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A note on general sum-connectivity index

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Abstract

For a simple finite graph G, general sum-connectivity index is defined for any real number α as $\chi_\alpha(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^\alpha$, which generalises both the first Zagreb index and the ordinary sum-connectivity index. In this paper, we present some new bounds for the general sum-connectivity index. We also present relation between general sum-connectivity index and general Randić index.

Keywords: *Simple graphs, general sum-connectivity index, general Randić index.*

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1. Introduction

We consider only finite simple graph in this paper. Let G be a finite simple graph on n vertices and m edges. We denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and it is defined as the number of edges incident with u. Let ω denotes the clique number of G which is the number of vertices in a largest complete subgraph of G. Let Δ and δ denote the maximum vertex degree and the minimum vertex degree of the graph G, respectively.

In chemical graph theory, one generally considers various graph-theoretical invariants of molecular graphs (also known as topological indices or molecular descriptors), and study how strongly are they correlated with various properties of the corresponding molecules. The first such topological index was introduced in 1947 by Wiener [17] and is used for correlation with boiling points of alkanes. Historically, the first vertex-degree-based topological indices were the graph invariants that nowadays are called Zagreb indices. Since then numerous graph invariants and their generalisations have been (and still continues to be) employed with varying degrees of success in QSAR (quantitative structure-activity relationship) and QSPR (quantitative structure - property relationship) studies.

The Zagreb indices are amongst the most studied invariants [13] and they are defined as sums of contributions dependent on the degrees of adjacent vertices over all edges of a graph. The Zagreb indices of a graph G, i.e., the *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$, were originally defined [7] as follows.

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2; \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The first Zagreb index of G can also be expressed as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

Generalised version of the first Zagreb index has also been introduced [9], known as *general first Zagreb index* or also called *general zeroth-order Randić index* [21] and is defined as $M_1^{\alpha}(G) = \sum_{u \in V(G)} d_G(u)^{\alpha}$. When $\alpha = 3$, $M_1^3(G) = \sum_{u \in V(G)} d_G(u)^3$ is known as the *forgotten index*, denoted by $F(G)$. One of the highly successful and widely used indices in QSPR and QSAR is the *Randić index* $R(G)$ [16]. It is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The Randić index has been extended to *general Randić index* [8], defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} [d_G(u)d_G(v)]^\alpha$$

for any real number α. Notice that $R_{-1/2}(G) = R(G)$ and $R_1(G) = M_2(G)$. Thus the general Randić index generalises the ordinary Randić index and the second Zagreb index.

Motivated by Randić and Zagreb indices, Zhou and Trinajstić defined *sum-connectivity index* $\chi(G)$ [19] and *general sum-connectivity index* $\chi_\alpha(G)$ [20], which are defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}$$

and

$$\chi_\alpha(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^\alpha$$

for any real number α. Notice that $\chi_{-1/2}(G) = \chi(G)$ and $\chi_1(G) = M_1(G)$. Thus the general sum-connectivity index generalises the ordinary sum-connectivity index and the first Zagreb index. Several results have been obtained for these generalised indices. For instance, various bounds for the general Randić index have been found in [10], [18] and [21]. And in [1], [11], [12] and [20], bounds for the general sum-connectivity index are obtained. Motivated by such results, we present some new bounds for the general sum-connectivity index in this paper. We also present relation between general sum-connectivity index and general Randić index.

2. Preliminaries

In this section, we recall some definitions and state some results that are needed in the proofs of our main results in the next section. A graph G is *regular* if $d_G(u)$ is constant for all $u \in V(G)$ and it is said to be *bi-degreed* if it has two distinct vertex degrees. A connected graph G is said to be *bi-regular* or *semi-regular bipartite* if it is bipartite with one of the two partite sets has constant vertex degree Δ while the other partite set has constant vertex degree δ. Obviously, regular graphs are bi-regular. The following result [3] gives necessary and sufficient condition for non-regular graphs to be bi-regular, more equivalent conditions could be found in [14].

Lemma 2.1. *Let G be a connected non-regular graph. Then G is bi-regular if and only if $d_G(u) + d_G(v)$ is constant for all $uv \in E(G)$.*

Next, we recall the following well-known result due to Pólya and Szegö which could be found in [10] and the reference therein.

Lemma 2.2 (Pólya-Szegö inequality). *Let $a_1, a_2, \dots, a_m$ and $b_1, b_2, \dots, b_m$ be two sequences of positive real numbers. If there exists real numbers A, a, B and b such that $0 < a \leq a_k \leq A < \infty$ and $0 < b \leq b_k \leq B < \infty$ for $k = 1, 2, \dots, m$, then*

$$\sum_{k=1}^{m} a_k^2 \sum_{k=1}^{m} b_k^2 \leq \frac{(ab + AB)^2}{4abAB} \left(\sum_{k=1}^{m} a_k b_k \right)^2$$

where the equality holds if and only if $a_1 = a_2 = \ldots = a_m$, $b_1 = b_2 = \ldots = b_m$, $a = a_1 = A$ and $b = b_1 = B$.

The next inequality is due to Hölder and could be found in [4].

Lemma 2.3 (Hölder's inequality). *Let $a_1, a_2, \dots, a_m$ and $b_1, b_2, \dots, b_m$ be two sequences of positive real numbers and $p, q > 1$ be such that $1/p + 1/q = 1$. Then*

$$\sum_{k=1}^{m} a_k b_k \leq \left(\sum_{k=1}^{m} {a_k}^p \right)^{1/p} \left(\sum_{k=1}^{m} {b_k}^q \right)^{1/q}.$$

Equality holds if and only if $\dfrac{{a_1}^p}{{b_1}^q} = \dfrac{{a_2}^p}{{b_2}^q} = \ldots = \dfrac{{a_m}^p}{{b_m}^q}$.

The following is a consequence of Hölder's inequality and could be found in [10] and the reference therein.

Lemma 2.4. *Let $a_1, a_2, \dots, a_m$ and $b_1, b_2, \dots, b_m$ be two sequences of positive real numbers and α, β be real numbers such that $\alpha + \beta = 1$ with $\alpha, \beta \neq 0, 1$. Then for $\alpha > 1$ we have*

$$\sum_{k=1}^{m} a_k b_k \geq \left(\sum_{k=1}^{m} (a_k)^{1/\alpha} \right)^{\alpha} \left(\sum_{k=1}^{m} (b_k)^{1/\beta} \right)^{\beta}.$$

Equality holds if and only if $\dfrac{(a_1)^{1/\alpha}}{(b_1)^{1/\beta}} = \dfrac{(a_2)^{1/\alpha}}{(b_2)^{1/\beta}} = \ldots = \dfrac{(a_m)^{1/\alpha}}{(b_m)^{1/\beta}}$.

Lastly, we present and prove the following lemma which is needed to prove our results in the next section.

Lemma 2.5. *Let G be a graph on n vertices and m edges. Then for any real number α we have*

$$\chi_\alpha(G)\chi_{-\alpha}(G) \leq \frac{m^2}{4}\left[\left(\frac{\delta}{\Delta}\right)^\alpha + \left(\frac{\Delta}{\delta}\right)^\alpha + 2\right].$$

Equality holds if and only if G is a regular graph.

Proof. We only consider the case when $\alpha > 0$ since we can similarly prove the case for $\alpha < 0$. Let $\alpha > 0$. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d_G(v_i)$ for any $i = 1, 2, \ldots, n$. Letting $a_k \to (d_i + d_j)^{\alpha/2}$ and $b_k \to (d_i + d_j)^{-\alpha/2}$ and choosing $a = (2\delta)^{\alpha/2}$, $A = (2\Delta)^{\alpha/2}$, $b = (2\Delta)^{-\alpha/2}$ and $B = (2\delta)^{-\alpha/2}$ in Lemma 2.2 with the sums running over the edges in G, we have

$$\sum_{v_iv_j \in E(G)} (d_i+d_j)^\alpha \sum_{v_iv_j \in E(G)} (d_i+d_j)^{-\alpha} \leq \frac{1}{4}\left[\left(\frac{\delta}{\Delta}\right)^{\alpha/2} + \left(\frac{\Delta}{\delta}\right)^{\alpha/2}\right]^2 \left(\sum_{v_iv_j \in E(G)} 1\right)^2$$

Thus

$$\chi_\alpha(G)\chi_{-\alpha}(G) \leq \frac{m^2}{4}\left[\left(\frac{\delta}{\Delta}\right)^\alpha + \left(\frac{\Delta}{\delta}\right)^\alpha + 2\right].$$

Notice that by Lemma 2.2 the above inequalities become equalities if and only if $a_1 = \ldots = a_k = \ldots = a = A$ and $b_1 = \ldots = b_k = \ldots = b = B$, i.e., if and only if $\delta = \Delta$, i.e., if and only if G is a regular graph. This proves the lemma. □

Remark 2.6. *If G is a triangle free graph on n vertices and $m \geq 1$ edges, then $2 \leq d_i + d_j \leq n$. Thus for $\alpha > 0$ we have*

$$\left(\frac{2}{n}\right)^\alpha m^2 \leq \chi_\alpha(G)\chi_{-\alpha}(G) \leq \left(\frac{n}{2}\right)^\alpha m^2.$$

Equality holds if and only if $d_i + d_j = n$ for all $v_iv_j \in E(G)$, i.e., G is a complete bipartite graph. The inequalities are reversed if $\alpha < 0$.

3. Main Results

In this section, we present and prove our main results. First, we prove the following result which gives a lower bound of the general sum-connectivity index in terms of the first Zagreb index and size of the considered graph. We note that this bound were also obtained in [20] by using Jensen's inequality, completely different from our approach presented here.

Proposition 3.1. *Let G be a graph with m edges. Then for $\alpha > 1$ we have*

$$\chi_\alpha(G) \geq M_1(G)^\alpha m^{1-\alpha}.$$

Equality holds if and only if G is bi-regular.

Proof. Let $\alpha + \beta = 1$ with $\alpha, \beta \neq 0, 1$ and let $\alpha > 1$. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = d_G(v_i)$ for any $i = 1, 2, \ldots, n$. Letting $a_k \to (d_i + d_j)^\alpha$ and $b_k \to 1^\beta$ in by Lemma 2.4 with the sums running over the edges in G, we have

$$\begin{aligned}
\chi_\alpha(G) &= \textstyle\sum_{v_iv_j \in E(G)} (d_i + d_j)^\alpha \cdot 1^\beta \\
&\geq \left[\textstyle\sum_{v_iv_j \in E(G)} (d_i + d_j)^{\alpha \cdot 1/\alpha}\right]^\alpha \left[\textstyle\sum_{v_iv_j \in E(G)} 1^{\beta \cdot 1/\beta}\right]^\beta \\
&= \left[\textstyle\sum_{v_iv_j \in E(G)} (d_i + d_j)\right]^\alpha m^\beta = M_1(G)^\alpha m^{1-\alpha}
\end{aligned}$$

Notice that by Lemma 2.4 the above inequality becomes equality if and only if a_k is constant for all k, i.e., if and only if $d_i + d_j = k$ for some constant $k > 0$ for all edges. Thus by Lemma 2.1 equality holds if and only if G is bi-regular. This completes the proof of the proposition. □

Since $M_1(G) \geq \dfrac{4m^2}{n}$, with equality if and only if G is a regular graph [20], the above Proposition 3.1 implies the following result which could also be found in [20].

Theorem 3.2. *Let G be a graph on n vertices and m edges. Then for $\alpha > 1$ we have*

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

Equality holds if and only if G is a regular graph.

Remark 3.3. *Notice that the lower bound for the general sum-connectivity index in terms of the first Zagreb index and the size of the graph obtained in the Proposition 3.1 generates many more lower bounds because there are many results on the lower bounds of the first Zagreb index. One such* *example we have in Theorem 3.2 and for more such bounds we refer the readers to the bounds obtained in a recent paper [15].*

Next, we present an upper bound for general sum-connectivity index in terms of Δ, δ, m and n.

Theorem 3.4. *Let G be a graph on n vertices and m edges. Then for $\alpha < -1$ we have*

$$\chi_\alpha(G) \leq 4^{\alpha-1} n^{-\alpha} m^{1+\alpha} \left[\left(\frac{\delta}{\Delta} \right)^\alpha + \left(\frac{\Delta}{\delta} \right)^\alpha + 2 \right].$$

Equality holds if and only if G is a regular graph.

Proof. Let $\alpha < -1$. Then $-\alpha > 1$ and by Theorem 3.2, we have

$$\chi_{-\alpha}(G) \geq 4^{-\alpha} n^\alpha m^{1-\alpha} \tag{3.1}$$

where the equality holds if and only if G is regular. And by Lemma 2.5, we have

$$\chi_\alpha(G) \leq \frac{m^2}{4} \left[\left(\frac{\delta}{\Delta} \right)^\alpha + \left(\frac{\Delta}{\delta} \right)^\alpha + 2 \right] \Big/ \chi_{-\alpha}(G) \tag{3.2}$$

From (3.1) and (3.2), we have

$$\begin{aligned} \chi_\alpha(G) &\leq \frac{m^2}{4} \left[\left(\frac{\delta}{\Delta} \right)^\alpha + \left(\frac{\Delta}{\delta} \right)^\alpha + 2 \right] \Big/ 4^{-\alpha} n^\alpha m^{1-\alpha} \\ &= 4^{\alpha-1} n^{-\alpha} m^{1+\alpha} \left[\left(\frac{\delta}{\Delta} \right)^\alpha + \left(\frac{\Delta}{\delta} \right)^\alpha + 2 \right]. \end{aligned}$$

Moreover, it is easy to see that the above inequality becomes equality if and only if $\Delta = \delta$, i.e., if and only if G is a regular graph. This completes the proof of the theorem. □

By Turán's theorem [21], $m \leq \dfrac{2(\omega - 1)}{\omega} n^2$. Thus, as a corollary, we present an upper bound for general sum-connectivity index involving ω.

Corollary 3.5. *Let G be a graph on n vertices and m edges. Then for $\alpha < -1$ we have*

$$\chi_\alpha(G) \leq 2^{-1+3\alpha} (\omega - 1)^{1+\alpha} \omega^{-1-\alpha} n^{2+\alpha} \left[\left(\frac{\delta}{\Delta} \right)^\alpha + \left(\frac{\Delta}{\delta} \right)^\alpha + 2 \right].$$

Lastly, we present a relation between general sum-connectivity index and Randić index.

Theorem 3.6. *Let G be a graph on n vertices and m edges. Then for $\alpha > 0$ we have*

$$2^{\alpha}\Delta^{-\alpha}R_{\alpha}(G) \leq \chi_{\alpha}(G) \leq 2^{\alpha}\delta^{-\alpha}R_{\alpha}(G).$$

Equality holds if and only if G is a regular graph. If $\alpha < 0$, then the above inequalities are reversed and the equality holds if and only if G is a regular graph.

Proof. Notice that for any real number α, we have

$$\chi_{\alpha}(G) = \sum_{v_iv_j \in E(G)} (d_i + d_j)^{\alpha} = \sum_{v_iv_j \in E(G)} (d_id_j)^{\alpha} \left(\frac{1}{d_i} + \frac{1}{d_j}\right)^{\alpha} \tag{3.3}$$

Since $0 < \delta \leq d_i \leq \Delta$ for any vertex v_i, $2^{\alpha}\Delta^{-\alpha} \leq \left(\frac{1}{d_i} + \frac{1}{d_j}\right)^{\alpha} \leq 2^{\alpha}\delta^{-\alpha}$, if $\alpha > 0$. Thus for $\alpha > 0$ equation (3.3) becomes

$$2^{\alpha}\Delta^{-\alpha}R_{\alpha}(G) \leq \chi_{\alpha}(G) \leq 2^{\alpha}\delta^{-\alpha}R_{\alpha}(G).$$

Notice that equality holds if and only if $\delta = \Delta$ i.e., G is a regular graph. Moreover, $2^{\alpha}\delta^{-\alpha} \leq \left(\frac{1}{d_i} + \frac{1}{d_j}\right)^{\alpha} \leq 2^{\alpha}\Delta^{-\alpha}$, if $\alpha < 0$. Thus for $\alpha < 0$ equation (3.3) becomes

$$2^{\alpha}\delta^{-\alpha}R_{\alpha}(G) \leq \chi_{\alpha}(G) \leq 2^{\alpha}\Delta^{-\alpha}R_{\alpha}(G).$$

Notice that equality holds if and only if $\delta = \Delta$ i.e., G is a regular graph. This completes the proof. □

It is proven in [21] that $R_{\alpha}(G) \leq \frac{\omega - 1}{\omega} M_1^{\alpha}(G)^2$. We thus have the following corollary.

Corollary 3.7. *Let G be a graph on n vertices and m edges. Then*

$$\chi_{\alpha}(G) \leq \frac{2^{\alpha}\delta^{-\alpha}(\omega - 1)}{\omega} M_1^{\alpha}(G)^2$$

if $\alpha > 0$ and

$$\chi_{\alpha}(G) \leq \frac{2^{\alpha}\Delta^{-\alpha}(\omega - 1)}{\omega} M_1^{\alpha}(G)^2$$

if $\alpha < 0$.

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