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A note on the general zeroth–order Randić coindex of graphs

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Abstract

Let G be a simple graph of minimum degree at least 1. Let $V = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G, and denote by d_i the degree of the vertex v_i for $i = 1, 2, \cdots, n$. If the two vertices v_i and v_j are not adjacent in G, we write $i \nsim j$. The general zeroth–order Randić coindex of G is defined as ${}^0\overline{R}_\alpha(G) = \sum_{i \nsim j,\ i \neq j}(d_i^{\alpha-1} + d_j^{\alpha-1})$, where α is an arbitrary real number. Denote by $\overline{G}$ the complement of G. In this note, by assuming that G is a tree, we derive new lower bounds on the numbers ${}^0\overline{R}_\alpha(G)$ and ${}^0\overline{R}_\alpha(\overline{G})$, and determine all the graphs attaining these bounds. As the special cases of the main results, we obtain bounds on the first Zagreb coindex ${}^0\overline{R}_2$ as well as on the forgotten topological coindex ${}^0\overline{R}_3$ (which is also called the Lanzhou index).

Keywords: topological index; general zeroth–order Randić coindex; first Zagreb coindex; forgotten topological coindex; Lanzhou index.

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1. Introduction

Let $G = (V, E)$ be a simple graph with the vertex set $V = \{v_1, v_2, \ldots, v_n\}$, edge set E and with the vertex–degree sequence $(d_1, d_2, \cdots, d_n)$ satisfying $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, where $n \geq 3$, $|E| = m$ and d_i is the degree of the vertex v_i for $i = 1, 2, \cdots, n$. The complement of G is the simple graph $\overline{G} = (V, \overline{E})$, with the vertex set equal to the vertex set of G and with the edge set $\overline{E}$ consisting of all the edges not present in G. Since the sum of the number of edges of G and $\overline{G}$ is equal to the number of edges of the complete graph K_n, the number of edges in $\overline{G}$ is $\overline{m} = \frac{n(n-1)}{2} - m$. If the vertices v_i and v_j are adjacent in G, we write $i \sim j$ and if they are not adjacent in 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 the labeling of vertices or edges, or on the drawings of the graphs. In chemical graph theory, such quantities are usually referred to as topological indices [6, 18–20]. Many of them are defined as simple functions of the degrees of the vertices of graph. Many degree based topological indices can be viewed as the contributions of pairs of adjacent vertices. But, equally important are the degree based topological indices that are defined over the non-adjacent pairs of vertices for computing some topological properties of graphs, and such topological indices are named as topological coindices.

The first Zagreb index is a vertex–degree–based graph invariant defined as

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

The quantity M_1 was first time considered in 1972 [7]. It was recognized to be a measure of the extent of branching of the carbon–atom skeleton of the underlying molecule. The first Zagreb index became one of the most popular and most extensively studied graph-based molecular structure descriptors.

Various generalizations of the first Zagreb index have been proposed. In [9] a so called general zeroth–order Randić index was introduced. It was conceived as

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

where α is an arbitrary real number (note that ${}^0R_\alpha(G)$ is well-defined also for $\alpha < 0$ because we already have assumed that $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, which means that G does not contain any isolated vertex). This index is also met under the names the first general Zagreb index [11] and variable first Zagreb index [14]. For specific values of α, specific notations

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and hence specific names are being used. For example, the choice $\alpha = 2$ gives the aforementioned first Zagreb index. For $\alpha = 3$, the so called forgotten topological index [4]

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

is gained. More details on the above-mentioned indices and their mathematical properties can be found in the surveys [1, 2, 8, 16] and in the references cited therein.

The notion of a coindex was introduced in [3]. The general zeroth–order Randić coindex was defined in [13] as

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

where α is an arbitrary real number. For its mathematical properties and bounds (both upper and lower), one can refer to [13, 15]. In [13], the authors proved that if $\alpha \geq 2$ then

$$\overline{{}^0R}_\alpha(G) = \sum_{i=1}^{n} (n-1-d_i) d_i^{\alpha-1}. \tag{1}$$

We remark here that (1) holds for any real number α because $d_i > 0$ for $i = 1, 2, \ldots, n$, and

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

It needs to be mentioned here that $\overline{{}^0R}_2$ is same as the first Zagreb coindex $\overline{M}_1$ that was proposed in [3] and $\overline{{}^0R}_3$ is equal to the forgotten topological coindex (or F-coindex for short) $\overline{F}$ that was introduced in [5]. In [21], the F-coindex was referred as the Lanzhou index. In this note, new lower bounds on the numbers $\overline{{}^0R}_\alpha(G)$ and $\overline{{}^0R}_\alpha(\overline{G})$ are established when G is a tree. All the trees attaining these bounds are also determined. Moreover, as the special cases of the main results, lower bounds on the first Zagreb coindex $\overline{M}_1$ as well as on the forgotten topological coindex (or the Lanzhou index) $\overline{F}$ are obtained.

2. Main results

Firstly, we recall a discrete inequality for real number sequences that is crucial in proving the main theorems of this note.

Lemma 2.1. *Let $p = (p_i)$, $i = 1, 2, \ldots, n$, be a non-negative real number sequence and let $a = (a_i)$, $i = 1, 2, \ldots, n$, be a sequence of positive real numbers. In [10] (see also [17]) it was proved that for any real r satisfying $r \leq 0$ or $r \geq 1$, it holds that*

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

When $0 \leq r \leq 1$, the opposite inequality in (2) is valid. Equality in (2) 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 satisfying $1 \leq t \leq n-1$.

As usual, the path and star graphs of order n are denoted by P_n and $K_{1,n-1}$, respectively. Next, we need to prove the following auxiliary result for trees.

Lemma 2.2. *Let T be a tree with the vertex–degree sequence $(d_1, d_2, \cdots, d_n)$ satisfying $d_1 \geq d_2 \geq \cdots \geq d_n$, where $n \geq 3$. If*

$$n - 1 \neq d_2 = \cdots = d_{n-2},$$

then $T \cong P_n$ or $T \cong K_{1,n-1}$, and vice versa.

Proof. Let $d_2 = \cdots = d_{n-2} > d_{n-1} = d_n = 1$. Then a tree T has only two vertices of degree 1, which implies that $T \cong P_n$. If $d_2 = \cdots = d_{n-2} = d_{n-1} = d_n = 1$, then $d_1 = n-1$, which means that $T \cong K_{1,n-1}$. □

Now, we are prepared to prove the first main result of this note. This result reveals a connection between $\overline{{}^0R}_\alpha(T)$ and $M_1(T)$, where T is a tree.

Theorem 2.1. *Let T be a tree of order $n \geq 4$ and maximum degree Δ. If α is any real number satisfying $\alpha \leq 1$ or $\alpha \geq 2$, then it holds that*

$$\overline{{}^0R}_\alpha(T) \geq 2(n-2) + (n-1-\Delta)\Delta^{\alpha-1} + \frac{\left(2(n^2-3n+3) - (n-1-\Delta)\Delta - M_1(T)\right)^{\alpha-1}}{(n^2-6n+\Delta+7)^{\alpha-2}}. \tag{3}$$

When $1 \leq \alpha \leq 2$, the opposite inequality in (3) is valid. Equality in (3) 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 (2) can be considered as

$$\left(\sum_{i=2}^{n-2} p_i\right)^{r-1} \sum_{i=2}^{n-2} p_i a_i^r \geq \left(\sum_{i=2}^{n-2} p_i a_i\right)^r . \tag{4}$$

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

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

that is

$$((n-1)(n-3) - 2m + \Delta + \delta + d_{n-1})^{\alpha-2} \left({}^0\overline{R}_\alpha(G) - (n-1-\Delta)\Delta^{\alpha-1} - (n-1-\delta)\delta^{\alpha-1} - (n-1-d_{n-1})d_{n-1}^{\alpha-1}\right)$$
$$\geq (2m(n-1) - M_1(G) - (n-1-\Delta)\Delta - (n-1-\delta)\delta - (n-1-d_{n-1})d_{n-1})^{\alpha-1} .$$

Let G be a tree, $G = T$. Then $m = n - 1$ and $d_{n-1} = d_n = \delta = 1$ (since every tree has at least two vertices of degree 1). In that case the above inequality becomes

$$(n^2 - 6n + 7 + \Delta)^{\alpha-2} \left({}^0\overline{R}_\alpha(T) - 2(n-2) - (n-1-\Delta)\Delta^{\alpha-1}\right) \geq (2(n^2 - 3n + 3) - (n-1-\Delta)\Delta - M_1(T))^{\alpha-1} , \tag{5}$$

from which (3) is obtained.

The opposite inequality, i.e. when $1 \leq \alpha \leq 2$, is proved analogously.

Equality in (5) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n - 1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_{n-2}$, for some t, $2 \leq t \leq n-3$, or $n - 1 \neq d_2 = \cdots = d_{n-2}$. Then, according to Lemma 2.2 we have that equality in (3) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$, or $T \cong K_{1,n-1}$. □

Corollary 2.1. *If T is a tree of order $n \geq 4$ and maximum degree Δ, then for any real number α satisfying $\alpha \leq 1$ or $\alpha \geq 2$, it holds that*

$${}^0\overline{R}_\alpha(T) \geq 2(n-2) + (n-1-\Delta)\Delta^{\alpha-1} + \frac{(2(n-2)^2 - (2n-3-\Delta)\Delta)^{\alpha-1}}{(n^2 - 6n + 7 + \Delta)^{\alpha-2}} .$$

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

Proof. The following inequality was proved in [12]

$$M_1(T) \leq 2(n-1) + (n-2)\Delta , \tag{6}$$

with equality if and only if $T \cong P_n$ or $T \cong K_{1,n-1}$. From the inequalities (6) and (3), we obtain the required result. □

From Corollary 2.1, we obtain lower bounds on the forgotten topological coindex $\overline{F}$ and on the first Zagreb coindex $\overline{M}_1$ of the trees.

Corollary 2.2. *If T is a tree of order $n \geq 4$ and maximum degree Δ, then*

$$\overline{F}(T) \geq 2(n-2) + (n-1-\Delta)\Delta^2 + \frac{(2(n-2)^2 - (2n-3-\Delta)\Delta)^2}{n^2 - 6n + 7 + \Delta} ,$$

with equality holding if and only if $T \cong P_n$, or $T \cong K_{1,n-1}$.

Corollary 2.3. *If T is a tree of order $n \geq 4$ and maximum degree Δ, then*

$$\overline{M}_1(T) \geq (n-2)[2(n-1) - \Delta] , \tag{7}$$

with equality holding if and only if $T \cong P_n$, or $T \cong K_{1,n-1}$.

Note that the inequalities (6) and (7) are equivalent because the equation $\overline{M}_1(G) = 2m(n-1) - M_1(G)$ holds for any graph G of order n and size m. In the next theorem, we determine a relationship between ${}^0\overline{R}_\alpha(\overline{T})$ and $M_1(T)$.

Theorem 2.2. *Let T be a tree of order $n \geq 4$ and maximum degree Δ. If $\alpha \leq 1$ and $T \ncong K_{1,n-1}$ or if $\alpha \geq 2$, then it holds that*

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

When $1 \leq \alpha \leq 2$, the opposite inequality in (8) is valid. Equality in (8) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $T \cong P_n$, or $T \cong K_{1,n-1}$ and $\alpha \geq 1$.

Proof. For $r=\alpha-1$, $\alpha\le 1$ or $\alpha\ge 2$, $p_i=d_i$, $a_i=n-1-d_i$, $i=1,2,\dots,n$, the inequality (4) transforms into

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

that is

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

When graph has a tree structure, we have $m=n-1$ and $d_{n-1}=d_n=\delta=1$, and the above inequality becomes

$$(2(n-2)-\Delta)^{\alpha-2}\left({}^0\overline{R}_\alpha(\overline{T})-2(n-2)^{\alpha-1}-\Delta(n-1-\Delta)^{\alpha-1}\right)\ge\Big(2(n^2-3n+3)-M_1(T)-\Delta(n-1-\Delta)\Big)^{\alpha-1},\tag{9}$$

from which (8) is obtained.

Equality in (9) holds if and only if $\alpha=1$, or $\alpha=2$, or $d_2=\cdots=d_{n-2}$. Having this in mind and Lemma 2.2 we conclude that equality in (8) holds if and only if either $\alpha=1$, or $\alpha=2$, or $T\cong P_n$, or $T\cong K_{1,n-1}$ and $\alpha\ge 1$. □

Corollary 2.4. *Let T be a tree of order $n\ge 4$ and maximum degree Δ. If $\alpha\le 1$ and $T\ncong K_{1,n-1}$ or if $\alpha\ge 2$, then it holds that*

$${}^0\overline{R}_\alpha(\overline{T})\ge 2(n-2)^{\alpha-1}+\Delta(n-1-\Delta)^{\alpha-1}+\frac{(2(n-2)^2-(2n-3-\Delta)\Delta)^{\alpha-1}}{(2(n-2)-\Delta)^{\alpha-2}}.\tag{10}$$

When $1\le\alpha\le 2$ the opposite inequality in (10) is valid. Equality in (10) holds if and only if either $\alpha=1$, or $T\cong P_n$, or $T\cong K_{1,n-1}$ and $\alpha\ge 1$.

From Corollary 2.4, we obtain lower bounds on the forgotten topological coindex $\overline{F}$ and on the first Zagreb coindex $\overline{M}_1$ of the complement of trees.

Corollary 2.5. *If T is a tree of order $n\ge 4$ and maximum degree Δ, then*

$$\overline{F}(\overline{T})\ge 2(n-2)^2+\Delta(n-1-\Delta)^2+\frac{(2(n-2)^2-(2n-3-\Delta)\Delta)^2}{2(n-2)-\Delta}.$$

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

Corollary 2.6. *If T is a tree of order $n\ge 4$ and maximum degree Δ, then*

$$\overline{M}_1(\overline{T})\ge(n-2)[2(n-1)-\Delta],\tag{11}$$

with equality holding if and only if $T\cong P_n$, or $T\cong K_{1,n-1}$.

It needs to be noted here that the inequalities (6), (7) and (11) are equivalent because it holds that $\overline{M}_1(\overline{G})=\overline{M}_1(G)=2m(n-1)-M_1(G)$ for any graph G of order n and size m. Next result follows from Corollaries 2.2 and 2.5.

Corollary 2.7. *If T is a tree of order $n\ge 4$ and maximum degree Δ, then*

$$\overline{F}(T)+\overline{F}(\overline{T})\ge(n-1)\left(2(n-2)+(n-1-\Delta)\Delta+\frac{(n-3)(2(n-2)^2-(2n-3-\Delta)\Delta)^2}{(2(n-2)-\Delta)(n^2-6n+7+\Delta)}\right).$$

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

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