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Some Remarks on the General Zeroth–Order Randić Coindex

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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 and size m, without isolated vertices. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n$, $d_i = d(v_i)$ a sequence of vertex degrees of G. The general zeroth–order Randić index is defined as ${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha$, where α is an arbitrary real number. The corresponding general zeroth–order Randić coindex is defined via ${}^0\overline{R}_\alpha(G) = \sum_{i=1}^n (n-1-d_i)d_i^\alpha$. Some new bounds for the general zeroth–order Randić coindex and relationship between ${}^0\overline{R}_\alpha(\overline{G})$ and ${}^0\overline{R}_{\alpha-1}(\overline{G})$ are obtained. For a particular values of parameter α a number of new bounds for different topological coindices are obtained as corollaries.

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple connected graph with n vertices, m edges and a sequence of vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$, $d_i = d(v_i)$. The complement of G, denoted as $\overline{G}$, has the same vertex set $V(G)$, and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G, that is $\overline{G} = (V, \overline{E})$. If vertices v_i and v_j of G are adjacent, we write $i \sim j$. On the other hand, if v_i and v_j are adjacent in $\overline{G}$, we write $i \nsim j$.

A topological index of a graph is a numerical quantity which is invariant under automorphisms of the graph. Topological indices are important and useful tools in mathematical chemistry, nanomaterials, pharmaceutical engineering, etc. used for quantifying information on molecules. Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph. Various mathematical properties of topological indices have been investigated, as well.

In [5] a so called general zeroth–order Randić index was introduced. It is defined as

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

where α is an arbitrary real number. It is also met under the names first general Zagreb index [6] and variable first Zagreb index [7].

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For specific values of α, specific notations (and hence specific names) are being used. Thus, for $\alpha = 2$, one of the most popular and most extensively studied graph-based molecular structure descriptors, the first Zagreb index [10]

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

is obtained.

For $\alpha = 3$, a so called forgotten topological index [9]

$$F(G) = \sum_{i=1}^{n} d_i^3\,,$$

is acquired, and for $\alpha = -1$, the inverse degree index [11]

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} = \sum_{i\sim j}\left(\frac{1}{d_i^2} + \frac{1}{d_j^2}\right)$$

is gained.

For various mathematical properties of the above topological indices one can refer to [1, 12–16] and references cited therein.

Let v_i be a vertex of the graph G and let $\Phi(v_i)$ be any quantity associated to v_i. In [2] the following graph invariant has been introduced

$$TI(G) = \sum_{i=1}^{n} \Phi(v_i)\,,$$

and in [3] it was proven that the following edge–decomposition of $TI(G)$ is valid

$$TI(G) = \sum_{i\sim j}\left(\frac{\Phi(v_i)}{d_i} + \frac{\Phi(v_j)}{d_j}\right).$$

If $\Phi(v_i) = d_i f(d_i)$, where f is a real function defined on the set $D = \{d_1, d_2, \dots, d_n\}$, then

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

Let $TI(G)$ be a vertex–degree based topological index defined by (1). In [1] a concept of coindices was introduced. The corresponding coindex of $TI(G)$, can be defined via [4]

$$\overline{TI}(G) = \sum_{i\nsim j}(f(d_i) + f(d_j)) = \sum_{i=1}^{n}(n-1-d_i)f(d_i)\,. \tag{2}$$

Obviously, in this case the sum runs over the edges of the complement of G.

If function f is defined on the set $\overline{D} = \{n-1-d_1, n-1-d_2, \dots, n-1-d_n\}$, then according to (1) and (2) we have that

$$TI(\overline{G}) = \sum_{i=1}^{n}(n-1-d_i)f(n-1-d_i)\,, \tag{3}$$

and

$$\overline{TI}(\overline{G}) = \sum_{i=1}^{n} d_i f(n-1-d_i)\,. \tag{4}$$

It is not difficult to verify that according to (1), (2), (3) as well as (4), the following result holds.

Lemma 1.1. *Let $TI(G)$ be a vertex–degree–based topological index defined as*

$$TI(G) = \sum_{i\sim j}(f(d_i) + f(d_j)) = \sum_{i=1}^{n} d_i f(d_i),$$

where f is a real function defined on set $D = \{d_1, d_2, \dots d_n\}$. Then we have that

$$TI(G) + \overline{TI}(G) = (n-1)\sum_{i=1}^{n} f(d_i), \tag{5}$$

and, if f is defined on the set $\overline{D} = \{n-1-d_1, n-1-d_2, \dots, n-1-d_n\}$, then we have

$$TI(\overline{G}) + \overline{TI}(\overline{G}) = (n-1)\sum_{i=1}^{n} f(n-1-d_i). \tag{6}$$

Having in mind (2), the general zeroth–order Randić coindex [21] can be defined as

$${}^0\overline{R}_\alpha(G) = \sum_{i\nsim j}\left(d_i^{\alpha-1} + d_j^{\alpha-1}\right) = \sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha-1}. \tag{7}$$

We have the following corollary of Lemma 1.1.

Corollary 1.2. *Let G be a simple graph without isolated vertices. Then, for any real α we have that*

$${}^0R_\alpha(G) + {}^0\overline{R}_\alpha(G) = (n-1)\sum_{i=1}^{n} d_i^{\alpha-1}, \tag{8}$$

and for $\alpha \geq 1$

$${}^0R_\alpha(\overline{G}) + {}^0\overline{R}_\alpha(\overline{G}) = (n-1)\sum_{i=1}^{n}(n-1-d_i)^{\alpha-1}. \tag{9}$$

The equality (8) for $\alpha \geq 1$ has been proven in [21] (see also [8]).

In this paper we establish some new bounds for the general zeroth–order Randić coindex and determine relationship between ${}^0\overline{R}_\alpha(\overline{G})$ and ${}^0\overline{R}_{\alpha-1}(\overline{G})$. For a particular values of parameter α a number of new bounds for different topological coindices are obtained as corollaries.

2. Preliminaries

The following analytical inequality will be frequently used in the proofs of main results of this paper (see eg. [17]).

Let $p = (p_i)$, $i, 2, \dots, n$, be a sequence of non-negative real numbers and $a = (a_i)$, $i = 1, 2, \dots, n$, a sequence of positive real numbers. Then, for any real r, $r \leq 0$ or $r \geq 1$, holds

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1}\sum_{i=1}^{n} p_i a_i^r \geq \left(\sum_{i=1}^{n} p_i a_i\right)^r. \tag{10}$$

For $0 \leq r \leq 1$, the opposite inequality holds. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, for some t, $1 \leq t \leq n-1$.

3. Main results

In the next theorem we will determine a relationship between ${}^0\overline{R}_\alpha(G)$ and ${}^0\overline{R}_{\alpha-1}(G)$, where α is a real number.

Theorem 3.1. *Let G, $G \ncong K_n$, be a simple graph of order $n \geq 3$ and size m without isolated vertices. Then, for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, we have*

$$ {}^0\overline{R}_\alpha(G) \leq (n-1){}^0\overline{R}_{\alpha-1}(G) - \frac{(n(n-1)^2 - 4m(n-1) + M_1(G))^{\alpha-1}}{((n-1)^2 ID(G) + 2m - 2n(n-1))^{\alpha-2}} . \tag{11} $$

If in addition, $G \ncong K_{1,n-1}$, then

$$ {}^0\overline{R}_\alpha(G) \geq {}^0\overline{R}_{\alpha-1}(G) + \frac{(2mn - M_1(G) - n(n-1))^{\alpha-1}}{(n^2 - 2m - (n-1)ID(G))^{\alpha-2}} . \tag{12} $$

If $1 \leq \alpha \leq 2$, the sense of inequalities reverses.

Equality in (11) *holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-2$.*

Equality in (12) *holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n \neq 1$, for some t, $1 \leq t \leq n-2$, or $n-1 \neq d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$.*

Proof. Based on (6) we have

$$ (n-1){}^0\overline{R}_{\alpha-1}(G) - {}^0\overline{R}_\alpha(G) = \sum_{i=1}^{n} (n-1-d_i)^2 d_i^{\alpha-2} . \tag{13} $$

On the other hand, for $r = \alpha - 1$, $\alpha \leq 1$ or $\alpha \geq 2$, $p_i = \frac{(n-1-d_i)^2}{d_i}$, $a_i = d_i$, $i = 1, 2, \dots, n$, the inequality (10) becomes

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

that is

$$ \Big((n-1)^2 ID(G) + 2m - 2n(n-1) \Big)^{\alpha-2} \sum_{i=1}^{n} (n-1-d_i)^2 d_i^{\alpha-2} \geq \Big(n(n-1)^2 + M_1(G) - 4m(n-1) \Big)^{\alpha-1} . $$

Since $G \ncong K_n$, we have that $(n-1)^2 ID(G) + 2m - 2n(n-1) \neq 0$, which implies that

$$ \sum_{i=1}^{n} (n-1-d_i)^2 d_i^{\alpha-2} \geq \frac{(n(n-1)^2 - 4m(n-1) + M_1(G))^{\alpha-1}}{((n-1)^2 ID(G) + 2m - 2n(n-1))^{\alpha-2}} . \tag{14} $$

From the above and inequality (13) we arrive at (11).

Similarly, based on (6) we have that

$$ {}^0\overline{R}_\alpha(G) - {}^0\overline{R}_{\alpha-1}(G) = \sum_{i=1}^{n} (n-1-d_i)(d_i-1) d_i^{\alpha-2} . \tag{15} $$

For $r = \alpha - 1$, $\alpha \leq 1$ or $\alpha \geq 2$, $p_i = \frac{(n-1-d_i)(d_i-1)}{d_i}$, $a_i = d_i$, $i = 1, 2, \dots, n$, the inequality (10) transforms into

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

that is

$$(n^2 - 2m - (n-1)ID(G))^{\alpha-2} \sum_{i=1}^{n} (n-1-d_i)(d_i-1)d_i^{\alpha-2} \geq (2mn - M_1(G) - n(n-1))^{\alpha-1}\,.$$

Since $G \ncong K_n$ and $G \ncong K_{1,n-1}$, we have that $n^2 - 2m - (n-1)ID(G) \neq 0$, which implies that

$$\sum_{i=1}^{n} (n-1-d_i)(d_i-1)d_i^{\alpha-2} \geq \frac{(2mn - M_1(G) - n(n-1))^{\alpha-1}}{(n^2 - 2m - (n-1)ID(G))^{\alpha-2}}\,. \tag{16}$$

Now, inequality (12) is obtained from (15) and (16).

It can be easily verified that according to (10) when $1 \leq \alpha \leq 2$, the opposite inequalities are valid in (11) and (12).

Equality in (14), and consequently in (11), holds if and only if $\alpha = 1$, or $\alpha = 2$, or $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-2$.

Equality in (16), and consequently in (12), holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n \neq 1$, for some t, $1 \leq t \leq n-2$, or $n-1 \neq d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$. □

Corollary 3.2. *Let G be a simple graph of order $n \geq 3$ and size m without isolated vertices. If $G \ncong K_n$, then*

$$\overline{F}(G) \leq 2m(n-1)^2 - (n-1)M_1(G) - \frac{(n(n-1)^2 - 4m(n-1) + M_1(G))^2}{(n-1)^2 ID(G) + 2m - 2n(n-1)}\,, \tag{17}$$

and

$$\overline{F}(G) \geq 2m(n-1) - M_1(G) + \frac{(2mn - M_1(G) - n(n-1))^2}{n^2 - 2m - (n-1)ID(G)}\,. \tag{18}$$

Equality in (17) *holds if and only if $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-2$.*

Equality in (18) *holds if and only if either $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n \neq 1$, for some t, $1 \leq t \leq n-2$, or $n-1 \neq d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \leq t \leq n-2$.*

Proof. The required inequalities are obtained from (11) and (12) for $\alpha = 3$, and from

$$\overline{M_1}(G) = 2m(n-1) - M_1(G)\,,$$

which was proven in [18]. □

The proofs of the following two theorems are fully analogous to that of Theorem 3.1, hence omitted.

Theorem 3.3. *Let G, $G \ncong K_n$, be a simple graph of order $n \geq 3$ and size m without isolated vertices. If $G \ncong K_n$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds*

$${}^{0}\overline{R}_\alpha(G) \geq \frac{(n(n-1) - 2m)^\alpha}{((n-1)ID(G) - n)^{\alpha-1}}\,.$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid.

Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $n-1 \neq d_1 = \cdots = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-2$.

Theorem 3.4. *Let G, $G \ncong K_n$, be a simple graph of order $n \geq 3$ and size m without isolated vertices. If $G \ncong K_n$, then for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

$${}^{0}\overline{R}_\alpha(G) \geq \frac{(2m(n-1) - M_1(G))^{\alpha-1}}{(n(n-1) - 2m)^{\alpha-2}}\,.$$

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

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

For particular values of parameter α, the following corollaries of Theorems 3.3 and 3.4 are obtained.

Corollary 3.5. *Let G, $G \ncong K_n$, be a simple graph of order $n \geq 3$ and size m, without izolated vertices. Then*

$$\begin{aligned}
\overline{ID}(G) &\geq \frac{((n-1)ID(G)-n)^2}{n(n-1)-2m}, \\
\overline{M}_1(G) &\geq \frac{(n(n-1)-2m)^2}{(n-1)ID(G)-n}, \\
\overline{F}(G) &\geq \frac{(n(n-1)-2m)^3}{((n-1)ID(G)-n)^2}, \\
\overline{F}(G) &\geq \frac{(2m(n-1)-M_1(G))^2}{n(n-1)-2m}.
\end{aligned}$$

Equalities hold if and only if $n-1 \neq d_1 = \cdots = d_n$, or $n-1 = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-2$.

In [19] the following inequality was proven:

$$M_1(G) \leq m\left(\frac{2m}{n-1} + n - 2\right),$$

with equality if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ (see [20]). Having in mind the above inequality we obtain the following corollaries of Theorem 3.4.

Corollary 3.6. *Let G be a simple graph with $n \geq 2$ vertices and m edges. Then, for any real α, $\alpha \geq 2$, we have that*

$$^0\overline{R}_\alpha(G) \geq \frac{(n(n-1)-2m)m^{\alpha-1}}{(n-1)^{\alpha-1}},$$

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

Corollary 3.7. *Let T be an arbitrary tree with $n \geq 2$ vertices. Then for any real α, $\alpha \geq 2$, holds*

$$^0\overline{R}_\alpha(T) \geq (n-1)(n-2),$$

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

In the next theorem we determine the lower bound for $^0\overline{R}_\alpha(\overline{G})$.

Theorem 3.8. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then, for any real α, $\alpha \geq 2$, holds*

$$^0\overline{R}_\alpha(\overline{G}) \geq \frac{(2m(n-1)-M_1(G))^{\alpha-1}}{(2m)^{\alpha-2}}. \tag{19}$$

For $1 \leq \alpha \leq 2$, the sense of (19) *reverses. Equality holds if and only if eiher $\alpha = 1$, or $\alpha = 2$, or G is regular.*

Proof. For $TI(G) = ^0R_\alpha(G)$ from (4) we have that

$$^0\overline{R}_\alpha(\overline{G}) = \sum_{i=1}^{n} d_i(n-1-d_i)^{\alpha-1}. \tag{20}$$

On the other hand, for $r = \alpha - 1$, $\alpha \geq 2$, $p_i = d_i$, $a_i = n-1-d_i$, $i = 1, 2, \ldots, n$, the inequality (10) becomes

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

that is

$$(2m)^{\alpha-2}\sum_{i=1}^{n} d_i(n-1-d_i)^{\alpha-1} \geq (2m(n-1)-M_1(G))^{\alpha-1}\,. \tag{21}$$

The inequality (19) is obtained from (20) and (21).

It can be easily proved that when $1 \leq \alpha \leq 2$, the opposite inequality holds in (19). Equality in (21), and hence in (19), holds if and only if either $\alpha = 1$, or $\alpha = 2$, or if G is regular. □

Corollary 3.9. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then, for any real α, $\alpha \geq 2$, holds*

$$^0\overline{R}_\alpha(\overline{G}) \geq \frac{m(n(n-1)-2m)^{\alpha-1}}{2^{\alpha-2}(n-1)^{\alpha-1}}\,.$$

Equality holds if and only if $G \cong K_n$.

Now we state a few inequalities of Nordhaus–Gaddum type (see [22]) which can be easily proved using (8), (9) and (10).

Theorem 3.10. *Let G be a simple graph of order $n \geq 2$ and size m without isolated vertices. Then, for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds*

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

When $0 \leq \alpha \leq 1$, the opposite inequality holds. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or G is regular.

Theorem 3.11. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. The, for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

$$^0R_\alpha(G) + {}^0\overline{R}_\alpha(G) \geq \frac{(n-1)(2m)^{\alpha-1}}{n^{\alpha-2}}\,.$$

When $1 \leq \alpha \leq 2$, the opposite inequality holds. Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or G is regular.

Theorem 3.12. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then, for any α, $\alpha \geq 2$, holds*

$$^0R_\alpha(\overline{G}) + {}^0\overline{R}_\alpha(\overline{G}) \geq \frac{(n-1)(n(n-1)-2m)^{\alpha-1}}{n^{\alpha-2}}\,.$$

When $1 \leq \alpha \leq 2$ the opposite inequality holds. Equality holds if and only if either $\alpha = 1$, or $\alpha = 2$, or G is regular.

In the next theorem we establish a relationship between $^0\overline{R}_{\alpha+1}(G)$, $^0\overline{R}_\alpha(G)$ and $^0\overline{R}_{\alpha-1}(G)$, where α is an arbitrary real number.

Theorem 3.13. *Let G be a simple graph of order $n \geq 2$ and size m, without isolated vertices. Then, for any real α, holds*

$$^0\overline{R}_{\alpha+1}(G) + \Delta\delta\,{}^0\overline{R}_{\alpha-1}(G) \leq (\Delta+\delta)\,{}^0\overline{R}_\alpha(G)\,. \tag{22}$$

Equality holds if and only if $d_i \in \{\delta, \Delta\}$, for $i = 1, 2, \ldots, n$.

Proof. For all i, $i = 1, 2, \ldots, n$, holds

$$(\Delta - d_i)(d_i - \delta) \geq 0\,. \tag{23}$$

that is

$$\Delta\delta + d_i^2 \leq (\Delta+\delta)d_i\,.$$

After multiplying the above inequality by $(n-1-d_i)d_i^{\alpha-2}$, where α is an arbitrary real number, we obtain

$$(n-1-d_i)d_i^{\alpha} + \Delta\delta(n-1-d_i)d_i^{\alpha-2} \le (\Delta+\delta)(n-1-d_i)d_i^{\alpha-1}\,.$$

Summing the above inequality over i, $i = 1, 2, \ldots, n$, gives

$$\sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha} + \Delta\delta\sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha-2} \le (\Delta+\delta)\sum_{i=1}^{n}(n-1-d_i)d_i^{\alpha-1}\,,$$

from which the inequality (22) is obtained.

Equality in (23), and consequently in (22), holds if and only if $d_i = \Delta$ or $d_i = \delta$, for every $i = 1, 2, \ldots, n$. □

For $\alpha = 1$ and $\alpha = 2$, we obtain the following corollary of Theorem 3.13.

Corollary 3.14. *Let G be a simple graph of order $n \ge 2$ and size m, without isolated vertices. Then*

$$\overline{M}_1(G) \le (\Delta+\delta)(n(n-1)-2m) - \Delta\delta((n-1)ID(G)-n)\,,$$

and

$$\overline{F}(G) \le (\Delta+\delta)(2m(n-1)-M_1(G)) - \Delta\delta(n(n-1)-2m)\,.$$

Equalities hold if and only if $d_i \in \{\Delta, \delta\}$, for every $i = 1, 2, \ldots, n$.

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