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On some mathematical properties of the general zeroth–order Randić coindex of graphs

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Abstract: Let $G = (V,E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple connected graph of order n, size m with vertex degree sequence $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta > 0$, $d_i = d(v_i)$. Denote by $\overline{G}$ a complement of G. If vertices v_i and v_j are adjacent in G, we write $i \sim j$, otherwise we write $i \nsim j$. The general zeroth–order Randić coindex of G is defined as ${}^0\overline{R}_\alpha(G) = \sum_{i \nsim j}(d_i^{\alpha-1} + d_j^{\alpha-1}) = \sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha-1}$, where α is an arbitrary real number. Similarly, general zeroth–order Randić coindex of $\overline{G}$ is defined as ${}^0\overline{R}_\alpha(\overline{G}) = \sum_{i=1}^{n} d_i(n-1-d_i)^{\alpha-1}$. New lower bounds for ${}^0\overline{R}_\alpha(G)$ and ${}^0\overline{R}_\alpha(\overline{G})$ are obtained. A case when G has a tree structure is also covered.

Keywords: Topological indices and coindices, first Zagreb index, forgotten index, general zeroth–order Randić index.

1 Introduction

Let $G = (V,E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple graph with $n \ge 3$ vertices, m edges and vertex degree sequence $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta > 0$, $d_i = d(v_i)$. The complement of G is the graph $\overline{G} = (V, \overline{E})$, with the same vertex set but whose edge set consists of the edges not present in G. Since the graph sum $G + \overline{G}$ on a n-node graph G is the complete graph K_n, the number of edges in $\overline{G}$ is $\overline{m} = \frac{n(n-1)}{2} - m$. If vertices v_i and v_j are adjacent in G, we write $i \sim j$. On the other hand, if v_i and v_j are adjacent in $\overline{G}$, we write $i \nsim j$.

In graph theory, an invariant is a numerical quantity of graphs that depends only on their abstract structure, not on labeling of vertices or edges, or on the drawings of the graphs. In chemical graph theory such quantities are also referred to as topological indices [6, 22–24]. Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph. Most degree based topological indices are viewed as the contributions of pairs of adjacent vertices. But equally important are degree based topological indices that consider the non-adjacent pairs of vertices for computing some topological properties of graphs which are named as coindices.

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One of the most popular and extensively studied graph based molecular structure descriptors is the first Zagreb index introduced in 1972 by Gutman and Trinajstić in [7]. It is defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i\sim j}(d_i + d_j)\,.$$

Various generalizations of the first Zagreb index have been proposed. In [10] a so called general zeroth–order Randić index was introduced. It was conceived as

$$^0R_\alpha(G) = \sum_{i=1}^{n} d_i^\alpha = \sum_{i\sim j}(d_i^{\alpha-1} + d_j^{\alpha-1})\,, \tag{1}$$

where α is an arbitrary real number. It is also met under the names the first general Zagreb index [13] and variable first Zagreb index [17].

For specific values of α, specific notations and hence specific names are being used. Thus, for $\alpha = 2$ the aforementioned first Zagreb index is obtained. For $\alpha = 3$, a so called forgotten topological index [5]

$$F(G) = \sum_{i=1}^{n} d_i^3 = \sum_{i\sim j}(d_i^2 + d_j^2)$$

is gained.

More details on these indices and their mathematical properties can be found in [1,2,8, 20] and references cited therein.

The notion of coindex was introduced in [4]. In this case sum runs over the edges of complement of G. The general zeroth–order Randić coindex was defined in [16] as

$$^0\overline{R}_\alpha(G) = \sum_{i\nsim j}(d_i^{\alpha-1} + d_j^{\alpha-1}) = \sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha-1}\,, \tag{2}$$

where α is an arbitrary real number. For its mathematical properties and upper and lower bounds one can refer to [18,19]. For $\alpha = 3$ the forgotten topological coindex, or F-coindex for short, is obtained [3] (see also [12]). In [25] this coindex is called the Lanzhou index.

From (1) and (2) it can be concluded that between $^0R_\alpha(G)$ and $^0\overline{R}_\alpha(G)$ the following relation exists [16] (see also [18])

$$^0R_\alpha(G) + {}^0\overline{R}_\alpha(G) = (n-1)\,{}^0R_{\alpha-1}(G)\,.$$

In this paper some new lower bounds for $^0\overline{R}_\alpha(G)$ are obtained. A case when G has a tree structure is discussed as well.

2 Preliminaries

In this section we recall one discrete inequality for real number sequences that will be used in proofs of theorems.

Let $p = (p_i)$, $i = 1,2,\dots,n$, be a non-negative real number sequence and $a = (a_i)$, $i = 1,2,\dots,n$, a sequence of positive real numbers. In [11] (see also [21]) it was proved that for any real r, $r \le 0$ or $r \ge 1$, holds

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \ge \left(\sum_{i=1}^{n} p_i a_i\right)^{r}. \tag{3}$$

When $0 \le r \le 1$, the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, for some t, $1 \le t \le n-1$.

3 Main results

In the next theorem we establish a connection between ${}^0\overline{R}_\alpha(G)$ and $M_1(G)$.

Theorem 3.1. *Let G, $G \ncong K_n$, be a simple connected graph with $n \ge 3$ vertices and m edges. Then, for any real α, $\alpha \le 1$ or $\alpha \ge 2$, holds*

$${}^0\overline{R}_\alpha(G) \ge (n-1)(\delta^{\alpha-1} + \Delta^{\alpha-1}) - \delta^\alpha - \Delta^\alpha + \frac{\left((n-1)(2m-\delta-\Delta) - M_1(G) + \delta^2 + \Delta^2\right)^{\alpha-1}}{((n-1)(n-2) - 2m + \delta + \Delta)^{\alpha-2}}. \tag{4}$$

When $1 \le \alpha \le 2$ the opposite inequality is valid. Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some t, $1 \le t \le n-2$, or $n-1 \ne \Delta = d_1 = d_2 = \cdots = d_{n-1} \ge d_n = \delta$.

Proof. The inequality (3) can be observed in the form

$$\left(\sum_{i=2}^{n-1} p_i\right)^{r-1} \sum_{i=2}^{n-1} p_i a_i^r \ge \left(\sum_{i=2}^{n-1} p_i a_i\right)^{r}. \tag{5}$$

For $r = \alpha - 1$, $\alpha \le 1$ or $\alpha \ge 2$, $p_i = n-1-d_i$, $a_i = d_i$, $i = 1,2,\dots,n$, the above inequality becomes

$$\left(\sum_{i=2}^{n-1} (n-1-d_i)\right)^{\alpha-2} \sum_{i=2}^{n-1} (n-1-d_i) d_i^{\alpha-1} \ge \left(\sum_{i=2}^{n-1} (n-1-d_i) d_i\right)^{\alpha-1}. \tag{6}$$

If $d_2 = \cdots = d_{n-1} = n-1$, that is if $G \cong K_n$, in (6) equality occurs. Since ${}^0\overline{R}_\alpha(K_n) = 0$, without affecting the generality, suppose that $G \ncong K_n$. Then, according to (6) we have that

$$\sum_{i=2}^{n-1} (n-1-d_i) d_i^{\alpha-1} \ge \frac{\left(\sum_{i=2}^{n-1} (n-1-d_i) d_i\right)^{\alpha-1}}{\left(\sum_{i=2}^{n-1} (n-1-d_i)\right)^{\alpha-2}}, \tag{7}$$

from which (4) is obtained.

The case when $1 \le \alpha \le 2$ is proved analogously.

Equality in (7), and consequently in (4), holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1} \ge d_n = \delta$, for some t, $1 \le t \le n-2$, or $n-1 \ne \Delta = d_1 \ge d_2 = \cdots = d_{n-1} \ge d_n = \delta$. □

Corollary 3.1. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\overline{F}(G) \geq (n-1)(\delta^2+\Delta^2) - \delta^3 - \Delta^3 + \frac{((n-1)(2m-\Delta-\delta) - M_1(G) + \delta^2 + \Delta^2)^2}{(n-1)(n-2) - 2m + \Delta + \delta}.$$

Equality holds if and only if $n-1 = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1} \geq d_n = \delta$, for some t, $1 \leq t \leq n-2$, or $n-1 \neq \Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$.

In the next theorem we determine a lower bound on ${}^0\overline{R}_\alpha(G)$ when G is a tree, $G \cong T$.

Theorem 3.2. *Let T be a tree with $n \geq 4$ vertices. Then, for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

$$ {}^0\overline{R}_\alpha(T) \geq 2(n-2) + \frac{(2(n^2-3n+3) - M_1(T))^{\alpha-1}}{(n-2)^{\alpha-2}(n-3)^{\alpha-2}}. \tag{8}$$

When $1 \leq \alpha \leq 2$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$ or $T \cong K_{1,n-1}$.

Proof. The inequality (3) can be considered as

$$\left(\sum_{i=1}^{n-2} p_i\right)^{r-1} \sum_{i=1}^{n-2} p_i a_i^r \geq \left(\sum_{i=1}^{n-2} p_i a_i\right)^r. \tag{9}$$

For $r = \alpha - 1$, $\alpha \leq 1$ or $\alpha \geq 2$, $p_i = n-1-d_i$, $a_i = d_i$, $i = 1,2,\ldots,n$, the above inequality transforms into

$$\left(\sum_{i=1}^{n-2} (n-1-d_i)\right)^{\alpha-2} \sum_{i=1}^{n-2} (n-1-d_i) d_i^{\alpha-1} \geq \left(\sum_{i=1}^{n-2} (n-1-d_i) d_i\right)^{\alpha-1}. \tag{10}$$

Let G be a tree with $n \geq 4$ vertices. Then, $m = n-1$ and $d_{n-1} = d_n = \Delta = 1$, since any tree has at least two vertices of degree 1. Now, the inequality (10) becomes

$$\begin{aligned} &(n(n-1) - 2(n-1) - 2(n-2))^{\alpha-2} \left(\sum_{i=1}^{n} (n-1-d_i) d_i^{\alpha-1} - 2(n-2)\right) \geq \\ &\geq \left(2(n-1)^2 - M_1(T) - 2(n-2)\right)^{\alpha-1}, \end{aligned} \tag{11}$$

that is

$$(n-2)^{\alpha-2}(n-3)^{\alpha-2}\left({}^0\overline{R}_\alpha(T) - 2(n-2)\right) \geq \left(2(n^2-3n+3) - M_1(T)\right)^{\alpha-1},$$

from which (8) is obtained.

Equality in (11) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_{n-2} \geq d_{n-1} = d_n = \delta = 1$, for some t, $1 \leq t \leq n-3$, or $n-1 \neq \Delta = d_1 = \cdots = d_{n-2} \geq d_{n-1} = d_n = \delta = 1$, which implies that equality in (8) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$, or $T \cong K_{1,n-1}$. □

Corollary 3.2. *Let T be a tree with $n \geq 4$ vertices. Then*

$$\overline{F}(T) \geq 2(n-2) + \frac{(2(n^2-3n+3) - M_1(T))^2}{(n-2)(n-3)}. \tag{12}$$

Equality holds if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$.

Corollary 3.3. *Let T be a tree with $n \geq 2$ vertices. Then*

$$\overline{F}(T) \geq (n-2)(n-1). \tag{13}$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. In [9] (see also [14]) the following inequality was proven

$$M_1(T) \leq n(n-1),$$

with equality if and only if $T = K_{1,n-1}$. From this and (12), the inequality (13) is obtained. □

The inequality (13) was proven in [25].

Denote by Γ_1 a class of connected graphs that do not have vertices of degree $n-1$. In the next theorem we determine a lower bound for ${}^0\overline{R}_\alpha(\overline{G})$ in terms of $M_1(G)$ and n, m, δ and Δ.

Theorem 3.3. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then, for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

$$\begin{aligned} {}^0\overline{R}_\alpha(\overline{G}) \geq\ & \Delta(n-1-\Delta)^{\alpha-1} + \\ & + \delta(n-1-\delta)^{\alpha-1} + \frac{((n-1)(2m-\Delta-\delta) - M_1(G) + \delta^2 + \Delta^2)^{\alpha-1}}{(2m-\Delta-\delta)^{\alpha-2}}. \end{aligned} \tag{14}$$

When $1 \leq \alpha \leq 2$, the opposite inequality is valid.

If G belong to the class Γ_1, then for any real $\alpha \leq 1$ inequality (14) *is valid.*

Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $\Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$ and $\alpha \geq 1$, or $n-1 \neq \Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$ and $\alpha \leq 1$.

Proof. For $r = \alpha - 1$, $\alpha \geq 2$, $p_i = d_i$, $a_i = n-1-d_i$, $i = 1,2,\ldots,n$, the inequality (5) becomes

$$\left(\sum_{i=2}^{n-1} d_i\right)^{\alpha-2} \sum_{i=2}^{n-1} d_i(n-1-d_i)^{\alpha-1} \geq \left(\sum_{i=2}^{n-1} d_i(n-1-d_i)\right)^{\alpha-1},$$

that is

$$\begin{aligned} {}^0\overline{R}_\alpha(\overline{G}) - \Delta(n-1-\Delta)^{\alpha-1} - \delta(n-1-\delta)^{\alpha-1} \geq & \\ \geq \frac{(2m(n-1) - M_1(G) - \Delta(n-1-\Delta) - \delta(n-1-\Delta))^{\alpha-1}}{(2m-\Delta-\delta)^{\alpha-2}}, & \end{aligned} \tag{15}$$

from which (14) is obtained.

The case when $1 \leq \alpha \leq 2$ is proved analogously. Similarly, it can be proved that when $\alpha \leq 1$ and G does not belong to class Γ_1 the inequality (14) is valid.

Equality in (15) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1-d_2 = n-1-d_3 = \cdots = n-1-d_{n-1}$, which implies that equality in (14) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $\Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$ and $\alpha = 1$, or $n-1 \neq \Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$ and $\alpha \leq 1$.. □

Corollary 3.4. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\overline{F}(\overline{G}) \geq \Delta(n-1-\Delta)^2 + \delta(n-1-\delta)^2 + \frac{((n-1)(2m-\Delta-\delta) - M_1(G) + \delta^2 + \Delta^2)^2}{2m-\Delta-\delta}.$$

Equality holds if and only if $\Delta = d_1 \geq d_2 = \cdots = d_{n-1} \geq d_n = \delta$.

The proof of the next theorem is similar to that of Theorem 3.2.

Theorem 3.4. *Let T be a tree with $n \geq 3$ vertices. Then, for any real $\alpha \geq 2$, holds*

$$^0\overline{R}_\alpha(\overline{T}) \geq 2(n-2)^{\alpha-2} + \frac{(2(n^2-3n+3) - M_1(T))^{\alpha-1}}{(2(n-2))^{\alpha-2}}. \tag{16}$$

When $1 \leq \alpha \leq 2$, the opposite inequality is valid. When $\alpha \leq 1$ and $T \ncong K_{1,n-1}$, the inequality (16) *is also valid.*

Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$.

Corollary 3.5. *Let T be a tree with $n \geq 3$ vertices. Then*

$$\overline{F}(\overline{T}) \geq 2(n-2) + \frac{(2(n^2-3n+3) - M_1(T))^2}{2(n-2)}. \tag{17}$$

Equality holds if and only if $T \cong P_n$.

From (8) and (16) we have that the following is valid:

Corollary 3.6. *Let T be a tree with $n \geq 4$ vertices. Then, for any real $\alpha \geq 2$, holds*

$$\begin{aligned} {}^0\overline{R}_\alpha(T) + {}^0\overline{R}_\alpha(\overline{T}) &\geq 2(n-2)\left(1 + (n-2)^{\alpha-3}\right) + \\ &+ \frac{(2(n^2-3n+3) - M_1(T))^{\alpha-1}\left(2^{\alpha-2} + (n-3)^{\alpha-2}\right)}{2^{\alpha-2}(n-2)^{\alpha-2}(n-3)^{\alpha-2}}. \end{aligned} \tag{18}$$

The inequality (18) *is also valid when $\alpha \leq 1$ and $T \ncong K_{1,n-1}$. When $1 \leq \alpha \leq 2$ the opposite inequality in* (18) *is valid. Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$.*

Corollary 3.7. *Let T be a tree with $n \geq 4$ vertices. Then*

$$\overline{F}(T) + \overline{F}(\overline{T}) \geq 4(n-2) + \frac{(n-1)\Big(2(n^2-3n+3) - M_1(T)\Big)^2}{2(n-2)(n-3)}.$$

Equality holds if and only if $T \cong P_n$.

References

[1] A. ALI, I. GUTMAN, E. MILOVANOVIĆ, I. MILOVANOVIĆ, *Sum of powers of the degrees of graphs: extremal results and bounds*, MATCH Commun. Math. Comput. Chem. 80 (2018) 5–84.

[2] B. BOROVIČANIN, K. C. DAS, B. FURTULA, I. GUTMAN, *Bounds for Zagreb indices*, MATCH Commun. Math. Comput. Chem. 78 (2017) 17–100.

[3] N. DE, S. M. A. NAYEEM, A. PAL, *The F–coindex of some graph operations*, SpringerPlus 5 (2016) #221.

[4] T. DOŠLIĆ, *Vertex–weighted Wiener polynomials for composite graphs*, Ars Math. Comp. 1 (2008) 66–80.

[5] B. FURTULA, I. GUTMAN, *A forgotten topological index*, J. Math. Chem. 53 (4) (2015) 1184–1190.

[6] I. GUTMAN, *Degree–based topological indices*, Croat. Chem. Acta 86 (2013) 351–361.

[7] I. GUTMAN, N. TRINAJSTIĆ, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. 17 (1972) 535–538.

[8] I. GUTMAN, E. MILOVANOVIĆ, I. MILOVANOVIĆ, *Beyond the Zagreb indices*, AKCE Int. J. Graph. Comb. 17 (2020) 74–85.

[9] I. GUTMAN, K. C. DAS, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. 50 (2004) 83–92.

[10] Y. HU, X. LI, T. XU, I. GUTMAN, *On molecular graphs with smallest and greatest zeroth–order Randić index*, MATCH Commun. Math. Comput. Chem. 54 (2005) 425–434.

[11] J. L. W. JENSEN, *Sur les functions convexes of les integralities entre les valuesmoyennes*, Acta Math. 30 (1906) 175–193.

[12] A. KHAKSARI, M. CHORBANI, *On the forgotten topological index*, J. Math. Chem. 8 (2017) 327–338.

[13] X. LI, J. ZHENG, *A unified approach to the extremal trees for different indices*, MATCH Commun. Math. Comput. Chem. 54 (2005) 195–208.

[14] X. LI, H. ZHAO, *Trees with the first three smallest and largest generalized topological indices*, MATCH Commun. Math. Comput. Chem. 50 (2004) 57–62.

[15] J. B. LIU, M. M. MATEJIĆ, E. I. MILOVANOVIĆ, I. Ž. MILOVANOVIĆ, *Some new inequalities for the forgotten index and coindex of graphs*, MATCH Commun. Math. Comput. Chem. 84 (2020) 719–738.

[16] T. MANSOUR, C. SONG, *The a and (a,b)-analogs of Zagreb indices and coindices of graphs*, Int. J. Comb. 2012 (2012) Art. ID 909285.

[17] A. MILIČEVIĆ, S. NIKOLIĆ, *On variable Zagreb indices*, Croat. Chem. Acta 77 (2004) 97–101.

[18] I. MILOVANOVIĆ, E. MILOVANOVIĆ, M. MATEJIĆ, *Some remarks on the general zeroth–order Randić coindex*, Filomat (in press).

[19] I. MILOVANOVIĆ, M. MATEJIĆ, E. MILOVANOVIĆ, *A note on the zeroth–order Randić coindex of graphs*, Contrib. Math. 1 (2020) 17–21.

[20] P. MILOŠEVIĆ, I. MILOVANOVIĆ, E. MILOVANOVIĆ, M. MATEJIĆ, *Some inequalities for general zeroth–order Randić index*, Filomat 33 (2019) 5251–5260.

[21] D. S. MITRINOVIĆ, J. E. PEČARIĆ, A. M. FINK, *Classical and new inequalities in analysis*, Kluwer Academic Publishers, Dorchrecht, 1993.

[22] R. TODESCHINI, V. CONSONNI, *Handbook of molecular descriptors*, Wiley VCH, Weinheim, 2000.

[23] R. TODESCHINI, V. CONSONNI, *New local vetrex invariants and molecular descriptors based on the vertex degrees*, MATCH Commun. Math. Comput. Chem. 64 (2010) 359–372.

[24] B. VUKIČEVIĆ, *Bond additive modeling 2. Mathematical properties of maximum radeg index*, Croat. Chem. Acta 83 (2010) 261–273.

[25] D. VUKIČEVIĆ, Q. LI, J. SEDLAR, T. DOŠLIĆ, *Lanzhou index*, MATCH Commun. Math. Comput. Chem. 80 (2018) 863–876.