notations from the previous section. Moreover, we denote as a triplet (u, v, w) the vertices used in the definition of the t_1^r-transform and we give the next lemma.

Lemma 11. *Let $G \in \mathcal{B}_n$, $P = [u, v, w, z] \subset G$ a simple path, such that $d(v) > 2, d(w) > 2$ and $N_G(v) \cap N_G(w) \subseteq \{u\}$. Then, regardless of the degrees of P's vertices, there exists a t_1^1-transform after which $d(v) = 2$ or $d(w) = 2$.*

Proof. If $P = C_3$, then $z = u$ and we can apply the t_1^1-transform for any of the triplets (u, v, w) or (u, w, v). For an elementary path, if there exists $y \in N_G(w) - \{v\}$ with $d(y) \geq d(u)$, we apply the t_1^1-transform for the triplet (u, v, w). Otherwise, we deduce that $d(u) < d(y)$, for all $y \in N_G(w) - \{v\}$, then $d(z) < d(u)$ and the triplet (z, w, v) satisfies the conditions of Lemma 6. ■

4.1 Bicyclic graphs with k pendants

First, we determine the extremal bicyclic graphs with fixed number of pendants by treating separately each of the three categories of bicyclic graphs.

We begin with the subset of the $\mathcal{A}_{p,q}$-graphs. Let $G \in \mathcal{A}_{p,q}$ be a graph that contains two cycles C_p, C'_q with a common vertex x and some possible trees attached to the cycles, denoted $T_1, \ldots, T_r, r \geq 1, T_i \neq \emptyset$, $1 \leq i \leq r$. We also have $T_i \in \mathcal{T}_{t_i,k_i}$ and $\sum_{i=1}^{r} t_i = n - p - q + 1$, $\sum_{i=1}^{r} k_i = k$. Denote $T_i \cap (C_p \cup C'_q) = \{x_i\}, 1 \leq i \leq r$. We will use the already defined t_1^r-transform, mentioning that this transformation has to be handled with care on the triplets $(u, v, w) \in G$, in order to fulfill the conditions of Lemma 6.

Step I. For each tree $T_i, 1 \leq i \leq r$, we first apply the t_1^r-transforms for all triplets $(u, v, w) \subset T_i$ with $d(u) = 1$ and $v \neq x_i$, hence the conditions from Lemma 6 are satisfied. Thus, all pendant paths will be pushed towards the vertex x_i.

Step II. We apply a new sequence of t_1^r-transforms, this time with the condition $d(u) = 2$, until we obtain $w = x_i$. We denote T'_i the trees obtained after steps I and II. Thus $T'_i \in \mathcal{T}^*_{t_i,k_i}$ for $1 \leq i \leq r$ and $G' = C_p \cup C'_q \cup T'_1 \cup \ldots \cup T'_r$.

Let us denote further $\mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)} = \{G \in \mathcal{A}_{p,q} | G = C_p \cup C'_q \cup T, T \cap C_p \cap C'_q = \{x\}, T \in \mathcal{T}^*_{n,k}$ with k paths from which n_i paths of length $i \geq 1\}$. Then we have $\mathcal{A}^*_{p,q,k} = \bigcup \mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$.

Step III. Now, we unify all resulted star-like subtrees attached to the graph's cycles. Following Lemma 11, for the graph G' we apply the t_1^1-transform for all triplets $(u, v, w) \subset C_p$ and $(u, v, w) \subset C'_q$, then the t_1^r-transform with $r > 1$, whenever possible. After this step, we obtain an $\mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$-graph.

We next treat the case of the $\mathcal{B}_{p,q,r}$-graphs.

Steps I-III. The first two steps are identical to the ones from the previous case. For step III, in a way similar to the $\mathcal{A}_{p,q}$-graphs, we apply the t_1^r-transforms in the $\mathcal{B}_{p,q,r}$ set for any triplet (u, v, w) situated on C_p or on C'_q or on P_r. One of the graphs from Fig. 2 is obtained, where $T_i \in \mathcal{T}^*_{t_i,k_i}, 0 \leq k_i \leq k, 1 \leq i \leq 3$.

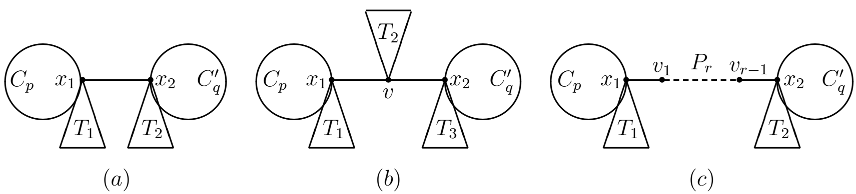

Figure 2: The three types of $\mathcal{B}_{p,q,r}$-graphs resulted after applying all t_1^r-transforms

Step IV. For each of these types of graphs from Fig. 2 we apply further the t_1^r-transform for the triplets (u, x_1, w) with $u \in N_G(x_1) - P_r, w \in P_r$, until we obtain $x_1 = x_2$. For this step these transformations are applied even when one or both of T_1 and T_2 are empty trees. Hence the end result is also an $\mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$-graph.

Now, we treat the category of the $\mathcal{C}_{p,q,r}$-graphs.

Steps I-III. As above, the first two steps remain unchanged. Next, we also start by applying the t_1^r-transforms for all triplets (u, v, w) with u, v, w belonging to P_r or $C_p - P_r$ or $C'_q - P_r$ which satisfy the conditions of Lemma 6. Then, one of the graphs from Fig. 3 is obtained, where $T_i \in T^*_{t_i,k_i}, 0 \leq k_i \leq k, 1 \leq i \leq 5$.

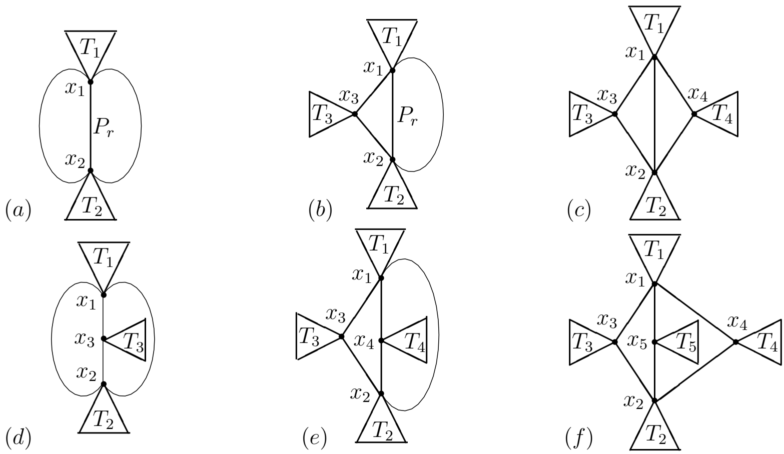

Figure 3: Types of $\mathcal{C}_{p,q,r}$-graphs after applying t_1^r-transforms

Step IV. To strictly increase the value of χ_α, we will continue the process of unifying all subtrees attached to the cycles in one of the vertices x_1 or x_2. But at the same time, we request that these transformations will keep unchanged the girth of the graph.

Lemma 12. *Let G be one of the $\mathcal{C}_{p,q,r}$-graphs from Fig. 3. There exists a sequence of transformations that strictly increases the value of the index χ_α for $\alpha > 1$, after which all pendant paths will be incident either to the vertex x_1 or to the vertex x_2. Moreover, this sequence of transformations keeps unchanged the girth of the graph.*

Proof. We assume that $k_1 \geq k_2 \geq 0$.

Case (a): $p - r > 2, q - r > 2$, $d(y) = 2$ for all $y \in (P_r)$, $r \geq 1$.

If $q-r \geq g$ we can apply the t_1^r-transform to the triplet (u, x_2, x_1), with $u \in N_G(x_2) \cap C_p$. An $\mathcal{A}_{p,q}^{(n_1,n_2,\ldots)}$-graph of girth g is obtained. Otherwise, this transformation would decrease the girth of the graph. In this case, we move the tree T_2 to the vertex x_1 which will make the index χ_α to strictly increase.

We denote $N_G(x_j) \cap T_j = \{x_{j1}, \ldots, x_{jk_j}\}$, $j \in \{1, 2\}$, then:

$$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{j=1}^{2} \sum_{i=1}^{k_1} \Big[(d(x_{ji}) + k_1 + k_2 + 3)^\alpha - (d(x_{ji}) + k_j + 3)^\alpha\Big]$$
$$+\beta\Big[(k_1 + k_2 + 5)^\alpha - (k_1 + 5)^\alpha + 5^\alpha - (k_2 + 5)^\alpha\Big],$$

where $\beta = 2$ for $r = 1$ and $\beta = 3$ for $r > 1$. The double sum is obviously strictly positive and the last square paranthesis is also strictly positive from Lemma 3.

Case (b): $p - r = 2, q - r > 2$, $d(y) = 2$ for all $y \in (P_r)$, $r \geq 1$.

Since the graph girth is 3, we can apply a t_1^r-transform for the triplet (y, x_2, x_1) and so, we reduce this type of graph to an $\mathcal{A}_{p,q}^{(n_1,n_2,\ldots)}$-graph also.

Case (c): $p - r = q - r = 2$, $d(y) = 2$ for all $y \in (P_r)$, $r \geq 1$.

If $r = 1$ we gather one at a time all the trees T_i $(i \in \{1, \ldots, 4\})$ in the vertex x_1, in any order we like. Thus the index will strictly increase. We begin, for example, with the tree T_3, knowing that $k_3 > 0$:

$$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{i=1}^{k_1} [(d(x_{1i}) + k_1 + k_3 + 3)^\alpha - (d(x_{1i}) + k_1 + 3)^\alpha]$$
$$+\sum_{i=1}^{k_3} [(d(y_{1i}) + k_1 + k_3 + 3)^\alpha - (d(y_{1i}) + k_3 + 2)^\alpha] + [(k_2 + 5)^\alpha - (k_2 + k_3 + 5)^\alpha]$$
$$+[(k_1 + k_2 + k_3 + 6)^\alpha - (k_1 + k_2 + 6)^\alpha] + [(k_1 + k_3 + k_4 + 5)^\alpha - (k_1 + k_4 + 5)^\alpha],$$

which is strictly positive since $k_1 \geq k_2$, $k_4 \geq 0$ and using Lemma 3. Then, we continue to increase the index χ_α moving in x_1 the other trees, with simplified computations.

If $r > 1$ we must first move the tree T_2 to ensure the increasing of χ_α:

$$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{j=1}^{2} \sum_{i=1}^{k_1} \Big[(d(x_{ji}) + k_1 + k_2 + 3)^\alpha - (d(x_{ji}) + k_j + 3)^\alpha\Big]$$
$$+\sum_{i=3}^{4} \Big\{ \Big[(k_1 + k_2 + k_i + 5)^\alpha - (k_1 + k_i + 5)^\alpha\Big] + \Big[(k_i + 5)^\alpha - (k_2 + k_i + 5)^\alpha\Big] \Big\}$$
$$+\Big[(k_1 + k_2 + 5)^\alpha - (k_1 + 5)^\alpha\Big] + \Big[5^\alpha - (k_2 + 5)^\alpha\Big] > 0.$$

Then, we continue to move in x_1 the other trees.

Case (d): If $q \geq g+1$ we apply the t_1^1-transform for the triplet (u, x_2, x_3), where $u \in N_G(x_2) \cap C_p$ and we reduce this case to the case (a). Otherwise, we first move the tree T_2 to the vertex x_1, then T_3 (performing similar computations as above).

Case (e): If $q \geq 5$ and $d(x_1) \geq d(x_3)$ we apply the t_1^1-transform for the triplet (x_3, x_2, x_4), then for (x_2, x_3, x_1) and we reduce this case to the case (a) with $r = 1$. Otherwise, we first move T_2 to x_1, then the other remaining trees.

Case (f): Since $p = q = 4$, no matter how we would apply the t_1^1-transform, the girth would become equal to 3, so we must move the subtrees to the vertex x_1 one by one, begining with the tree T_2. ■

Now we can give our next theorem.

Theorem 4. *Let G^* be a graph which maximizes the general sum-connectivity index for $\alpha > 1$ in the set of bicyclic graphs of order n with $0 \leq k < n-4$ pendant vertices. Then we have:*

(a) $G^* \in \mathcal{A}_{p,q,0}$ with $p \geq 3, q \geq 3$, if $k = 0$;

(b) $G^* \simeq A_{3,3,k}^{(n_1,n_2,\ldots)}$ with $n_1 = 2k+5-n, n_2 = n-k-5, n_i = 0$ for $i \geq 3$, if $k > 0$ and $k+4 < n \leq 2k+4$;

(c) $G^* \in \mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$ with $n_1 = 0$, if $k > 0$ and $n > 2k+4$.

Proof. From the proof of the last lemma we conclude that for the group of the $\mathcal{C}_{p,q,r}$-graphs we strictly increased the value of the index χ_α by applying t_1^r-transforms such that an $\mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$ or another $\mathcal{C}_{p,q,r,k}^{(n_1,n_2,\ldots)}$-graph was obtained. Since for the family of the $\mathcal{B}_{p,q,r}$-graphs we also obtained an $\mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$-graph, it remains to decide which of these two types of graphs maximizes the value of the index χ_α.

Case (a): $k = 0$.

If $r > 1$, following the notations from Fig. 3, we denote $u \in N_G(x_1) - P_r$ and also $w \in N_G(x_2) \cap P_r$. We apply the t_1^1-transform for the triplet (u, x_1, w), thus any $\mathcal{C}_{p,q,r,0}$-graph with $r > 1$ will be transformed into a $\mathcal{C}_{p',q',1,0}$-graph, with a greater value for the index χ_α. So, let $A^* \in \mathcal{A}_{p,q,0}$ and $C^* \in \mathcal{C}_{p,q,1,0}$, then we have

$$\chi_\alpha(A^*) - \chi_\alpha(C^*) = 2(6^\alpha - 5^\alpha) + 6^\alpha - 2 \cdot 5^\alpha + 4^\alpha > 0,$$

from the Jensen's inequality.

For $k > 1$, we first need to give a transformation wich extracts an internal edge uv from a cycle of length $p > 3$ or from a pendant path of length $r > 2$ and reattaches it in extension to any path of length one xx'. Let $uv \in E(G)$ an internal edge such that $d(v) = 2$ and $\{v'\} = N_G(v) - \{u\}$. Now we define $t_4(G) = G - uv - vv' + uv' + xv'$. We can write $d(x) = k + \beta, \beta \in \{3, 4\}$, $d(u) = 2 + \beta', \beta' \in \{0, 1\}$ and $d(v') \in \{1, 2, k + 3\}$, depending on the position of the edge uv in the graph G. Thus:

$$\chi_\alpha(t_4(G)) - \chi_\alpha(G) = (k + 5 + \beta')^\alpha - (k + 4)^\alpha + 3^\alpha - (4 + \beta')^\alpha > 0,$$

from Lemma 3.

By decreasing the number of paths of length one, the value of χ_α will strictly increase, thus obtaining two graphs $A^* \in \mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$ and $C^* \in \mathcal{C}_{p,q,r,k}^{(n_1,n_2,\ldots)}$ that maximize the index χ_α, each in their respective category. Now we compare the values of the index χ_α for these two graphs.

Case (b): $k > 0$ and $n \leq 2k + 4$.

In this case $A^* \in \mathcal{A}_{3,3,k}^{(n_1,n_2,\ldots)}$ with $n_1 = 2k + 5 - n, n_2 = n - k - 5, n_i = 0$ for $i \geq 3$ and $C^* \in \mathcal{C}_{3,3,1,k}^{(n_1,n_2,\ldots)}$ with $n_1 = 2k + 4 - n, n_2 = n - k - 4, n_i = 0$ for $i \geq 3$ and

$$\chi_\alpha(A^*) = 2 \cdot 4^\alpha + (n - k - 1)(k + 6)^\alpha + (2k + 5 - n)(k + 5)^\alpha + (n - k - 5)3^\alpha,$$

$$\chi_\alpha(C^*) = 2 \cdot 5^\alpha + (n - k - 2)(k + 5)^\alpha + (2k + 4 - n)(k + 4)^\alpha + (n - k - 4)3^\alpha + (k + 6)^\alpha,$$

so we have:

$$\begin{aligned}
&\chi_\alpha(A^*) - \chi_\alpha(C^*) \\
&= (n-k-2)(k+6)^\alpha + (3k+7-2n)(k+5)^\alpha + (2k+4-n)(k+4)^\alpha - 2\cdot 5^\alpha + 2\cdot 4^\alpha - 3^\alpha \\
&= (n - k - 2)(k + 6)^\alpha + (3k + 6 - 2n)(k + 5)^\alpha + (2k + 4 - n)(k + 4)^\alpha \\
&\quad + (k + 5)^\alpha - 2 \cdot 5^\alpha + 2 \cdot 4^\alpha - 3^\alpha \\
&\geq (n - k - 2)\Big[(k + 6)^\alpha - (k + 5)^\alpha\Big] + (2k + 4 - n)\Big[(k + 4)^\alpha + (k + 5)^\alpha\Big] \\
&\quad + (6^\alpha - 2 \cdot 5^\alpha + 4^\alpha) + 4^\alpha - 3^\alpha.
\end{aligned}$$

Since $k + 4 < n \leq 2k + 4$, we have $n - k - 2 > 2$ and $2k + 4 - n \geq 0$, so using Jensen's inequality we obtain $\chi_\alpha(A^*) > \chi_\alpha(C^*)$.

Case (c): $k > 0$ and $n > 2k + 4$.

Now we have $A^* \in \mathcal{A}_{p,q,k}^{(n_1,n_2,\ldots)}$and $C^* \in \mathcal{C}_{p,q,1,k}^{(n_1,n_2,\ldots)}$ with $n_1 = 0$. Thus

$$\chi_\alpha(A^*) - \chi_\alpha(C^*) = (k + 2)\Big[(k + 6)^\alpha - (k + 5)^\alpha\Big] + (k + 6)^\alpha + 4^\alpha - 2 \cdot 5^\alpha > 0,$$

then the conclusion. ■

4.2 Bicyclic graphs with given girth g

Since all operations performed before keep unchanged the graph's girth, we shall use the $\mathcal{A}^*_{p,q,k}$ and $C^*_{p,q,r,k}$- graphs obtained in the proof of Lemma 12. We remember the t_2-transform defined in the previous section and we have a similar result.

Lemma 13. *Let $G \in \mathcal{A}^*_{p,q,k} \cup C^*_{p,q,r,k}$ and $G' = t_2(G)$ be two graphs. Then we have $\chi_\alpha(G') > \chi_\alpha(G)$.*

Proof. Denoting $N_G(x) = \{x'_1, \ldots, x'_k\}$, $d(x) = k + \beta$, where $\beta = 4$ for $G \in \mathcal{A}^*_{p,q,k}$ and $\beta = 3$ for $G \in C^*_{p,q,r,k}$, we have:
$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{i=1}^{k+2-d(v)} \Big[(d(x'_i) + k + \beta + 1)^\alpha - (d(x'_i) + k + \beta)^\alpha\Big] + (k + \beta + 2)^\alpha - 4^\alpha$,
which is stricly positive, taking into account that $d(v) \in \{1, 2\}$. ∎

Similar to the strategy used for the topological indices based on vertices, we apply the t_2-transform whenever possible, without changing the graph's girth. Thus we also obtain $A^*_{p,q}$ or $C^*_{p,q,r}$-graphs. As such, we give the next lemma.

Lemma 14. *Let $C^*_{p,q,r} \in \mathcal{B}^g_n$ be a graph such that $\chi_\alpha(C^*_{p,q,r}) \geq \chi_\alpha(C^*_{p',q',r'})$ for any $C^*_{p',q',r'} \in \mathcal{B}^g_n$. Then $C^*_{p,q,r} = C^*_{g,g,\frac{g}{2}}$ for g an even number and $C^*_{p,q,r} \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.*

Proof. We follow the same reasoning as in the results obtained in the previous section on indices based on vertices. All we have to do is to remake the computations for the t_3-transform, in order to show that it strictly increases the index χ_α:
$\chi_\alpha(G') - \chi_\alpha(G) = 2\Big[(k+6)^\alpha - (k+5)^\alpha\Big] + k\Big[(k+5)^\alpha - (k+4)^\alpha\Big] + 5^\alpha + (k+5)^\alpha - 2 \cdot 4^\alpha > 0.$ ∎

Theorem 5. *Let G^* be a bicyclic graph of order n and girth $g \geq 3$ which maximizes the index χ_α for $\alpha > 1$. Then G^* is the graph $C^*_{g,g,\frac{g}{2}}$ for g an even number and $G^* \simeq C^*_{g,g,\frac{g-1}{2}}$ for g odd.*

Proof. Following all above facts, we conclude that we need to compare the values of the index χ_α for $A^*_{g,g}$ and $C^*_{g,g,\frac{g-\beta}{2}}$, where $\beta = 0$ for g even and $\beta = 1$ for g odd.

For $r > 1$ we have:

$$\begin{aligned}
&\chi_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) - \chi_\alpha(A^*_{g,g})\\
&\quad = (n-3r-2\beta+1)(n-3r-2\beta+5)^\alpha + 3(n-3r-2\beta+6)^\alpha + (3r+2\beta-6)4^\alpha + 3 \cdot 5^\alpha\\
&\qquad -(n-4r-2\beta+1)(n-4r-2\beta+6)^\alpha - 4(n-4r-2\beta+7)^\alpha - (4r+2\beta-4)4^\alpha.
\end{aligned}$$

We denote $a = n - 3r - 2\beta$, then we have

$$\begin{aligned}
&\chi_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) - \chi_\alpha(A^*_{g,g}) \\
&\quad = (a+1)(a+5)^\alpha + 3(a+6)^\alpha + (n-a-6)4^\alpha + 3\cdot 5^\alpha \\
&\qquad -(a+1-r)(a+6-r)^\alpha - 4(a+7-r)^\alpha - (n-a+r-4)4^\alpha \\
&\quad = a\Big[(a+5)^\alpha - (a+6-r)^\alpha\Big] + 3\Big[(a+6)^\alpha - (a+7-r)^\alpha\Big] + \Big[(a+5)^\alpha - (a+7-r)^\alpha\Big] \\
&\qquad +(r-1)\Big[(a+6-r)^\alpha - 4^\alpha\Big] + 3\Big[5^\alpha - 4^\alpha\Big].
\end{aligned}$$

Since $r > 1$, we have $a+6-r < a+5$, so the first three square parenthesis are (strictly) positive. Remembering also that the number of pendants for the graph $A^*_{g,g}$ is $n-4r-2\beta+1 \geq 0$, it follows that $a = n-3r-2\beta \geq r-1$, so $a+6-r \geq 5$, thus the next square paranthesis is strictly positive also. Hence the conclusion.

If $r = 1$ it follows that $\chi_\alpha(C^*_{g,g,\frac{g-\beta}{2}}) - \chi_\alpha(A^*_{g,g}) = n^\alpha + (n+2)^\alpha - 2(n+1)^\alpha > 0$ from Jensen's inequality. ■

Remark 3. We note that the graph obtained in the last theorem is the same with the graph that maximizes the indices PM_2, ${}^0R_\alpha$ for $\alpha \in (-\infty, 0) \cup (1, \infty)$, χ_α for $\alpha > 1$ and minimizes the index PM_1.

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