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EXTREMAL RESULTS CONCERNING THE GENERAL SUM-CONNECTIVITY INDEX IN SOME CLASSES OF CONNECTED GRAPHS

Ioan Tomescu

Faculty of Mathematics and Computer Science, University of Bucharest, Romania

ioan@fmi.unibuc.ro

Abstract This paper surveys extremal properties of general sum-connectivity index $\chi_\alpha(G)$ in several classes of connected graphs of given order for some values of the parameter α: a) trees; b) connected unicyclic or bicyclic graphs; c) graphs of given connectivity.
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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. The minimum degree of G is denoted $\delta(G)$ and the complement of G is $\overline{G}$. The girth of a graph G containing cycles is the length of a shortest cycle of G. The distance between vertices u and v of a connected graph, denoted by $d(u, v)$, is the length of a shortest path between them. The diameter of G is the maximum distance between vertices of G. If $A \subset V(G)$ and $u \in V(G)$, the distance between u and A is $d(u, A) = \min_{v \in A} d(u, v)$. If $x \in V(G)$, $G - x$ denotes the subgraph of G obtained by deleting x and its incident edges.
A similar notation is $G - xy$, where $xy \in E(G)$. $K_{p,q}$ will denote the complete bipartite graph, where the partite sets contain p and q vertices, respectively. Given a graph G, a subset S of $V(G)$ is said to be an independent set of G if every two vertices of S are not adjacent. The maximum number of vertices in an independent set of G is called the independence number of G and is denoted by $\alpha(G)$. $K_{1,n-1}$ and P_n will denote, respectively, the star and the path on n vertices. For two vertex-disjoint graphs G and H, the join $G + H$ is obtained by joining by edges each vertex of G to all vertices of H and the union $G \cup H$ has vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

The connectivity of a graph G, written $\kappa(G)$, is the minimum size of a vertex set S such that $G - S$ is disconnected or has only one vertex. A graph G is said to be k-connected if its connectivity is at least k. Similarly, the edge-connectivity of G, written $\kappa'(G)$, is the minimum size of a disconnecting set of edges. For every graph G we have $\kappa(G) \le \kappa'(G)$. Since a tree on n vertices is a bipartite graph, at least one partite set, which is an independent set, has at least $n/2$ vertices, which implies that for any tree T we have $\alpha(T) \ge \lceil n/2 \rceil$ and this bound is reached for paths. Also, $\alpha(T) \le n-1$ and the equality holds only for the star graph. For every $n \ge 2$ and $n/2 \le s \le n-1$ the spur $SP_{n,s}$ [4] is a tree consisting of $2s-n+1$ edges and $n-s-1$ paths of length 2 having a common endvertex; in other words, it is obtained from a star $K_{1,s}$ by attaching a pendant edge to $n-s-1$ pendant vertices of $K_{1,s}$. We have $\alpha(SP_{n,s}) = s$. A bistar of order n, denoted by $BS(p,q)$, consists of two vertex disjoint stars, $K_{1,p}$ and $K_{1,q}$, where $p+q = n-2$, and a new edge joining the centers of these stars. For $n \ge 3$ and $0 \le k \le n-3$, let $C_{n-k,k}$ denote the unicyclic graph of order n consisting of a cycle C_{n-k} and k pendant edges attached to a unique vertex of C_{n-k}. For other notations in graph theory, we refer [1].

The general sum-connectivity index of graphs was proposed by Zhou and Trinajstić [18]. 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 [17] 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

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

The zeroth-order general Randić index, denoted by ${}^0R_\alpha(G)$ is defined as

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

where α is a real number. For $\alpha = 2$ this index is also known as first Zagreb index (see [7]).

These graph invariants, that are useful for chemical purposes, were named topological indices, or, less confusing, molecular structure-descriptors. Their main use is for designing so-called quantitative structure-property relations, QSPR and quantitative structure-activity relations, QSAR. In this context structure means molecular stucture, property some physical or chemical property, and activity some pharmacologic, biologic, toxicologic, or similar property [7].

In the next sections we shall present some results about graphs having maximum or minimum general sum-connectivity index in various classes of connected graphs for some values of the parameter α.

2. GENERAL SUM-CONNECTIVITY INDEX FOR TREES

In the paper proposing new index $\chi_\alpha(G)$ [18] the following result was deduced:

Theorem 2.1. *Let T be a tree with $n \geq 4$ vertices. If $\alpha > 0$, then:*

$$2 \cdot 3^\alpha + (n-3)4^\alpha \leq \chi_\alpha(T) \leq (n-1)n^\alpha$$

with left (right, respectively) equality if and only if $T = P_n$ ($T = K_{1,n-1}$, respectively). If $\alpha < 0$, then the above inequalities on $\chi_\alpha(T)$ are reversed, where the upper bound holds for $\alpha \geq 1 - \frac{\log 2}{\log(4/3)} \approx -1.4094$.

The maximum value for the general sum-connectivity indices of n-vertex trees and the corresponding extremal trees for $\alpha < \gamma_0$, where $\gamma_0 \approx -4.3586$ is the unique root of the equation $(4^x - 5^x)/(5^x - 6^x) = 3$ has been deduced in [6]:

Theorem 2.2. *In the set of n-vertex trees T with $n \geq 4$, if $\alpha < \gamma_0$ maximum of $\chi_\alpha(T)$ if reached if and only if T consists of $(n-1)/2$ copies of P_3 having a common endvertex if n is odd and of $(n-4)/2$ copies of P_3 and a copy of P_4 having a common endvertex if n is even.*

For every integers n, p with $2 \leq p \leq n-1$, let $S_{n,p}$ denote the tree with p pendant vertices formed by attaching $p-1$ pendant vertices to an endvertex of the path P_{n-p+1}. In particular $S_{n,2} = P_n$ and $S_{n,n-1} = K_{1,n-1}$. Minimum value of $\chi_\alpha(T)$ for trees of given diameter and $-1 \leq \alpha < 0$ has been deduced in [11] using graph transformations and some parametric inequalities:

Theorem 2.3. *For every $-1 \leq \alpha < 0$ in the set of trees T having order $n \geq 3$ and diameter equal to d $(2 \leq d \leq n-1)$, $\chi_\alpha(T)$ is minimum if and only if $T = S_{n,n-d+1}$.*

An ordering of the trees T having minimum $\chi_\alpha(T)$ was also obtained in [11]:

Theorem 2.4. *For every $-1 \leq \alpha < 0$ there exists $n_0(\alpha) > 0$ such that for every $n \geq n_0(\alpha)$ the trees T having smallest $\chi_\alpha(T)$ are $K_{1,n-1}$, $BS(n-3,1)$, $BS(n-4,2)$, $S_{n,n-3}$ and $BS(n-5,3)$ (in this order). Also we have $n_0(-1) = 16$.*

If we restrict ourselves to the set of trees with given order and number of pendant vertices, we have the following result [11]:

Theorem 2.5. *Let T be a tree with $n \geq 5$ vertices and p pendant vertices, where $3 \leq p \leq n-2$ and $-1 \leq \alpha < 0$. Then $\chi_\alpha(T)$ is minimum if and only if $T = S_{n,p}$.*

The following theorem characterizes trees T of given order and independence number with maximum $\chi_\alpha(T)$ for $\alpha > 1$ [13]:

Theorem 2.6. *Let $n \geq 2$, $n/2 \leq s \leq n-1$ and T be a tree of order n with independence number s. Then for every $\alpha > 1$, both $\chi_\alpha(T)$ and ${}^0R_\alpha(T)$ are maximum if and only if $T = S_{n,s}$, the spur graph.*

3. GENERAL SUM-CONNECTIVITY INDEX FOR CONNECTED UNICYCLIC AND BICYCLIC GRAPHS

A connected unicyclic graph of order n has a unique cycle and n edges; it can be obtained from a tree T of order n by adding a new edge between two nonadjacent vertices of T. Similarly, a connected bicyclic graph has two linear independent cycles. It has $n + 1$ edges and can be deduced from a tree T of order n by adding two edges between two pairs of nonadjacent vertices of T.
The first results about connected unicyclic graphs of given order having minimum general sum-connectivity index were deduced in [5]. In order to show these results let $S_n(a, b, c)$ be the n-vertex graph obtained by attaching $a-2, b-2$ and $c-2$ pendant vertices to the three vertices of a triangle, respectively, where $a + b + c = n + 3$ and $a \geq b \geq c \geq 2$.

Theorem 3.1. *Among the set of n-vertex unicyclic graphs with $n \geq 5$, for $\alpha > 0$, cycle C_n is the unique graph with the minimum general sum-connectivity index and for $-1 \leq \alpha < 0$, $S_n(n-1, 2, 2)$ and $S_n(n-2, 3, 2)$ are respectively the unique graphs with the minimum and the second minimum general sum-connectivity indices.*

Note that $S_n(n-1, 2, 2)$ consists of a triangle and $n-3$ pendant vertices incident to the same vertex of this triangle. This extremal graph has girth equal to 3. If G has girth $k \geq 4$ extremal graphs are given by the next theorem [12]:

Theorem 3.2. *Let G be a connected unicyclic graph of order n and girth k, where $n \geq k \geq 4$ and $-1 \leq \alpha < 0$. Then $\chi_\alpha(G) \geq \chi_\alpha(C_{k,n-k})$, and equality holds if and only if $G = C_{k,n-k}$, where $C_{k,n-k}$ denotes the cycle C_k with $n-k$ pendant edges attached to a single vertex of C_k.*

Let $A(n, k)$ denote the set of unicyclic graphs of order n consisting of C_k, $n-k-1$ pendant edges incident to a vertex $x \in V(C_k)$ and one pendant edge incident to a vertex $y \in V(C_k)$, such that $d(x, y) \geq 2$. In the set of connected unicyclic graphs of order n and girth k, where $n \geq k+2 \geq 6$ and $-1 \leq \alpha < 0$ the graphs having the second minimum general sum-connectivity index are graphs in $A(n, k)$ [12].
A characterization of connected unicyclic graphs of order n having k pendant vertices and minimum general sum-connectivity index was done for $-1 \leq \alpha < 0$ in [14]:

Theorem 3.3. *Let G be a connected unicyclic graph of order $n \geq 3$ with k pendant vertices $(0 \leq k \leq n-3)$. If $-1 \leq \alpha < 0$ then $\chi_\alpha(G) \geq f(n, k) = k(k+3)^\alpha + 2(k+4)^\alpha + (n-k-2)4^\alpha$. Equality holds if and only if $G = C_{n-k,k}$, the graph consisting of C_{n-k} and k pendant edges incident to a unique vertex of this cycle.*

Since function $f(n, k)$ is increasing in k, we get:

Corollary 3.1. *If $-1 \leq \alpha < 0$, in the class of unicyclic connected graphs G of order n, $\chi_\alpha(G)$ is minimum if and only if $G = C_{3,n-3}$,*

property also stated by Theorem 3.1.
The extremal connected bicyclic graphs of order n for $\alpha \geq 1$ were deduced in [9] and [10] as follows:

Theorem 3.4. *The unique graph with the largest general sum-connectivity index for $\alpha \geq 1$ among all connected bicyclic graphs of order n, consists of two triangles having a common edge and other $n - 4$ pendant edges incident to a vertex of degree three of this graph.*

Theorem 3.5. *The set of graphs which minimize the general sum-connectivity index in the set of the connected bicyclic graphs of order n for $\alpha \geq 1$ is $A \cup B$, where A is the set of graphs consisting of two vertex disjoint cycles C_p and C_q, joined by a path P_r and B the set of those graphs formed by two cycles C_{p+r} and C_{q+r}, having in common a path P_r, provided $r \geq 2$.*

4. GENERAL SUM-CONNECTIVITY INDEX FOR *K*-CONNECTED GRAPHS

First we consider the minimum $\chi_\alpha(G)$ in the class of graphs G of order $n \geq 3$ and minimum degree $\delta(G) \geq 2$, when $-1 \leq \alpha < \alpha_0$, where $\alpha_0 \approx -0.866995$ is the unique root of the equation $4(4^x - 5^x) = 6^x$. A similar investigation was done when graphs G are triangle-free for $-1 \leq \alpha < \beta_0$, where $\beta_0 = \frac{\ln 6/5}{\ln 4/5} \approx -0.81706$. The proofs of the next two theorems use induction, several approximations of exponential functions by polynomials using Taylor formula and some properties of convex functions, like Jensen's inequality [15].

Theorem 4.1. *Let G be a graph of order $n \geq 3$ with $\delta(G) \geq 2$. If $-1 \leq \alpha < \alpha_0$ then $\chi_\alpha(G) \geq f(n) = 2(n-2)(n+1)^\alpha + 2^\alpha(n-1)^\alpha$. Equality holds if and only if $G = K_2 + \overline{K_{n-2}}$.*

Theorem 4.2. *Let $-1 \leq \alpha < \beta_0$ and G be a triangle-free graph of order $n \geq 4$ with $\delta(G) \geq 2$. Then $\chi_\alpha(G) \geq g(n) = 2(n-2)n^\alpha$ and equality is reached if and only if $G = K_{2,n-2}$.*

Since all 2-connected graphs G have $\delta(G) \geq 2$ and both $K_2 + \overline{K_{n-2}}$ and $K_{2,n-2}$ are 2-connected, we deduce the following corollaries.

Corollary 4.1. *If G is a 2-connected graph of order $n \geq 3$ and $-1 \leq \alpha < \alpha_0$, then $\chi_\alpha(G) \geq f(n)$. The extremal graph is $K_2 + \overline{K_{n-2}}$.*

Corollary 4.2. *Let G be a triangle-free 2-connected graph of order $n \geq 4$ and $-1 \leq \alpha < \beta_0$. We have $\chi_\alpha(G) \geq g(n)$ and equality holds if and only if $G = K_{2,n-2}$.*

We proposed the following conjecture [15]:

Let $n, k \in \mathbb{N}, n \geq 4, k \leq n/2$ and $-1 \leq \alpha < \beta_0$. Then for any triangle-free graph of order n with $\delta(G) \geq k \geq 2$ we have $\chi_\alpha(G) \geq k(n-k)n^\alpha$ with equality if and only if $G = K_{k,n-k}$.

This property is true for $\alpha = -1$ [2] and for $k = 2$ and $-1 \leq \alpha < \beta_0$ by Theorem 4.2. If the conjecture is true, then the property also holds for k-connected graphs. The following theorem shows extremal graph G of order n with $\kappa(G) = k$ which maximizes $\chi_\alpha(G)$ for $\alpha \geq 1$ [16].

Theorem 4.3. *Let G be an n-vertex graph, $n \geq 3$, with vertex connectivity k, $1 \leq k \leq n-1$ and $\alpha \geq 1$. Then ${}^0R_\alpha(G)$ and $\chi_\alpha(G)$ are maximum if and only if $G = K_k + (K_1 \cup K_{n-k-1})$.*

Note that the graph $K_k + (K_1 \cup K_{n-k-1})$ is the graph of order n obtained by joining by edges k vertices of K_{n-1} to a new vertex. Since for every graph G, $\kappa(G) \leq \kappa'(G)$ holds, we have [16]:

Corollary 4.3. *Let G be an n-vertex graph, $n \geq 3$, with edge connectivity k, $1 \leq k \leq n-1$ and $\alpha \geq 1$. Then ${}^0R_\alpha(G)$ and $\chi_\alpha(G)$ are maximum if and only if $G = K_k + (K_1 \cup K_{n-k-1})$.*

For $\alpha > 0$ the 2-connected graph having minimum $\chi_\alpha(G)$ is the cycle C_n [16]:

Theorem 4.4. *Let G be a 2-(connected or edge-connected) graph with $n \geq 3$ vertices. Then for $\alpha > 0$, ${}^0R_\alpha(G)$ and $\chi_\alpha(G)$ are minimum if and only if $G = C_n$.*

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