MAXIMUM GENERAL SUM-CONNECTIVITY INDEX WITH $-1 \le \alpha < 0$ FOR BICYCLIC GRAPHS

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In the present paper, we show that in the class of connected bicyclic graphs G of order $n \ge 4$, the set of graphs G having maximum general sum-connectivity index $\chi_\alpha(G)$ consists of two vertex disjoint cycles joined by an edge or two cycles having a common edge, if $-1 \le \alpha < 0$. This extends the corresponding result by Zhu, Chang and Wei on the harmonic index of bicyclic graphs [Ars Combinatoria, **110** (2013), 97–104].

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1. INTRODUCTION

Let G be a simple graph having vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $u \in V(G)$ is denoted $d(u)$. If $d(u) = 1$ then u is called pendant; a pendant edge is an edge containing a pendant vertex. $N(v)$ is the set of vertices adjacent to v. For $A \subset E(G)$, $G - A$ denotes the graph deduced from G by deleting the edges of A and the graph obtained by the deletion of an edge $uv \in E(G)$ is denoted $G - uv$. Conversely, if $A \subset E(\overline{G})$, $G + A$ is the graph obtained from G by adding the edges of A. Attaching a path P_r to a vertex v of a graph means adding an edge between v and a terminal vertex of the path. If $r = 1$, then we attach a pendant vertex.

For other notations in graph theory, we refer [1].

The general sum-connectivity index of graphs was proposed by Zhou and Trinajstić [9]. It is denoted by $\chi_\alpha(G)$ and defined as

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

where α is a real number. The sum-connectivity index, previously proposed by the same authors [8] is $\chi_{-1/2}(G)$. A particular case of the general sum-connectivity index is the harmonic index, denoted by $H(G)$ and defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d(u)+d(v)}=2\chi_{-1}(G).$$

Zhu, Chang and Wei [10] proved that in the set of connected bicyclic graphs of order $n\geq 4$ maximum harmonic index is reached for several graphs which consist of two vertex disjoint cycles joined by an edge or two cycles having an edge in common. Tache [5] studied the maximum general sum-connectivity index for bicyclic graphs of order $n\geq 4$ for $\alpha\geq 1$. In this case, the extremal graph is unique and consists of two cycles C_3 having a common edge and $n-4$ pendant vertices adjacent to a vertex of degree three of this graph. Other extremal properties of the sum-connectivity or general sum-connectivity index for trees, unicyclic graphs and general graphs were proposed in [2, 3, 6, 7].

These graph invariants, which are useful for chemical purposes, were named "topological indices" or, less confusing, "molecular structure-descriptors" and their main use is for designing so-called quantitative structure-property relations ($QSPR$) and quantitative structure-activity relations ($QSAR$) in chemistry [4].

In this paper, we study the maximum general sum-connectivity index $\chi_\alpha(G)$ in the class of connected bicyclic graphs G of order $n\geq 4$ and extend the results of Zhu, Chang and Wei for every $-1\leq\alpha<0$ (including here the case of the harmonic index).

In Section 2, we define two transformations which strictly increase the general sum-connectivity index of a graph, which will be used in the last section. In Section 3, we determine the connected bicyclic graphs G of order $n\geq 4$ reaching maximum $\chi_\alpha(G)$ for $-1\leq\alpha<0$.

2. PRELIMINARY RESULTS

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

LEMMA 2.2. *Consider a connected graph G with $|V(G)|\geq 3$ and two adjacent vertices $v,w\in V(G)$. Let H be the graph obtained from G by attaching a path $P=u_1,\ldots,u_p$ $(p\geq 1)$ to v such that u_p is the pendant vertex of the path P in H. Let $H'=H-\{vw\}+\{u_pw\}$. If $3\leq d_H(v)\leq 5$ and $2\leq d_H(w)\leq 3$ then we have $\chi_\alpha(H')>\chi_\alpha(H)$ for $-1\leq\alpha<0$.*

Proof. Denote $d=d_H(v)$ and let $N_H(v)\backslash\{u_1,w\}=\{x_1,\ldots,x_{d-2}\}$. If $p=1$, then for $\alpha<0$ we have: $\Delta=\chi_\alpha(H')-\chi_\alpha(H)=(d_H(w)+2)^\alpha-$

$(d_H(w)+d)^\alpha + \sum_{i=1}^{d-2} [(d_H(x_i)+d-1)^\alpha - (d_H(x_i)+d)^\alpha] > 0$ for every $d \ge 3$. If $p \ge 2$, then

$$\Delta = \chi_\alpha(H') - \chi_\alpha(H) = S + \sum_{i=1}^{d-2} [(d_H(x_i)+d-1)^\alpha - (d_H(x_i)+d)^\alpha],$$

where $S = (d+1)^\alpha - (d+2)^\alpha + (d_H(w)+2)^\alpha - (d_H(w)+d)^\alpha + 4^\alpha - 3^\alpha$. We shall prove that $S \ge 0$ for every $3 \le d \le 5$ and $2 \le d_H(w) \le 3$ if $\alpha < 0$. Since the function $(x+2)^\alpha - (x+d)^\alpha$ is strictly decreasing in $x > 0$ for $d \ge 3$ it follows that $(d_H(w)+2)^\alpha - (d_H(w)+d)^\alpha \ge 5^\alpha - (d+3)^\alpha$, therefore $S \ge \varphi(d,\alpha)$, where

(1) $$\varphi(d,\alpha) = (d+1)^\alpha - (d+2)^\alpha - (d+3)^\alpha + 5^\alpha + 4^\alpha - 3^\alpha.$$

For $d = 3$ (1) yields $\varphi(3,\alpha) = 2 \cdot 4^\alpha - 3^\alpha - 6^\alpha$. Equation $\varphi(3,\alpha) = 0$ has roots $\alpha_0 = 0$ and $\alpha_2 = -1$ and $\varphi(3,\alpha) \ge 0$ for every $-1 \le \alpha < 0$ [11]. For $d = 4$ we get $\varphi(4,\alpha) = 4^\alpha - 3^\alpha + 2 \cdot 5^\alpha - 6^\alpha - 7^\alpha$, equation $\varphi(4,\alpha) = 0$ has roots α_0 and $\alpha_3 \approx -1.162$, $\varphi(4,\alpha)$ being strictly positive for $\alpha_3 < \alpha < 0$.

Similarly, for $d = 5$, $\varphi(5,\alpha) = 4^\alpha + 5^\alpha + 6^\alpha - 3^\alpha - 7^\alpha - 8^\alpha$ has roots α_0 and $\alpha_4 \approx -1.284$ and $\varphi(5,\alpha) > 0$ for $\alpha_4 < \alpha < 0$. Consequently, $\Delta > S \ge 0$ for every $-1 \le \alpha < 0$. $\square$

3. MAIN RESULT

THEOREM 3.1. *Let G be a connected bicyclic graph of order $n \ge 4$. If $-1 \le \alpha < 0$ then $\chi_\alpha(G) \le 6^\alpha + 4 \cdot 5^\alpha + (n-4)4^\alpha$. Equality holds if and only if G consists of two vertex disjoint cycles joined by an edge or two cycles having a common edge.*

Proof. Let G be a graph with the above-mentioned properties having a maximum general sum-connectivity index. It follows that G has $n+1$ edges. If $n = 4$ G is unique and consists of two triangles having a common edge; it is denoted $C_4 + e$. We have $\chi_\alpha(C_4 + e) = 6^\alpha + 4 \cdot 5^\alpha$ and the property holds. Let $n \ge 5$. For a graph H by successively deleting pendant vertices we obtain another graph, denoted $S(H)$ and called the skeleton of H. G being connected and bicyclic, it is clear that $S(G)$ belongs to one of the following five classes, denoted A, B, C, D, E: A consists of two cycles having a common vertex; B and C are composed from two vertex disjoint cycles joined by a path P_r of length $r-1 \ge 2$ and $r-1 = 1$, respectively and D and E consist of two cycles having a common path P_r with $r \ge 3$ and $r = 2$, respectively. It is clear that G is composed from $S(G)$ and some vertex disjoint trees, each having exactly a common vertex with $S(G)$. Since $\chi_\alpha(G)$ is maximum, by Lemma 2.1 it follows that all these trees may be only pendant paths. Also, Lemma 2.2 implies that every such graph containing at least one pendant path cannot be extremal, so we have $S(G) = G$ and $G \in A \cup B \cup C \cup D \cup E$. If $G \in A$ we obtain $\chi_\alpha(G) = f_1(\alpha) = 4 \cdot 6^\alpha + (n-3)4^\alpha$; if $G \in B \cup D$ then $\chi_\alpha(G) = f_2(\alpha) = 6 \cdot 5^\alpha + (n-5)4^\alpha$ and for $G \in C \cup E$ we have $\chi_\alpha(G) = f_3(\alpha) = 6^\alpha + 4 \cdot 5^\alpha + (n-4)4^\alpha$.

We deduce that $f_3(\alpha) > f_1(\alpha)$ is equivalent to $4 \cdot 5^\alpha - 4^\alpha - 3 \cdot 6^\alpha > 0$ for $-1 \le \alpha < 0$. But equation $4 \cdot 5^\alpha - 4^\alpha - 3 \cdot 6^\alpha = 0$ has roots $\alpha_0 = 0$ and $\alpha_5 \approx -4.358$ (equivalently, α_5 is the unique root of the equation $\frac{4^\alpha - 5^\alpha}{5^\alpha - 6^\alpha} = 3$) and $f_3(\alpha) > f_1(\alpha)$ for $\alpha_5 < \alpha < 0$. Also $f_3(\alpha) > f_2(\alpha)$ is equivalent to $6^\alpha - 2 \cdot 5^\alpha + 4^\alpha > 0$, which is true by Jensen's inequality since the function x^α is strictly convex for $-1 \le \alpha < 0$. $\square$

Because $H(G) = 2\chi_{-1}(G)$, the result also holds for the harmonic index.

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