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ORIGINAL PAPER

On general sum-connectivity index

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Abstract We report some properties especially lower and upper bounds in terms of other graph invariants for the general sum-connectivity index which generalizes both the ordinary sum-connectivity index and the first Zagreb index. Additionally, we give the Nordhaus-Gaddum-type result for the general sum-connectivity index.

Keywords Randić connectivity index · Sum-connectivity index · General Randić connectivity index · General sum-connectivity index

1 Introduction

The well-known Randić connectivity index, proposed by Randić in 1975 [1], is the most used molecular descriptor in QSPR and QSAR [*e.g.*, 2–6]. In view of its successful applications in QSPR and QSAR, some people gave physicochemical interpretation of this molecular descriptor [4–10]. The history of this index is described in [11,12]. Mathematical properties of this index have also been reported [*e.g.*, 13,14].

Let G be a simple graph with vertex-set $V(G)$ and edge-set $E(G)$. For $u \in V(G)$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of v is $d_u = d_G(u) = |\Gamma(u)|$. The Randić connectivity index $R = R(G)$ of G is defined as:

$$R = R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-1/2}.$$

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The sum-connectivity index of the graph G, denoted by $\chi = \chi(G)$, is defined as [15]:

$$\chi = \chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-1/2}.$$

For convenience, we may call $R(G)$ the product-connectivity index of G. These two molecular descriptors are highly intercorrelated quantities; for example, the value of the correlation coefficient is 0.99088 for 134 trees representing the lower alkanes taken from [16]. In [15], we gave several basic properties for the sum-connectivity index, especially lower and upper bounds in terms of graph (structural) invariants, determined the unique tree with fixed numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and with the maximum, second maximum and third maximum values of the sum-connectivity index, and discussed properties of the sum-connectivity index for a class of trees representing acyclic hydrocarbons. In [17], some properties of the sum-connectivity index for trees and unicyclic graphs with fixed maximum degree were obtained.

The ordinary Randić connectivity index has been extended to the general Randić connectivity index defined as [13,18]:

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

where α is a real number. The properties of the general Randić connectivity index may be found in [*e.g.*, 13,19,20]. Similarly, the general sum-connectivity index is defined as:

$$\chi_\alpha = \chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

Evidently, $R_{-1/2}$ is the ordinary Randić connectivity index, while $\chi_{-1/2}$ is the ordinary sum-connectivity index. Recall that the first and the second Zagreb indices are defined as [21–24]:

$$M_1 = M_1(G) = \sum_{u \in V(G)} d_u^2$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v$$

which are occasionally employed as molecular descriptors in QSPR and QSAR [*e.g.*, 25,26]. Mathematical and computational properties of Zagreb indices have also been reported [*e.g.*, 27–37]. We note that $R_1 = M_2$ and $\chi_1 = M_1$. Thus, the general Randić connectivity index generalizes both the ordinary Randić connectivity index and the second Zagreb index, while the general sum-connectivity index generalizes both the ordinary sum-connectivity index and the first Zagreb index.

In this report, we give some basic properties, especially lower and upper bounds in terms of other graph invariants, of the general sum-connectivity index, and also give the Nordhaus-Gaddum-type result [38] for it.

2 Preliminaries

Let P_n and S_n be respectively the path and the star with n vertices. Let K_n be the complete graph with n vertices. A bipartite graph G is a graph whose vertex-set V can be partitioned into two subsets (partite sets) V_1 and V_2 such that every edge of G connects a vertex in V_1 and a vertex in V_2. The graph $G \cup H$ denotes the vertex-disjoint union of graphs G and H. Let $\overline{G}$ be the complement of the graph G.

Recall that if a real valued function $f(x)$ defined on an interval has a second derivative $f''(x)$ then a necessary and sufficient condition for it to be strictly convex on that interval is that $f''(x) > 0$. For positive integer k, if $f(x)$ is strictly convex, then (by Jensen's inequality) we have $f\left(\sum_{i=1}^{k} \frac{x_i}{k}\right) \leq \frac{1}{k}\sum_{i=1}^{k} f(x_i)$ with equality if and only if $x_1 = x_2 = \cdots = x_k$, and if $-f(x)$ is strictly convex, then the inequality is reversed.

3 Bounds for the general sum-connectivity index

Proposition 1 *Let G be a graph with $m \geq 1$ edges. If $0 < \alpha < 1$, then $\chi_\alpha(G) \leq M_1(G)^\alpha m^{1-\alpha}$, and if $\alpha < 0$ or $\alpha > 1$, then $\chi_\alpha(G) \geq M_1(G)^\alpha m^{1-\alpha}$, and either equality holds if and only if $d_u + d_v$ is a constant for any edge uv.*

Proof If $0 < \alpha < 1$, then $-x^\alpha$ for $x > 0$ is strictly convex, and thus:

$$\left[\frac{1}{m}M_1(G)\right]^\alpha = \left[\frac{1}{m}\sum_{uv\in E(G)}(d_u + d_v)\right]^\alpha \geq \frac{1}{m}\sum_{uv\in E(G)}(d_u + d_v)^\alpha = \frac{1}{m}\chi_\alpha(G),$$

i.e., $\chi_\alpha(G) \leq M_1(G)^\alpha m^{1-\alpha}$ with equality if and only if $d_u + d_v$ is a constant for any edge uv. Similarly, if $\alpha < 0$ or $\alpha > 1$, then x^α for $x > 0$ is strictly convex, and thus $\chi_\alpha(G) \geq M_1(G)^\alpha m^{1-\alpha}$ with equality if and only if $d_u + d_v$ is a constant for any edge uv. □

There is a number of reports on the upper bounds for the first Zagreb index [27–30,32,34–37], from which and Proposition 1, we may deduce upper bounds for χ_α when $0 < \alpha < 1$ and lower bounds for χ_α when $\alpha < 0$. Also lower bounds for the first Zagreb index lead to lower bounds for χ_α when $\alpha > 1$. We give such examples.

(a) Let G be a graph with n vertices and $m \geq 1$ edges. Then [27,28] $M_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$ with equality if and only if $G = K_n$, S_n or $K_1 \cup K_{n-1}$, and thus if $0 < \alpha < 1$, then:

$$\chi_\alpha(G) \leq m\left(\frac{2m}{n-1}+n-2\right)^\alpha \quad \text{if} \quad 0<\alpha<1$$
$$\chi_\alpha(G) \geq m\left(\frac{2m}{n-1}+n-2\right)^\alpha \quad \text{if} \quad \alpha<0$$

with equality in either case if and only if $G = K_n$, S_n or $K_1 \cup K_{n-1}$.

(b) Let G be a graph with n vertices and m edges. Then [29,30]:

$$M_1(G) \geq f(n,m) = 2m\left(2\left\lfloor\frac{2m}{n}\right\rfloor+1\right) - n\left\lfloor\frac{2m}{n}\right\rfloor\left(\left\lfloor\frac{2m}{n}\right\rfloor+1\right)$$

with equality if and only if the difference of the degrees of any two vertices of G is at most one. Thus, for $\alpha > 1$:

$$\chi_\alpha(G) \geq f(n,m)^\alpha m^{1-\alpha}$$

with equality if and only if either G is regular or G is a bipartite semi-regular graph (bipartite graph for which vertices in the same partite sets have equal degree) of degrees of two consecutive integers. A somewhat simple bound is as follows. Let G be a graph with n vertices and m edges. By the Cauchy-Schwarz inequality:

$$\chi_1(G) = M_1(G) \geq \frac{1}{n}\left(\sum_{u\in V(G)} d_u\right)^2 = \frac{4m^2}{n}.$$

Thus, for $\alpha > 1$:

$$\chi_\alpha(G) \geq 4^\alpha n^{-\alpha} m^{1+\alpha}$$

with equality if and only if G is regular.

Proposition 2 *Let G be a graph with $n \geq 2$ vertices. If $0 < \alpha < 1$, then $\chi_\alpha(G) \geq M_1(G)^\alpha$ with equality if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$, and if $\alpha < 0$, then $\chi_\alpha(G) \leq 2^{-1+\alpha}n(n-1)$ with equality if and only if $G = K_2$.*

Proof If $0 < \alpha < 1$, then $\chi_\alpha(G) \geq \left[\sum_{uv\in E(G)}(d_u + d_v)\right]^\alpha = M_1(G)^\alpha$ with equality if and only if $|E(G)| \leq 1$, i.e, $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$. If $\alpha < 0$ and $G \neq \overline{K_n}$, then by setting δ and Δ to be respectively the minimum and maximum degree of G_1 on n_1 vertices, obtained from G by deleting possible isolated vertices, we have:

$$\chi_\alpha(G) \leq \sum_{uv\in E(G_1)} (2\delta)^\alpha \leq \frac{n_1\Delta}{2}(2\delta)^\alpha = 2^{-1+\alpha}n_1\Delta\delta^\alpha \leq 2^{-1+\alpha}n(n-1)$$

with equalities if and only if G is regular and $\Delta\delta^\alpha = n-1$, i.e., $G = K_2$. □

If G is a graph with n vertices and m edges, then for $\alpha > 1$, as $d_u + d_v \leq 2(n-1)$ for $u, v \in V(G)$, we have: $\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha \leq m(2n-2)^\alpha$ with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

Proposition 3 *Let G be a tree with $n \geq 4$ vertices. If $\alpha > 0$, then*:

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

with left (right, respectively) equality if and only if $G = P_n$ ($G = S_n$, respectively). If $\alpha < 0$, then the above inequalities on $\chi(G)$ are reversed, where the upper bound holds for $\alpha \geqslant 1 - \dfrac{\log 2}{\log(4/3)}$.

Proof We only prove the case $\alpha > 0$. The case $\alpha < 0$ is similar. Suppose that $\alpha > 0$. Let uv be any edge of G. Obviously, $d_u + d_v \leq n$. Thus:

$$\chi_\alpha(G) \leq \sum_{uv \in E(G)} n^\alpha = (n-1)n^\alpha$$

with equality if and only if $d_u + d_v = n$ for every edge uv of G if and only if G is a complete bipartite graph that is a tree, i.e., $G = S_n$.

Suppose that Q is 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. Let $d_1 = d_{G_1}(u)$ and $d_x = d_Q(x)$ for vertex x of G_1 or G_2 that is also in Q. Then $d_1 \geq 3$. If $a = 1$ and $b = 1$, then:

$$\begin{aligned}\chi_\alpha(G_2) - \chi_\alpha(G_1) &= 3^\alpha + (d_1+1)^\alpha + \sum_{xu \in E(Q)} (d_1 - 1 + d_x)^\alpha \\ &\quad - \left[2(d_1+1)^\alpha + \sum_{xu \in E(Q)} (d_1 + d_x)^\alpha\right] \\ &= 3^\alpha - (d_1+1)^\alpha + \sum_{xu \in E(Q)} \left[(d_1 - 1 + d_x)^\alpha - (d_1 + d_x)^\alpha\right] < 0.\end{aligned}$$

If $a \geq 2$ and $b = 1$, then:

$$\chi_\alpha(G_2) - \chi_\alpha(G_1) = 4^\alpha - (d_1+2)^\alpha + \sum_{xu \in E(Q)} \left[(d_1 - 1 + d_x)^\alpha - (d_1 + d_x)^\alpha\right] < 0.$$

If $a \geq 2$ and $b \geq 2$, then $f(x) = 2 \cdot 4^\alpha + (x+1)^\alpha - 3^\alpha - 2(x+2)^\alpha$ for $x \geqslant 2$ is decreasing as this is equivalent to $(x+1)^{\alpha-1} \leq 2(x+2)^{\alpha-1}$, i.e., $\left(\frac{x+1}{x+2}\right)^{\alpha-1} \leq 2$, which is obviously true, and thus $2 \cdot 4^\alpha + (d_1+1)^\alpha - 3^\alpha - 2(d_1+2)^\alpha = f(d_1) \leq f(3) < f(2) = 0$, and we have:

$$\chi_\alpha(G_2) - \chi_\alpha(G_1) = 2 \cdot 4^\alpha + (d_1+1)^\alpha - 3^\alpha - 2(d_1+2)^\alpha + \sum_{xu \in E(Q)} \left[(d_1 - 1 + d_x)^\alpha - (d_1 + d_x)^\alpha\right] < 0.$$

It follows that $\chi_\alpha(G_1) > \chi_\alpha(G_2)$. If $G \neq P_n$, then by applying the above transformation to the tree G, we have $\chi_\alpha(G) > \chi_\alpha(P_n)$. □

A necessary condition for a molecular descriptor to be an acceptable measure of branching is that within the set of all n-vertex trees its values should be extremal for P_n and S_n [*e.g.*, 39]. By Proposition 3, χ_α satisfies this basic requirement for $\alpha \neq 0$ and $\alpha \geqslant 1 - \frac{\log 2}{\log(4/3)}$. In particular, both $\chi_{-1/2}$ and χ_{-1} provide a measure of molecular branching. For the general Randić connectivity index, $R_{-1/2}$ provides a measure of molecular branching [40] as if G is an n-vertex tree, then $R_{-1/2}(S_n) \leq R_{-1/2}(G) \leq R_{-1/2}(P_n)$ with left (right, respectively) equality if and only if $G = S_n$ ($G = P_n$, respectively), however, R_{-1} does not as the inequality $R_{-1}(G) \leq R_{-1}(P_n)$ does not hold when n is sufficiently large [41].

Proposition 4 *Let G be a triangle-free graph with n vertices and $m \geq 1$ edges. If $\alpha > 0$, then*:

$$\chi_\alpha(G) \leq mn^\alpha$$

with equality if and only if G is a complete bipartite graph. If $\alpha < 0$, then the above inequality on $\chi_\alpha(G)$ is reversed.

Proof For any edge uv of G, $d_u + d_v \leq n$ and thus for $\alpha > 0$:

$$\chi_\alpha(G) \leq \sum_{uv \in E(G)} n^\alpha = mn^\alpha$$

with equality if and only if $d_u + d_v = n$ for every edge uv of G, i.e., G is a complete bipartite graph. The proof for the case $\alpha < 0$ is similar. □

4 Nordhaus-Gaddum-type result for the general sum-connectivity index

Finally, we give the result for the general sum-connectivity index of Nordhaus-Gaddum-type, i.e., bounds for the sum of the general sum-connectivity indices of a graph and its complement in terms of the number of vertices of the graph.

Proposition 5 *Let G be a graph with $n \geq 2$ vertices.*

(i) *If $\alpha > 0$, then*:

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \leq 2^{-1+\alpha} n(n-1)^{1+\alpha}$$

with equality if and only if $G = K_n$ *or* $G = \overline{K_n}$,

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \geq 2^{-1}n(n-1)^{\alpha+1} \quad for\ \alpha \geq 1$$

with equality if and only if G *is a regular graph of degree* $\frac{n-1}{2}$, *and*

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) > 2^{-\alpha}n^\alpha(n-1)^{2\alpha} \quad for\ 0 < \alpha < 1.$$

(ii) *If* $\alpha < 0$, *then*:

$$2^{-1+\alpha}n(n-1)^{\alpha+1} \leq \chi_\alpha(G) + \chi_\alpha(\overline{G}) < 2^\alpha n(n-1)$$

with left equality if and only if $G = K_n$ *or* $G = \overline{K_n}$.

Proof Let m and $\overline{m}$ be respectively the numbers of edges of G and $\overline{G}$. Then $m + \overline{m} = \frac{n(n-1)}{2}$. If $\alpha > 0$, then:

$$\begin{aligned}\chi_\alpha(G) + \chi_\alpha(\overline{G}) &= \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^\alpha + \sum_{uv \in E(\overline{G})} \left[d_{\overline{G}}(u) + d_{\overline{G}}(v)\right]^\alpha \\ &\leq m(2n-2)^\alpha + \overline{m}(2n-2)^\alpha \\ &= (m+\overline{m})(2n-2)^\alpha = 2^{-1+\alpha}n(n-1)^{1+\alpha}\end{aligned}$$

with equality if and only if either $d_u = d_v = n-1$ for every edge $uv \in E(G)$ or $E(G) = \emptyset$, i.e., $G = K_n$ or $G = \overline{K_n}$. Similarly, if $\alpha < 0$, then $\chi_\alpha(G) + \chi_\alpha(\overline{G}) \geq 2^{-1+\alpha}n(n-1)^{1+\alpha}$ with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

It is easily seen that:

$$\begin{aligned}\chi_1(G) + \chi_1(\overline{G}) &= \sum_{u \in V(G)} \left[d_G(u)^2 + d_{\overline{G}}(u)^2\right] \\ &\geq \sum_{u \in V(G)} \frac{\left[d_G(u) + d_{\overline{G}}(u)\right]^2}{2} = \frac{n(n-1)^2}{2}\end{aligned}$$

with equality if and only if $d_G(u) = d_{\overline{G}}(u)$ for all $u \in V(G)$, i.e., G is a regular graph of degree $\frac{n-1}{2}$. If $\alpha > 1$, then x^α is strictly convex and thus:

$$\begin{aligned}&\chi_\alpha(G) + \chi_\alpha(\overline{G}) \\ &\quad\geq (m+\overline{m})\left[\frac{\sum_{uv \in E(G)}(d_G(u) + d_G(v)) + \sum_{uv \in E(\overline{G})}(d_{\overline{G}}(u) + d_{\overline{G}}(v))}{m+\overline{m}}\right]^\alpha \\ &\quad= (m+\overline{m})^{1-\alpha}\left[\chi_1(G) + \chi_1(\overline{G})\right]^\alpha \\ &\quad\geq (m+\overline{m})^{1-\alpha}\left[\frac{n(n-1)^2}{2}\right]^\alpha \\ &\quad= 2^{-1}n(n-1)^{1+\alpha}\end{aligned}$$

with equality if and only if G is a regular graph of degree $\frac{n-1}{2}$. If $0 < \alpha < 1$, then:

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) \geq \left[\sum_{uv\in E(G)} (d_G(u) + d_G(v)) + \sum_{uv\in E(\overline{G})} (d_{\overline{G}}(u) + d_{\overline{G}}(v))\right]^\alpha$$

$$= \left[\chi_1(G) + \chi_1(\overline{G})\right]^\alpha \geq \left[\frac{n(n-1)^2}{2}\right]^\alpha \geq 2^{-\alpha} n^\alpha (n-1)^{2\alpha}$$

and thus $\chi_\alpha(G) + \chi_\alpha(\overline{G}) > 2^{-\alpha} n^\alpha (n-1)^{2\alpha}$. This is because a graph G with $|E(G) \cup E(\overline{G})| \leq 1$ is not possible to be a regular graph of degree $\frac{n-1}{2}$ for $n \geq 2$.

If $\alpha < 0$, then by Proposition 2,

$$\chi_\alpha(G) + \chi_\alpha(\overline{G}) < 2^{-1+\alpha} n(n-1) + 2^{-1+\alpha} n(n-1) = 2^\alpha n(n-1).$$

The proof is now completed. □

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