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On the Bounds of Zeroth–Order General Randić Index

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Abstract. The zeroth–order general Randić index, ${}^0R_\alpha(G)$, of a connected graph G, is defined as ${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha$, where d_i is the degree of the vertex v_i of G and α arbitrary real number. We consider linear combinations of the ${}^0R_\alpha(G)$ of the form ${}^0R_\alpha(G) - (\Delta + \delta){}^0R_{\alpha-1}(G) + \Delta\delta\,{}^0R_{\alpha-2}(G)$ and ${}^0R_\alpha(G) - 2a\,{}^0R_{\alpha-1}(G) + a^2\,{}^0R_{\alpha-2}(G)$, where a is an arbitrary real number, and determine their bounds. As corollaries, various upper and lower bounds of ${}^0R_\alpha(G)$ and indices that represent some special cases of ${}^0R_\alpha(G)$ are obtained.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. The degree of a vertex v_i is denoted by $d_i = d(v_i)$, such that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. In particular, Δ and δ are maximum and minimum degrees of G, respectively. A graph G is called regular if all vertices of G have the same vertex degree. A graph G is called bi-degreed if it has two distinct vertex degrees.

In graph theory, a graph invariant is any property of graphs that depends only on the abstract structure, not on graph representations such as particular labellings or drawings of the graph. A graph invariant may be a polynomial (e.g., the characteristic polynomial), a set of numbers (e.g., the spectrum of a graph), or a numerical value. Numerical indices which quantitate topological characteristics of graphs are called topological indices [1]. Topological indices play an important role in studying quantitative structure–activity relationships (QSAR) and quantitative structure–property relationships (QSPR) for predicting different physico–chemical properties of chemical compounds. It is observed that some topological indices are very close to various chemical and biological properties such as boiling point, surface tension, etc. Over the years many topological indices were proposed and studied based on degree, distance and other parameters of graph. The first Zagreb index is the degree–based index introduced in [2] during the study of total π-electron energy of alternant hydrocarbons. It is defined as

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

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During the years the first Zagreb index became one of the most popular and most extensively studied graph-based molecular structure descriptors. More on its applications and mathematical properties can be found in surveys [3–7].

A generalization of the first Zagreb index, known as zeroth–order general Randić index was defined in [8] as

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

where α is an arbitrary real number. This index is also met in the literature under the names variable first Zagreb index [9], or first general Zagreb index [10]. Some special cases include:

- the modified first Zagreb index [7] (see also [10]), obtained for $\alpha=-2$, that is

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

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

$$ID(G)=\sum_{i=1}^{n}\frac{1}{d_i}\,,$$

- and the so called forgotten topological index [12], obtained for $\alpha=3$

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

In the present paper we consider linear combinations of the topological index $^{0}R_{\alpha}(G)$ of the form

$$^{0}R_{\alpha}(G)-(\Delta+\delta)^{0}R_{\alpha-1}(G)+\Delta\delta^{0}R_{\alpha-2}(G)\,, \tag{1}$$

and

$$^{0}R_{\alpha}(G)-2a\ ^{0}R_{\alpha-1}(G)+a^2\ ^{0}R_{\alpha-2}(G)\,, \tag{2}$$

where a is an arbitrary real number, and determine their bounds. This enables us to generalize and improve a number of results reported in the literature. Namely, by taking various values for parameter a we obtain a plentiful of new/old bounds for the various topological indices, including $^{0}R_{\alpha}(G)$, $M_1(G)$, $^{m}M_1(G)$, $F(G)$, $ID(G)$. Also, we establish a relationship between most commonly used irregularity measures of graphs.

2. Preliminaries

In this section we recall an analytical inequality for the real number sequences that will be frequently used in proofs of theorems.

Lemma 2.1. [13] *Let $p=(p_i)$, $i=1,2,\dots,n$, be as sequence of non–negative real numbers and $a=(a_i)$, $i=1,2,\dots,n$, sequence of positive real numbers. Then, for any r, $r\le 0$ or $r\ge 1$, holds*

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

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 $p_1=p_2=\cdots=p_t=0$ and $a_{t+1}=\cdots=a_n$, or $p_{t+1}=\cdots=p_n=0$ and $a_1=a_2=\cdots=a_t$, for some t, $1\le t\le n-1$.

The inequality (3) is known in the literature as Jensen's inequality. This is only one of many variations of this inequality. For the history of this inequality one can refer to [14] as well as monograph [34].

3. Main results

In the next theorem we determine bounds for the linear combination ${}^0R_\alpha(G) - (\Delta+\delta){}^0R_{\alpha-1}(G) + \Delta\delta{}^0R_{\alpha-2}(G)$ in terms of ${}^mM_1(G)$, $ID(G)$.

Theorem 3.1. *Let G be a connected graph of order $n \geq 4$ and size m. If $d_i \in \{\Delta, \delta\}$, for every i, $1 \leq i \leq n$, then for any real α holds*

$$ {}^0R_\alpha(G) = p\Delta^\alpha + q\delta^\alpha\,, \qquad p+q=n\,. \tag{4}$$

If $d_i \notin \{\Delta, \delta\}$, for at least one i, $2 \leq i \leq n-1$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds

$$ {}^0R_\alpha(G) \leq (\Delta+\delta)\,{}^0R_{\alpha-1}(G) - \Delta\delta\,{}^0R_{\alpha-2}(G) - \frac{(n(\Delta+\delta)-2m-\Delta\delta ID(G))^\alpha}{((\Delta+\delta)ID(G)-n-\Delta\delta\,{}^mM_1(G))^{\alpha-1}}\,. \tag{5}$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $\Delta = d_1 > d_2 = \cdots = d_{n-1} > d_n = \delta$, or $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = \delta$, for some t and r such that $1 \leq t < r \leq n-1$.

Proof. For $r = \alpha$, $\alpha \leq 0$ or $\alpha \geq 1$, $p_i = \frac{(\Delta-d_i)(d_i-\delta)}{d_i^2}$, $a_i = d_i$, $1 \leq i \leq n$, the inequality (3) becomes

$$ \left(\sum_{i=1}^n \frac{(\Delta-d_i)(d_i-\delta)}{d_i^2}\right)^{\alpha-1} \sum_{i=1}^n (\Delta-d_i)(d_i-\delta)d_i^{\alpha-2} \geq \left(\sum_{i=1}^n \frac{(\Delta-d_i)(d_i-\delta)}{d_i}\right)^\alpha\,. \tag{6}$$

Bearing in mind that

$$\begin{aligned}
\sum_{i=1}^n \frac{(\Delta-d_i)(d_i-\delta)}{d_i^2} &= \sum_{i=1}^n \left(\frac{\Delta+\delta}{d_i} - 1 - \frac{\Delta\delta}{d_i^2}\right) = \\
&= (\Delta+\delta)ID(G) - n - \Delta\delta\,{}^mM_1(G)\,, \\
\sum_{i=1}^n (\Delta-d_i)(d_i-\delta)d_i^{\alpha-2} &= \sum_{i=1}^n \left((\Delta+\delta)d_i^{\alpha-1} - \Delta\delta d_i^{\alpha-2} - d_i^\alpha\right) = \\
&= (\Delta+\delta)\,{}^0R_{\alpha-1}(G) - \Delta\delta\,{}^0R_{\alpha-2}(G) - {}^0R_\alpha(G)\,, \\
\sum_{i=1}^n \frac{(\Delta-d_i)(d_i-\delta)}{d_i} &= \sum_{i=1}^n \left((\Delta+\delta) - d_i - \frac{\Delta\delta}{d_i}\right) = \\
&= n(\Delta+\delta) - 2m - \Delta\delta ID(G)\,,
\end{aligned}$$

from the above identities and (6) we obtain that

$$ ((\Delta+\delta)ID(G)-n-\Delta\delta\,{}^mM_1(G))^{\alpha-1}\left((\Delta+\delta)\,{}^0R_{\alpha-1}(G) - \Delta\delta\,{}^0R_{\alpha-2}(G) - {}^0R_\alpha(G)\right) \geq $$

$$ \geq (n(\Delta+\delta)-2m-\Delta\delta ID(G))^\alpha\,. $$

Since $n \geq 4$ and $d_i \notin \{\Delta, \delta\}$, for at least one i, $2 \leq i \leq n-1$, we have that

$$ (\Delta+\delta)ID(G) - n - \Delta\delta\,{}^mM_1(G) > 0 $$

and

$$ n(\Delta+\delta) - 2m - \Delta\delta ID(G) > 0\,, $$

from which we obtain (5).

The case when $0 \leq \alpha \leq 1$ can be proved analogously.

If $n \geq 4$ and $d_i \notin \{\Delta, \delta\}$ for at least one i, $2 \leq i \leq n-1$, equality in (6), and consequently in (5), holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $\Delta = d_1 > d_2 = \cdots = d_{n-1} > d_n = \delta$, or $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = \delta$, for some t and r such that $1 \leq t < r \leq n-1$. □

Remark 3.2. *The inequality* (5) *is stronger than*

$$ {}^0R_\alpha(G) - (\Delta+\delta)\,{}^0R_{\alpha-1}(G) + \Delta\delta\,{}^0R_{\alpha-2}(G) \le 0\,, $$

which was proven in [24] (*see also* [15, 16]).

Corollary 3.3. *Let G be a connected graph of order $n \ge 5$ and size m. If $d_i \in \{\Delta, \delta\}$, for every i, $1 \le i \le n$, then*

$$ M_1(G) = p\Delta^2 + q\delta^2 \qquad and \qquad F(G) = p\Delta^3 + q\delta^3\,, \quad p+q=n\,. $$

If $d_i \notin \{\Delta, \delta\}$ for at least one i, $2 \le i \le n-1$, then

$$ M_1(G) \le 2m(\Delta+\delta) - n\Delta\delta - \frac{(n(\Delta+\delta) - 2m - \Delta\delta ID(G))^2}{(\Delta+\delta)ID(G) - n - \Delta\delta\,{}^mM_1(G)}\,, \tag{7} $$

and

$$ F(G) \le (\Delta+\delta)M_1(G) - 2m\Delta\delta - \frac{(n(\Delta+\delta) - 2m - \Delta\delta ID(G))^3}{((\Delta+\delta)ID(G) - n - \Delta\delta\,{}^mM_1(G))^2}\,. \tag{8} $$

Equalities hold if and only if $\Delta = d_1 > d_2 = \cdots = d_{n-1} > d_n = \delta$, or $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = \delta$, for some t and r such that $1 \le t < r \le n-1$.

Remark 3.4. *The inequality* (7) *was proven in* [29]*. Let us note that inequalities* (7) *and* (8)*, are, respectively, stronger than*

$$ M_1(G) \le 2m(\Delta+\delta) - n\Delta\delta\,, $$

and

$$ F(G) \le (\Delta+\delta)M_1(G) - 2m\Delta\delta\,, $$

which were proved in [17] (*see also* [18–22])*, and* [24] (*see also* [15, 18, 23–27]).

Corollary 3.5. *Let G be a connected graph of order $n \ge 5$ and size m. If $d_i \notin \{\Delta, \delta\}$ for at least one i, $2 \le i \le n-1$, then*

$$ F(G) \le 2m(\Delta^2+\delta^2+\Delta\delta) - n\Delta\delta(\Delta+\delta) - \frac{(n(\Delta+\delta) - 2m - \Delta\delta ID(G))^3}{((\Delta+\delta)ID(G) - n - \Delta\delta\,{}^mM_1(G))^2}\,. \tag{9} $$

Remark 3.6. *The inequality* (9) *is stronger than*

$$ F(G) \le 2m(\Delta^2+\delta^2+\Delta\delta) - n\Delta\delta(\Delta+\delta)\,, $$

which was proven in [16].

The proof of the next theorem is analogous to that of Theorem 3.1, hence omitted.

Theorem 3.7. *Let G be a connected graph of order $n \ge 4$ and size m. If $d_i \notin \{\Delta, \delta\}$ for at least one i, $2 \le i \le n-1$, then for any real α, $\alpha \le 1$ or $\alpha \ge 2$, holds*

$$ {}^0R_\alpha(G) \le (\Delta+\delta)\,{}^0R_{\alpha-1}(G) - \Delta\delta\,{}^0R_{\alpha-2}(G) - \frac{(2m(\Delta+\delta) - n\Delta\delta - M_1(G))^{\alpha-1}}{(n(\Delta+\delta) - 2m - \Delta\delta ID(G))^{\alpha-2}}\,. $$

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

Corollary 3.8. *Let G be a connected graph with $n \geq 4$ vertices and m edges. If $d_i \notin \{\Delta, \delta\}$, for at least one i, $2 \leq i \leq n-1$, then*

$$F(G) \leq (\Delta+\delta)M_1(G) - 2m\Delta\delta - \frac{(2m(\Delta+\delta) - n\Delta\delta - M_1(G))^2}{n(\Delta+\delta) - 2m - \Delta\delta ID(G)}.$$

Equality holds if and only if if either $\alpha = 1$, or $\alpha = 2$, or $\Delta = d_1 > d_2 = \cdots = d_{n-1} > d_n = \delta$, or $\Delta = d-1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = \delta$, for some t and r such that $1 \leq t < r \leq n-1$.

In the next theorem we determine bounds for the linear combination ${}^0R_\alpha(G) - 2a\,{}^0R_{\alpha-1}(G) + a^2\,{}^0R_{\alpha-2}(G)$, where a is an arbitrary real number.

Theorem 3.9. *Let G be a connected graph of order $n \geq 5$ and size m, and a an arbitrary real number. If $d_2 = \cdots = d_{n-1} = a \neq 0$, then for any real α holds*

$${}^0R_\alpha(G) = \Delta^\alpha + \delta^\alpha + (n-2)a^\alpha.$$

If $d_i \neq a$ for at least one i, $2 \leq i \leq n-1$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds

$$\begin{aligned} &{}^0R_\alpha(G) - 2a\,{}^0R_{\alpha-1}(G) + a^2\,{}^0R_{\alpha-2}(G) \geq \\ &\geq (\Delta-a)^2\Delta^{\alpha-2} + (\delta-a)^2\delta^{\alpha-2} + \frac{\left(a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta}\right)^\alpha}{\left(n - 2aID(G) + a^2\,{}^mM_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2}\right)^{\alpha-1}}. \end{aligned} \tag{10}$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_{n-1} \neq a$, or $a = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1}$, or $d_2 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1} = a$, for some t, $2 \leq t \leq n-2$.

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

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

For $r = \alpha$, $\alpha \leq 0$ or $\alpha \geq 1$, $p_i = \frac{(d_i-a)^2}{d_i^2}$, $a_i = d_i$, $i = 2, \dots, n-1$, the above inequality becomes

$$\left(\sum_{i=2}^{n-1} \frac{(d_i-a)^2}{d_i^2}\right)^{\alpha-1} \sum_{i=2}^{n-1} (d_i-a)^2 d_i^{\alpha-2} \geq \left(\sum_{i=2}^{n-1} \frac{(d_i-a)^2}{d_i}\right)^\alpha. \tag{11}$$

The following identities are valid

$$\begin{aligned} \sum_{i=2}^{n-1} \frac{(d_i-a)^2}{d_i^2} &= \sum_{i=1}^{n} \frac{(d_i-a)^2}{d_i^2} - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2} = \\ &= \sum_{i=1}^{n} \left(\frac{a^2}{d_i^2} - \frac{2a}{d_i} + 1\right) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2} = \\ &= n - 2aID(G) + a^2\,{}^mM_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2}, \end{aligned}$$

$$\begin{aligned} &\sum_{i=2}^{n-1} (d_i-a)^2 d_i^{\alpha-2} = \sum_{i=1}^{n} (d_i-a)^2 d_i^{\alpha-2} - (\Delta-a)^2\Delta^{\alpha-2} - (\delta-a)^2\delta^{\alpha-2} = \\ &= \sum_{i=1}^{n} (d_i^\alpha - 2ad_i^{\alpha-1} + a^2 d_i^{\alpha-2}) - (\Delta-a)^2\Delta^{\alpha-2} - (\delta-a)^2\delta^{\alpha-2} = \\ &= {}^0R_\alpha(G) - 2a\,{}^0R_{\alpha-1}(G) + a^2\,{}^0R_{\alpha-2}(G) - (\Delta-a)^2\Delta^{\alpha-2} - (\delta-a)^2\delta^{\alpha-2}, \end{aligned}$$

$$\begin{aligned}\sum_{i=2}^{n-1} \frac{(d_i-a)^2}{d_i} &= \sum_{i=1}^{n} \frac{(d_i-a)^2}{d_i} - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta} = \\ &= \sum_{i=1}^{n} \left(\frac{a^2}{d_i} - 2a + d_i\right) - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta} = \\ &= a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta}\,.\end{aligned}$$

From the above identities and inequality (11) we obtain

$$\begin{aligned}&\left(n - 2aID(G) + a^2\, {}^{m}M_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2}\right)^{\alpha-1} \Big({}^{0}R_\alpha(G) - \\ &\quad -2a\, {}^{0}R_{\alpha-1}(G) + a^2\, {}^{0}R_{\alpha-2}(G) - (\Delta-a)^2\Delta^{\alpha-2} - (\delta-a)^2\delta^{\alpha-2}\Big) \geq \\ &\qquad \geq \left(a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta}\right)^{\alpha}\,.\end{aligned} \tag{12}$$

If $d_i \neq a$ for at least one i, $2 \leq i \leq n-1$, then

$$n - 2aID(G) + a^2\, {}^{m}M_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2} > 0$$

and

$$a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta} > 0\,.$$

Now from (12) the inequality (10) follows.

By a similar procedure, the case $0 \leq \alpha \leq 1$ can be proved.

When $d_i \neq a$ for at least one i, $2 \leq i \leq n-1$, equality in (12), and consequently in (10), holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_{n-1} \neq a$, or $a = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1}$, or $d_2 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1} = a$, for some t, $2 \leq t \leq n-2$. □

The proof of the next theorem is analogous to that of Theorem 3.9, hence omitted.

Theorem 3.10. *Let G be a connected graph with $n \geq 4$ vertices and m edges, and a be an arbitrary real number. When $d_2 = \cdots = d_n = a \neq 0$, then for any real α, holds*

$${}^{0}R_\alpha(G) = \Delta^\alpha + (n-1)a^\alpha\,.$$

If $d_i \neq a$ for some i, $2 \leq i \leq n$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds

$$\begin{aligned}&{}^{0}R_\alpha(G) - 2a\, {}^{0}R_{\alpha-1}(G) + a^2\, {}^{0}R_{\alpha-2}(G) \geq \\ &\geq (\Delta-a)^2\Delta^{\alpha-2} + \frac{\left(a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta}\right)^{\alpha}}{\left(n - 2aID(G) + a^2\, {}^{m}M_1(G) - \frac{(\Delta-a)^2}{\Delta^2}\right)^{\alpha-1}}\,.\end{aligned}$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_n = \delta \neq a$, or $a = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$, or $d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta = a$, for some t, $2 \leq t \leq n-1$.

Theorem 3.11. *Let G be a connected graph of order $n \geq 3$, size m, and a be an arbitrary real number. If $d_1 = \cdots = d_n = a$, then, for any real α holds*

$$^0R_\alpha(G) = na^\alpha .$$

If $d_i \neq a$, for at least one i, $1 \leq i \leq n$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, holds

$$^0R_\alpha(G) - 2a\,^0R_{\alpha-1}(G) + a^2\,^0R_{\alpha-2}(G) \geq \frac{(a^2ID(G) - 2na + 2m)^\alpha}{(n - 2aID(G) + a^2\,^mM_1(G))^{\alpha-1}} .$$

When $0 \leq \alpha \leq 1$ the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_1 = \cdots = d_n \neq a$, or $a = \Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$, or $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta = a$, for some t, $1 \leq t \leq n-1$.

4. Corollaries and applications

4.1. Simple graphs

According to the Theorems 3.9, 3.10 and 3.11, for a particular values of parameters a and α, we obtain a number of new/old bounds for various topological indices.

Corollary 4.1. *Let G be a connected graph with $n \geq 4$ vertices and m edges, and let a be an arbitrary real number. If $d_i \neq a$, for at least one i, $2 \leq i \leq n-1$, then*

$$M_1(G) \geq (\Delta - a)^2 + (\delta - a)^2 + 4ma - na^2 + + \frac{\left(a^2ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta}\right)^2}{n - 2aID(G) + a^2\,^mM_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2}} . \tag{13}$$

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

Remark 4.2. *The inequality* (13) *was proven in* [29].

Corollary 4.3. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_i \neq a$, for at least one i, $2 \leq i \leq n$, then we have*

$$M_1(G) \geq (\Delta - a)^2 + 4ma - na^2 + \frac{\left(a^2ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta}\right)^2}{n - 2aID(G) + a^2\,^mM_1(G) - \frac{(\Delta-a)^2}{\Delta^2}} . \tag{14}$$

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

Corollary 4.4. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_i \neq a$, for at least one i, $1 \leq i \leq n$, then we have*

$$M_1(G) \geq 4ma - na^2 + \frac{(a^2ID(G) - 2na + 2m)^2}{n - 2aID(G) + a^2\,^mM_1(G)} . \tag{15}$$

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

Corollary 4.5. *Let G be a connected graph with $n \geq 3$ vertices and m edges, and let a be an arbitrary real number. If $d_i \neq a$, for at least one i, $2 \leq i \leq n-1$, then we have*

$$F(G) \geq (\Delta - a)^2\Delta + (\delta - a)^2\delta + 2aM_1(G) - 2ma^2 + \frac{\left(a^2ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta} - \frac{(\delta-a)^2}{\delta}\right)^3}{\left(n - 2aID(G) + a^2\,^mM_1(G) - \frac{(\Delta-a)^2}{\Delta^2} - \frac{(\delta-a)^2}{\delta^2}\right)^2} .$$

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

If $d_i \neq a$ for at least one i, $2 \leq i \leq n$, then

$$F(G) \geq (\Delta - a)^2\Delta + 2aM_1(G) - 2ma^2 + \frac{\left(a^2 ID(G) - 2na + 2m - \frac{(\Delta-a)^2}{\Delta}\right)^3}{\left(n - 2aID(G) + a^2\, {}^{m}M_1(G) - \frac{(\Delta-a)^2}{\Delta^2}\right)^2}.$$

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

If $d_i \neq a$ for at least one i, $1 \leq i \leq n$, then we have

$$F(G) \geq 2aM_1(G) - 2ma^2 + \frac{\left(a^2 ID(G) - 2na + 2m\right)^3}{\left(n - 2aID(G) + a^2\, {}^{m}M_1(G)\right)^2}.$$

Equality holds if and only if $d_1 = \cdots = d_n \neq a$.

For $a = 0$ we have the following corollary of Theorems 3.9–3.11.

Corollary 4.6. *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, we have*

$$
\begin{aligned}
{}^{0}R_\alpha(G) &\geq \Delta^\alpha + \delta^\alpha + \frac{(2m - \Delta - \delta)^\alpha}{(n-2)^{\alpha-1}}, && (16)\\
{}^{0}R_\alpha(G) &\geq \Delta^\alpha + \frac{(2m - \Delta)^\alpha}{(n-1)^{\alpha-1}}, && (17)\\
{}^{0}R_\alpha(G) &\geq \frac{(2m)^\alpha}{n^{\alpha-1}}. && (18)
\end{aligned}
$$

When $0 \leq \alpha \leq 1$, the opposite inequalities are valid. Equality in (16) *holds if and only if $d_2 = \cdots = d_{n-1}$, in* (17) *if and only if $d_2 = \cdots = d_n$, and in* (18) *if and only if $d_1 = \cdots = d_n$.*

Remark 4.7. *For $\alpha \geq 1$ the inequality* (18) *was proven in* [30].

Corollary 4.8. *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$
\begin{aligned}
{}^{m}M_1(G) &\geq \frac{\Delta^2 + \delta^2}{\Delta^2\delta^2} + \frac{(n-2)^3}{(2m - \Delta - \delta)^2}, && (19)\\
{}^{m}M_1(G) &\geq \frac{1}{\Delta^2} + \frac{(n-1)^3}{(2m - \Delta)^2}, \\
{}^{m}M_1(G) &\geq \frac{n^3}{(2m)^2}, && (20)\\
ID(G) &\geq \frac{\Delta + \delta}{\Delta\delta} + \frac{(n-2)^2}{2m - \Delta - \delta}, && (21)\\
ID(G) &\geq \frac{1}{\Delta} + \frac{(n-1)^2}{2m - \Delta}, \\
ID(G) &\geq \frac{n^2}{2m}, && (22)\\
M_1(G) &\geq \Delta^2 + \delta^2 + \frac{(2m - \Delta - \delta)^2}{n-2}, && (23)\\
M_1(G) &\geq \Delta^2 + \frac{(2m - \Delta)^2}{n-1}, && (24)\\
M_1(G) &\geq \frac{4m^2}{n}, && (25)
\end{aligned}
$$

$$F(G) \geq \Delta^3 + \delta^3 + \frac{(2m - \Delta - \delta)^3}{(n-2)^2}, \tag{26}$$

$$F(G) \geq \Delta^3 + \frac{(2m - \Delta)^3}{(n-1)^2}, \tag{27}$$

$$F(G) \geq \frac{8m^3}{n^2}. \tag{28}$$

Remark 4.9. *The inequality* (19) *was proven in* [1] (*see also* [31]) *as a particular case of one more general result. The inequality* (20) *was proven in* [36], *the inequality* (21) *in* [32] *and as a special case of one more general result in* [26]. *The inequality* (22) *was proven in* [35], (23) *in* [33], (24) *in* [41], (25) *in* [37] (*see also* [30, 38, 40]), *and* (28) *in* [9] (*see also* [39]).

For $a = \delta$ and $a = \Delta$, we obtain the following corollary of Theorem 3.9.

Corollary 4.10. *Let G be a connected graph with $n \geq 4$ vertices and m edges. If $d_i \neq \Delta$ for at least one i, $2 \leq i \leq n-1$, then for any real α, $\alpha \leq 0$ or $\alpha \geq 1$, we have that*

$$^0R_\alpha(G) - 2\Delta\, ^0R_{\alpha-1}(G) + \Delta^2\, ^0R_{\alpha-2}(G) \geq (\Delta - \delta)^2\delta^{\alpha-2} + \frac{\left(\Delta^2 ID(G) - 2n\Delta + 2m - \frac{(\Delta-\delta)^2}{\delta}\right)^\alpha}{\left(n - 2\Delta ID(G) + \Delta^2\, ^mM_1(G) - \frac{(\Delta-\delta)^2}{\delta^2}\right)^{\alpha-1}} \tag{29}$$

and

$$^0R_\alpha(G) - 2\delta\, ^0R_{\alpha-1}(G) + \delta^2\, ^0R_{\alpha-2}(G) \geq (\Delta - \delta)^2\Delta^{\alpha-2} + \frac{\left(\delta^2 ID(G) - 2n\delta + 2m - \frac{(\Delta-\delta)^2}{\Delta}\right)^\alpha}{\left(n - 2\delta ID(G) + \delta^2\, ^mM_1(G) - \frac{(\Delta-\delta)^2}{\Delta^2}\right)^{\alpha-1}}. \tag{30}$$

When $0 \leq \alpha \leq 1$ opposite inequalities are valid.

Equality in (29) *holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_{n-1} \neq \Delta$, or $\Delta = d_1 = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_{n-1}$, for some t, $1 \leq t \leq n-2$.*

Equality in (30) *holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_{n-1} \neq \delta$, or $d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n = \delta$, for some t, $2 \leq t \leq n-1$.*

Remark 4.11. *A graph G is regular if and only if $d_1 = d_2 = \cdots = d_n > 0$. A connected graph is called irregular if it contains at least two vertices with different degrees. In many applications and problems it is of importance to know how much a given graph deviates from being regular, i.e. how great its irregularity is. For this purpose, various quantitative measures of graph irregularity have been proposed. Denote with $irr(G)$ a topological index such that $irr(G) > 0$ if G is irregular, and $irr(G) = 0$ if and only if G is a regular graph* (*see e.g.* [42–44]).

According to the inequalities (20), (22), (25) *and* (28), *we can define the following irregularity measures:*

$$irr_1(G) = {}^mM_1(G) - \frac{n^3}{4m^2},$$

$$irr_2(G) = ID(G) - \frac{n^2}{2m},$$

$$irr_3(G) = M_1(G) - \frac{4m^2}{n},$$

$$irr_4(G) = F(G) - \frac{8m^3}{n^2}.$$

Some of the above irregularity measures, such as $irr_3(G)$ (Edward's irregularity measure), are well known see [37, 43]. In the following couple of theorems we establish relationship between various irregularity measures.

Theorem 4.12. *Let G be an irregular graph with $n \geq 4$ vertices and m edges. Then we have*

$$irr_4(G) \geq \frac{4m}{n} irr_3(G) + \frac{\frac{4m^4}{n^4} irr_2(G)^3}{\left(\frac{m}{n} irr_1(G) - irr_2(G)\right)^2} . \tag{31}$$

Proof. For $r = 3$, $p_i = \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i^2}$, $a_i = d_i$, $i = 1, 2, \ldots, n$, the inequality (3) becomes

$$\left(\sum_{i=1}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i^2} \right)^2 \sum_{i=1}^{n} \left(d_i - \frac{2m}{n}\right)^2 d_i \geq \left(\sum_{i=1}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i} \right)^3 . \tag{32}$$

If G is regular, then in (32) equality is attained. Therefore, without affecting the generality, we assume that G is irregular.

Since

$$\begin{aligned}
\sum_{i=1}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i^2} &= \sum_{i=1}^{n} \left(1 - \frac{4m}{n}\frac{1}{d_i} + \frac{4m^2}{n^2}\frac{1}{d_i^2} \right) = \\
&= n - \frac{4m}{n} ID(G) + \frac{4m^2}{n^2} {}^{m}M_1(G) = \\
&= \frac{4m^2}{n^2} {}^{m}M_1(G) - n + 2n - \frac{4m}{n} ID(G) = \\
&= \frac{4m^2}{n^2} \left({}^{m}M_1(G) - \frac{n^3}{4m^2} \right) - \frac{4m}{n} \left(ID(G) - \frac{n^2}{2m} \right) = \\
&= \frac{4m}{n} \left(\frac{m}{n} irr_1(G) - irr_2(G) \right) ,
\end{aligned}$$

$$\begin{aligned}
\sum_{i=1}^{n} \left(d_i - \frac{2m}{n}\right)^2 d_i &= \sum_{i=1}^{n} \left(d_i^3 - \frac{4m}{n} d_i^2 + \frac{4m^2}{n^2} d_i \right) = \\
&= F(G) - \frac{4m}{n} M_1(G) + \frac{8m^3}{n^2} = \\
&= F(G) - \frac{8m^3}{n^2} - \frac{4m}{n} M_1(G) + \frac{16m^3}{n^2} = \\
&= irr_4(G) - \frac{4m}{n} irr_3(G) ,
\end{aligned}$$

$$\begin{aligned}
\sum_{i=1}^{n} \frac{\left(d_i - \frac{2m}{n}\right)^2}{d_i} &= \sum_{i=1}^{n} \left(d_i - \frac{4m}{n} + \frac{4m^2}{n^2}\frac{1}{d_i} \right) = \\
&= 2m - 4m + \frac{4m^2}{n^2} ID(G) = \frac{4m^2}{n^2} \left(ID(G) - \frac{n^2}{2m} \right) = \\
&= \frac{4m^2}{n^2} irr_2(G) .
\end{aligned}$$

From the above identities and inequality (32) we obtain the following inequality

$$\left(\frac{4m}{n} \left(\frac{m}{n} irr_1(G) - irr_2(G) \right) \right)^2 \left(irr_4(G) - \frac{4m}{n} irr_3(G) \right) \geq \left(\frac{4m^2}{n^2} irr_2(G) \right)^3 ,$$

from which we obtain (31). $\square$

The proof of the next theorem is analogous to that of Theorem 4.12, hence omitted.

Theorem 4.13. *Let G be a connected irregular graph with $n \geq 4$ vertices and m edges. Then*

$$irr_3(G) \geq \frac{\frac{4m^3}{n^3} irr_2(G)^2}{\frac{m}{n} irr_1(G) - irr_2(G)} .$$

4.2. Trees

In this section we consider graphs with tree structure, $G \cong T$, and point out to the corollaries of the main results.

Corollary 4.14. *Let T be a tree with $n \geq 5$ vertices. If $d_i \in \{\Delta, 1\}$, for all i, $1 \leq i \leq n$, then for any real α we have*

$$ {}^0R_\alpha(T) = p\Delta^\alpha + q , \qquad p + q = n .$$

If $d_i \notin \{\Delta, 1\}$ for at least one i, $2 \leq i \leq n-2$, then for any rala α, $\alpha \leq 0$ or $\alpha \geq 1$, we have

$$ {}^0R_\alpha(T) \leq (\Delta+1)\, {}^0R_{\alpha-1}(T) - \Delta\, {}^0R_{\alpha-2}(T) - \frac{(n\Delta - n + 2 - \Delta ID(T))^\alpha}{((\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T))^{\alpha-1}} . \tag{33}$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or T is a tree such that $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = 1$, for some t and r, $1 \leq t < r \leq n-2$.

Corollary 4.15. *Let Tbe a tree with $n \geq 5$ vertices. If $d_i \notin \{\Delta, 1\}$, for at least one i, $2 \leq i \leq n-2$, then we have*

$$M_1(T) \leq (n-2)\Delta + 2(n-1) - \frac{(n\Delta - n + 2 - \Delta ID(T))^2}{(\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T)} , \tag{34}$$

and

$$F(T) \leq (\Delta+1)M_1(T) - 2(n-1)\Delta - \frac{(n\Delta - n + 2 - \Delta ID(T))^3}{((\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T))^2} .$$

Equalities hold if and only if T is a tree such that $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_r > d_{r+1} = \cdots = d_n = 1$, for some t and r, $1 \leq t < r \leq n-2$.

Corollary 4.16. *Let Tbe a tree with $n \geq 5$ vertices. If $d_i \notin \{\Delta, 1\}$, for at least one i, $2 \leq i \leq n-2$, then we have*

$$F(T) \leq 2(n-1) + (n-2)\Delta(\Delta+1) - \frac{(n\Delta - n + 2 - \Delta ID(T))^3}{((\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T))^2} . \tag{35}$$

Remark 4.17. *The inequalities* (34) *and* (35) *are stronger than*

$$M_1(T) \leq 2(n-1) + (n-2)\Delta ,$$

and

$$F(T) \leq 2(n-1) + (n-2)\Delta(\Delta+1) ,$$

which were proven in [23].

Corollary 4.18. *Let Tbe a tree with $n \geq 5$ vertices. If $d_i \notin \{\Delta, 1\}$, for at least one i, $2 \leq i \leq n-2$, then we have*

$$M_1(T) \leq n(n-1) - \frac{(n\Delta - n + 2 - \Delta ID(T))^2}{(\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T)} , \tag{36}$$

and

$$F(T) \leq (n-1)(n^2 - 2n + 2) - \frac{(n\Delta - n + 2 - \Delta ID(T))^3}{((\Delta+1)ID(T) - n - \Delta\, {}^mM_1(T))^2} . \tag{37}$$

Remark 4.19. *The inequalities* (36) *and* (37) *are stronger than*

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

and

$$F(T) \le (n-1)(n^2-2n+2)\,,$$

which were proven in [5] *and* [28]*, respectively.*

Corollary 4.20. *Let T be a tree with $n \ge 2$ vertices. Then, for any real α, $\alpha \le 0$ or $\alpha \ge 1$, we have that*

$$^0R_\alpha(T) \ge 2 + (n-2)2^\alpha\,. \tag{38}$$

When $0 \le \alpha \le 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $T \cong P_n$.

Corollary 4.21. *Let T be a tree with $n \ge 2$ vertices. Then*

$$^mM_1(T) \ge \frac{n+6}{4}\,, \tag{39}$$

$$ID(T) \ge \frac{n+2}{2}\,, \tag{40}$$

$$M_1(T) \ge 4n-6\,, \tag{41}$$

$$F(T) \ge 8n-14\,. \tag{42}$$

Equalities hold if and only if $T \cong P_n$.

Remark 4.22. *The inequality* (39) *was proven in* [45] (*see also* [36, 46])*, the inequality* (40) *in* [28], (41) *in* [28]*, and* (42) *in* [5].

Corollary 4.23. *Let T be a tree with $n \ge 5$ vertices. If $d_i \ne 1$ for at least one i, $1 \le i \le n-2$, then for any real α, $\alpha \le 0$ or $\alpha \ge 1$, we have that*

$$^0R_\alpha(T) - 2\,{}^0R_{\alpha-1}(T) + {}^0R_{\alpha-2}(T) \ge \frac{(ID(T)-2)^\alpha}{(n-2ID(T)+{}^mM_1(T))^{\alpha-1}}\,.$$

When $0 \le \alpha \le 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $\Delta = d_1 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $1 \le t \le n-2$.

Corollary 4.24. *Let T be a tree with $n \ge 5$ vertices. If $d_i \ne a$ for at least one i, $1 \le i \le n-2$, then*

$$M_1(T) \ge 3n-4+\frac{(ID(T)-2)^2}{n-2ID(T)+{}^mM_1(T)}\,,$$

and

$$F(T) \ge 2M_1(T)-2(n-1)+\frac{(ID(T)-2)^3}{(n-2ID(T)+{}^mM_1(T))^2}\,.$$

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

Since any tree has at least two vertices of order 1, $d_n = d_{n-1} = 1$, the following result can be easily proved.

Theorem 4.25. *Let T be a tree with $n \ge 5$ vertices. If $d_i \ne 1$ for at least one i, $2 \le i \le n-2$, then for any real α, $\alpha \le 0$ or $\alpha \ge 1$, holds*

$$^0R_\alpha(T) - 2\,{}^0R_{\alpha-1}(T) + 2\,{}^0R_{\alpha-2}(T) \ge (\Delta-1)^2\Delta^{\alpha-2} + \frac{\left(ID(T)-2-\frac{(\Delta-1)^2}{\Delta}\right)^\alpha}{\left(n-2ID(T)+{}^mM_1(T)-\frac{(\Delta-1)^2}{\Delta^2}\right)^{\alpha-1}}\,.$$

When $0 \le \alpha \le 1$, the opposite inequality is valid. Equality holds if and only if either $\alpha = 0$, or $\alpha = 1$, or $d_2 = \cdots = d_{n-2} \ne 1$, or or $d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n = 1$, for some t, $2 \le t \le n-2$.

Corollary 4.26. *Let T be a tree with $n \geq 5$ vertices. If $d_i \neq 1$ for at least one i, $2 \leq i \leq n-2$, then we have*

$$M_1(T) \geq 3n - 4 + (\Delta - 1)^2 + \frac{\left(ID(T) - 2 - \frac{(\Delta-1)^2}{\Delta}\right)^2}{n - 2ID(T) + {}^{m}M_1(T) - \frac{(\Delta-1)^2}{\Delta^2}} . \tag{43}$$

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

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