Remarks on general zeroth-order Randić and general sum-connectivity indices

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Abstract: Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple connected graph with n vertices, m edges and vertex degree sequence $d_1 \geq d_2 \geq \dots \geq d_n > 0$, $d_i = d(v_i)$. General zeroth-order Randić index of G is defined as ${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha$, and general sum-connectivity index as $\chi_\alpha(G) = \sum_{i \sim j} (d_i + d_j)^\alpha$, where α is an arbitrary real number. In this paper we establish a relationship between ${}^0R_{\alpha+\beta}(G)$, ${}^0R_{\alpha-\beta}(G)$ and ${}^0R_\alpha(G)$, as well as $\chi_{\alpha+\beta}(G)$, $\chi_{\alpha-\beta}(G)$ and $\chi_\alpha(G)$, where α and β are arbitrary real numbers. By the appropriate choice of parameters α and β , a number of new/old inequalities that reveal relationships between various vertex and edge degree-based topological indices are obtained.

1 Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with n vertices, m edges and $\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0$, $d_i = d(v_i)$, and $\Delta_e = d(e_1) + 2 \geq d(e_2) + 2 \geq \dots \geq d(e_m) + 2 = \delta_e$ be sequences of vertex and edge degrees in G , respectively. With $i \sim j$ we denote adjacency of vertices v_i and v_j in G . As usual, $L(G)$ denotes a line graph of G .

A graph invariant, or topological index, is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. Gutman and Trinajstić in [9] introduced a vertex-degree-based topological index, later named the first Zagreb index, $M_1(G)$, as

$$M_1(G) = \sum_{i=1}^n d_i^2.$$

In [13] degree 2 in the previous expression is replaced with an arbitrary real number α , i.e. generalization of the first Zagreb index is introduced, known as the general zeroth-order

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Randić index as

$${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha.$$

It is also met under names general first Zagreb index [16] and variable first Zagreb index [22].

In addition to the aforementioned first Zagreb index $M_1(G) = {}^0R_2(G)$, in this paper we are interested in the following special cases of invariant ${}^0R_\alpha(G)$: ${}^mM_1(G) = {}^0R_{-2}(G)$ (the modified first Zagreb index [28]), $ID(G) = {}^0R_{-1}(G)$ (the inverse degree or modified total adjacency index [5] and [28]), ${}^0R(G) = {}^0R_{-1/2}(G)$ (zeroth-order Randić index), $F(G) = {}^0R_3(G)$ (forgotten topological index [8]). More on these topological indices can be found in [1, 3, 10, 17, 20] and in the references cited therein.

As shown in [22, 28], the first Zagreb index can be also expressed as

$$M_1(G) = \sum_{i \sim j} (d_i + d_j).$$

The sum-connectivity index, $SCI(G)$, is defined as [35]

$$SCI(G) = \sum_{i \sim j} (d_i + d_j)^{-1/2}.$$

A generalization of the previous two degree-based graph invariant was introduced in [36], and named general sum-connectivity index, $\chi_\alpha(G)$. It is defined as

$$\chi_\alpha(G) = \sum_{i \sim j} (d_i + d_j)^\alpha,$$

where α is an arbitrary real number.

Let $e = \{v_i, v_j\}$ be an arbitrary edge of graph G . Then $d(e) = d_i + d_j - 2$, and consequently we have

$$\chi_\alpha(G) = \sum_{i=1}^m (d(e_i) + 2)^\alpha.$$

Therefore $\chi_\alpha(G)$ is also edge-degree-based topological index. In this paper we are interested in the following special cases of this topological index: ${}^mHM(G) = \chi_{-2}(G)$ (the modified hyper-Zagreb index), $H(G) = 2\chi_{-1}(G)$ (the harmonic index [5]), $HM(G) = \chi_2(G)$ (the hyper-Zagreb index [33]).

One can easily see that

$$HM(G) = F(G) + 2M_2(G),$$

where

$$M_2(G) = \sum_{i \sim j} d_i d_j$$

is the second Zagreb index defined in [11].

In this paper we prove inequalities that establish relations between topological indices ${}^0R_{\alpha+\beta}(G)$, ${}^0R_{\alpha-\beta}(G)$ and ${}^0R_{\alpha}(G)$, as well as $\chi_{\alpha+\beta}(G)$, $\chi_{\alpha-\beta}(G)$ and $\chi_{\alpha}(G)$, where α and β are arbitrary real numbers. In special cases, for the appropriate choice of parameters α and β , we obtain a number of old/new inequalities for different vertex and edge degree-based topological indices.

2 Preliminaries

In this section we recall one discrete analytical inequality for real number sequences that will be used in the paper.

Let $p = (p_i)$ be nonnegative and $x = (x_i)$ be positive real number sequences with the properties $p_1 + p_2 + \dots + p_n = 1$ and $0 < r \leq x_i \leq R < +\infty$, $i = 1, 2, \dots, n$. Then [29] (see also [27])

$$\sum_{i=1}^n p_i x_i + rR \sum_{i=1}^n \frac{p_i}{x_i} \leq r + R, \quad (1)$$

with equality if and only if $x_i \in \{r, R\}$ for every $i = 1, 2, \dots, n$.

3 Relations between ${}^0R_{\alpha+\beta}(G)$, ${}^0R_{\alpha-\beta}(G)$ and ${}^0R_{\alpha}(G)$

In the following theorem we establish relations between graph invariants ${}^0R_{\alpha+\beta}(G)$, ${}^0R_{\alpha-\beta}(G)$ and ${}^0R_{\alpha}(G)$.

Theorem 1. *Let G be a simple connected graph with $n \geq 2$ vertices. Then for any real numbers α and β hold*

$${}^0R_{\alpha+\beta}(G) - (\Delta^\beta + \delta^\beta) {}^0R_{\alpha}(G) + (\Delta\delta)^\beta {}^0R_{\alpha-\beta}(G) \leq 0. \quad (2)$$

Equality holds if and only if $\beta = 0$ or $d_i \in \{\delta, \Delta\}$ for every $i = 1, 2, \dots, n$.

Proof. Let $\beta \geq 0$. For $p_i = \frac{d_i^\alpha}{\sum_{i=1}^n d_i^\alpha}$, $x_i = d_i^\beta$, $i = 1, 2, \dots, n$, $r = \delta^\beta$ and $R = \Delta^\beta$, the inequality (1) transforms into

$$\frac{\sum_{i=1}^n d_i^{\alpha+\beta}}{\sum_{i=1}^n d_i^\alpha} + (\Delta\delta)^\beta \frac{\sum_{i=1}^n d_i^{\alpha-\beta}}{\sum_{i=1}^n d_i^\alpha} \leq \Delta^\beta + \delta^\beta, \quad (3)$$

i.e.

$$\frac{{}^0R_{\alpha+\beta}(G)}{{}^0R_{\alpha}(G)} + (\Delta\delta)^\beta \frac{{}^0R_{\alpha-\beta}(G)}{{}^0R_{\alpha}(G)} \leq \Delta^\beta + \delta^\beta,$$

wherefrom (2) is obtained.

In a similar way the inequality (2) is obtained when $\beta \leq 0$.

Equality in (3), i.e. in (2), holds if and only if $\beta = 0$ or $d_i \in \{\delta, \Delta\}$ for every $i = 1, 2, \dots, n$. $\square$

Corollary 1. *Let G be a simple connected graph with $n \geq 2$ vertices. Then for any real numbers α and β hold*

$${}^0R_{\alpha-\beta}(G){}^0R_{\alpha+\beta}(G) \leq \frac{{}^0R_{\alpha}(G)^2}{4} \left(\sqrt{\frac{\Delta^\beta}{\delta^\beta}} + \sqrt{\frac{\delta^\beta}{\Delta^\beta}} \right)^2. \quad (4)$$

Equality holds if and only if $\beta = 0$ or G is a regular graph.

Proof. By applying the arithmetic–geometric mean inequality for real numbers (see e.g. [27]) to the following inequality

$${}^0R_{\alpha+\beta}(G) + (\Delta\delta)^\beta {}^0R_{\alpha-\beta}(G) \leq (\Delta^\beta + \delta^\beta) {}^0R_{\alpha}(G),$$

we get

$$2\sqrt{(\Delta\delta)^\beta {}^0R_{\alpha+\beta}(G){}^0R_{\alpha-\beta}(G)} \leq (\Delta^\beta + \delta^\beta) {}^0R_{\alpha}(G),$$

wherefrom (4) follows. $\square$

Corollary 2. *Let G be a simple connected graph with $n \geq 2$ vertices. Then for any real number α holds*

$${}^0R_{\alpha+1}(G) - (\Delta + \delta) {}^0R_{\alpha}(G) + \Delta\delta {}^0R_{\alpha-1}(G) \leq 0, \quad (5)$$

$${}^0R_{2\alpha}(G) - (\Delta^\alpha + \delta^\alpha) {}^0R_{\alpha}(G) + n(\Delta\delta)^\alpha \leq 0,$$

$${}^0R_{\alpha}(G) - n(\Delta^\alpha + \delta^\alpha) + (\Delta\delta)^\alpha {}^0R_{-\alpha}(G) \leq 0, \quad (6)$$

$${}^0R_{\alpha+1}(G){}^0R_{\alpha-1}(G) \leq \frac{{}^0R_{\alpha}(G)^2}{4} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2, \quad (7)$$

$$2(\Delta\delta)^{\alpha/2} \sqrt{n {}^0R_{2\alpha}(G)} \leq (\Delta^\alpha + \delta^\alpha) {}^0R_{\alpha}(G), \quad (8)$$

$$2(\Delta\delta)^{\alpha/2} \sqrt{{}^0R_{\alpha}(G){}^0R_{-\alpha}(G)} \leq n(\Delta^\alpha + \delta^\alpha).$$

Remark 1. *The inequalities (5) and (7) were proven in [23], whereas (6) and (8) in [30].*

Corollary 3. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta, \quad (9)$$

$$M_1(G) \leq \frac{m^2}{n} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2, \quad (10)$$

$$F(G) \leq 2m(\Delta^2 + \delta^2) - ID(G)(\Delta\delta)^2, \\ F(G) \leq (\Delta + \delta)M_1(G) - 2m\delta\Delta, \quad (11)$$

$$F(G) \leq \frac{M_1(G)^2}{8m} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2, \quad (12)$$

$$ID(G) \leq \frac{n(\Delta + \delta) - 2m}{\Delta\delta},$$

$${}^mM_1(G) \leq \frac{(\Delta + \delta)ID(G) - n}{\Delta\delta},$$

$${}^mM_1(G) \leq \frac{ID(G)^2}{4n} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2,$$

$${}^mM_1(G)M_1(G) \leq \frac{n^2(\Delta^2 + \delta^2)^2}{4(\Delta\delta)^2},$$

$$\frac{2}{(\Delta\delta)^{1/4}} \sqrt{nID(G)} \leq \left(\frac{1}{\sqrt{\Delta}} + \frac{1}{\sqrt{\delta}} \right) {}^0R(G),$$

$$M_2(G) \leq m(\Delta^2 + \delta^2) - \frac{1}{2}(\Delta\delta)^2 ID(G),$$

$$M_2(G) \leq \frac{1}{2}(\Delta + \delta)M_1(G) - m\Delta\delta,$$

$$M_2(G) \leq \frac{M_1(G)^2}{16m} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2,$$

$$F(G) \leq 2m(\Delta + \delta)^2 - (2m + n(\Delta + \delta))\Delta\delta.$$

Remark 2. *The inequality (9) was proven in [4] (see also [12, 18]), the inequality (10) in [7, 15, 19, 34], the inequality (11) in [14], and (12) in [23].*

4 Relations between $\chi_{\alpha+\beta}(G)$, $\chi_{\alpha-\beta}(G)$ and $\chi_{\alpha}(G)$

In the next theorem we prove the inequality that establishes relation between topological indices $\chi_{\alpha+\beta}(G)$, $\chi_{\alpha-\beta}(G)$ and $\chi_{\alpha}(G)$.

Theorem 2. *Let G be a simple connected graph with $m \geq 2$ edges. Then for any real numbers α and β hold*

$$\chi_{\alpha+\beta}(G) - (\Delta_e^\beta + \delta_e^\beta) \chi_{\alpha}(G) + (\Delta_e \delta_e)^\beta \chi_{\alpha-\beta}(G) \leq 0. \quad (13)$$

Equality holds if and only if $\beta = 0$ or $d(e_i) + 2 \in \{\delta_e, \Delta_e\}$ for every $i = 1, 2, \dots, m$.

Proof. Let $\beta \geq 0$. For $p_i = \frac{(d(e_i) + 2)^\alpha}{\sum_{i=1}^m (d(e_i) + 2)^\alpha}$, $x_i = (d(e_i) + 2)^\beta$, $i = 1, 2, \dots, m$, $r = \delta_e^\beta$ and $R = \Delta_e^\beta$, the inequality (1) becomes

$$\frac{\sum_{i=1}^m (d(e_i) + 2)^{\alpha+\beta}}{\sum_{i=1}^m (d(e_i) + 2)^\alpha} + (\Delta_e \delta_e)^\beta \frac{\sum_{i=1}^m (d(e_i) + 2)^{\alpha-\beta}}{\sum_{i=1}^m (d(e_i) + 2)^\alpha} \leq \Delta_e^\beta + \delta_e^\beta, \quad (14)$$

i.e.

$$\frac{\chi_{\alpha+\beta}(G)}{\chi_{\alpha}(G)} + (\Delta_e \delta_e)^\beta \frac{\chi_{\alpha-\beta}(G)}{\chi_{\alpha}(G)} \leq \Delta_e^\beta + \delta_e^\beta,$$

wherefrom we get (13).

Similarly, the inequality (13) is obtained when $\beta \leq 0$.

Equality in (14), and consequently in (13), holds if and only if $\beta = 0$ or $d(e_i) + 2 \in \{\delta_e, \Delta_e\}$ for every $i = 1, 2, \dots, m$. $\square$

By a similar procedure as in case of Corollary 1, the following corollary of Theorem 2 is proved.

Corollary 4. *Let G be a simple connected graph with $m \geq 2$ edges. Then for any real numbers α and β hold*

$$\chi_{\alpha+\beta}(G) \chi_{\alpha-\beta}(G) \leq \frac{\chi_{\alpha}(G)^2}{4} \left(\sqrt{\frac{\Delta_e^\beta}{\delta_e^\beta}} + \sqrt{\frac{\delta_e^\beta}{\Delta_e^\beta}} \right)^2.$$

Equality holds if and only if $\beta = 0$ or $L(G)$ is a regular graph.

Corollary 5. *Let G be a simple connected graph with $m \geq 2$ edges. Then for any real number α holds*

$$\chi_{\alpha+1}(G) - (\Delta_e + \delta_e) \chi_\alpha(G) + \Delta_e \delta_e \chi_{\alpha-1}(G) \leq 0, \quad (15)$$

$$\begin{aligned} \chi_{2\alpha}(G) - (\Delta_e^\alpha + \delta_e^\alpha) \chi_\alpha(G) + m(\Delta_e \delta_e)^\alpha &\leq 0, \\ \chi_\alpha(G) - m(\Delta_e^\alpha + \delta_e^\alpha) + (\Delta_e \delta_e)^\alpha \chi_{-\alpha}(G) &\leq 0, \\ \chi_{\alpha+1}(G) \chi_{\alpha-1}(G) &\leq \frac{\chi_\alpha(G)^2}{4} \left(\sqrt{\frac{\Delta_e}{\delta_e}} + \sqrt{\frac{\delta_e}{\Delta_e}} \right)^2, \end{aligned} \quad (16)$$

$$\begin{aligned} 2(\Delta_e \delta_e)^{\alpha/2} \sqrt{m \chi_{2\alpha}(G)} &\leq (\Delta_e^\alpha + \delta_e^\alpha) \chi_\alpha(G), \\ 2(\Delta_e \delta_e)^{\alpha/2} \sqrt{\chi_\alpha(G) \chi_{-\alpha}(G)} &\leq m(\Delta_e^\alpha + \delta_e^\alpha). \end{aligned} \quad (17)$$

Remark 3. *The inequalities (15) and (16) were proven in [24]. The inequality (17) is stronger than inequality*

$$2(\Delta \delta)^{\alpha/2} \sqrt{m \chi_{2\alpha}(G)} \leq (\Delta^\alpha + \delta^\alpha) \chi_\alpha(G),$$

proven in [31].

Corollary 6. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$\begin{aligned} {}^m HM(G) &\leq \frac{1}{\Delta_e \delta_e} \left(\frac{(\Delta_e + \delta_e) H(G)}{2} - m \right), \\ {}^m HM(G) &\leq \frac{1}{(\Delta_e \delta_e)^2} (\Delta_e^2 + \delta_e^2 - HM(G)), \\ {}^m HM(G) &\leq \frac{H(G)^2}{16m} \left(\sqrt{\frac{\Delta_e}{\delta_e}} + \sqrt{\frac{\delta_e}{\Delta_e}} \right)^2, \\ {}^m HM(G) HM(G) &\leq \frac{m^2 (\Delta_e^2 + \delta_e^2)^2}{4(\Delta_e \delta_e)^2}, \\ H(G) &\leq \frac{2}{\Delta_e \delta_e} (m(\Delta_e + \delta_e) - M_1(G)), \\ 2M_1(G) H(G) &\leq m^2 \left(\sqrt{\frac{\Delta_e}{\delta_e}} + \sqrt{\frac{\delta_e}{\Delta_e}} \right)^2, \end{aligned} \quad (18)$$

$$HM(G) \leq (\Delta_e + \delta_e) M_1(G) - m \Delta_e \delta_e, \quad (19)$$

$$HM(G) \leq \frac{M_1(G)^2}{4m} \left(\sqrt{\frac{\Delta_e}{\delta_e}} + \sqrt{\frac{\delta_e}{\Delta_e}} \right)^2, \quad (20)$$

$$SCI(G) \geq \frac{(\Delta_e \delta_e)^{1/4}}{\sqrt{\Delta_e} + \sqrt{\delta_e}} \sqrt{2mH(G)}.$$

Remark 4. The inequalities (19) and (20) were proven in [25], and in special cases in [24] and [21]. More about this type of inequalities can be found in [26].

The inequality (18) is stronger than inequality

$$2M_1(G)H(G) \leq m^2 \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}} \right)^2,$$

which was proven in [32].

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