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SOME REMARKS ON THE SUM OF POWERS OF THE DEGREES OF GRAPHS

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ABSTRACT. Let $G = (V, E)$ be a simple graph with $n \geq 3$ vertices, m edges and vertex degree sequence $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. Denote by $S = \{1, 2, \dots, n\}$ an index set and by $J = \{I = (r_1, r_2, \dots, r_k) \,|\, 1 \leq r_1 < r_2 < \cdots < r_k \leq n\}$ a set of all subsets of S of cardinality k, $1 \leq k \leq n-1$. In addition, denote by $d_I = d_{r_1} + d_{r_2} + \cdots + d_{r_k}$, $1 \leq k \leq n-1$, $1 \leq r_1 < r_2 < \cdots < r_k \leq n-1$, the sum of k arbitrary vertex degrees, where $\Delta_I = d_1 + d_2 + \cdots + d_k$ and $\delta_I = d_{n-k+1} + d_{n-k+2} + \cdots + d_n$. We consider the following graph invariant $S_{\alpha,k}(G) = \sum_{I \in J} d_I^\alpha$, where α is an arbitrary real number, and establish its bounds. A number of known bounds for various topological indices are obtained as special cases.

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, be a simple graph of order $n \geq 3$ and size m, without isolated vertices and vertex degree sequence $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(v_i)$.

Denote by $S = \{1, 2, \dots, n\}$ an index set and by $J = \{I = (r_1, r_2, \dots, r_k) \,|\, 1 \leq r_1 < r_2 < \cdots < r_k \leq n\}$ a set of all subsets of S of cardinality k, $1 \leq k \leq n-1$. In addition, denote by $d_I = d_{r_1} + d_{r_2} + \cdots + d_{r_k}$, $1 \leq k \leq n-1$, $1 \leq r_1 < r_2 < \cdots < r_k \leq n-1$, the sum of k arbitrary vertex degrees, where $\Delta_I = d_1 + d_2 + \cdots + d_k$ and $\delta_I = d_{n-k+1} + d_{n-k+2} + \cdots + d_n$. It is easy to verify that $\delta_I \leq d_I \leq \Delta_I$ for each I, $I \in J$.

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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.

Define the invariant $S_{\alpha,k}(G)$ in the following way

$$S_{\alpha,k}(G) = \sum_{I\in J} d_I^{\alpha},$$

where α is an arbitrary real number. It can be easily seen that for $k=1$ the invariant $S_{\alpha,k}(G)$ reduces to the zeroth-order general Randić index [10]:

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

This index is also met under names general first Zagreb index [15] and variable first Zagreb index [18]. Some special cases of this index are: $M_1(G) = {}^0R_2(G)$ (the first Zagreb index [8]), $F(G) = {}^0R_3(G)$ (forgotten topological index [7]), $ID(G) = {}^0R_{-1}(G)$ (the inverse degree index [5]).

In this paper some new bounds for $S_{\alpha,k}(G)$ are obtained. Besides, a number of known bounds for various graph invariants are obtained as special cases.

2. Preliminaries

In this section we recall a couple of discrete analytical inequalities for real number sequences that will be used in the proofs of theorems.

Let $p=(p_i)$, and $a=(a_i)$, $i=1,2,\dots,n$, be a nonnegative and positive real number sequences, respectively. Then, for any real r, such that $r\le 0$ or $r\ge 1$, holds [14]

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \ge \left(\sum_{i=1}^{n} p_i a_i\right)^{r}. \tag{2.1}$$

If $0\le r\le 1$, then the sense of (2.1) reverses. 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 $a_{t+1}=a_{t+2}=\cdots=a_n$ for some t, $1\le t\le n-1$.

Let $x=(x_i)$ and $a=(a_i)$, $i=1,2,\dots,n$, be two positive real number sequences. Then for all r, $r\ge 0$, holds [23]

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum_{i=1}^{n} x_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^{r}}, \tag{2.2}$$

with equality if and only if $r=0$ or $\frac{x_1}{a_1}=\frac{x_2}{a_2}=\cdots=\frac{x_n}{a_n}$.

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3. Main results

In the following theorem we establish a relation between $S_{\alpha,k}(G)$ and $S_{\alpha-1,k}(G)$.

Theorem 3.1. *Let G be a simple connected non-regular gragh with $n \geq 3$ vertices and m edges. Then for any k, $1 \leq k \leq n-1$, and for any real number α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

$$\begin{aligned} S_{\alpha,k}(G) &\geq \delta_I S_{\alpha-1,k}(G) \\ &+ \frac{k^{\alpha-2}\binom{n-1}{k-1}((n-k)M_1(G)+2m(2m(k-1)-(n-1)\delta_I))^{\alpha-1}}{(n-1)^{\alpha-1}(2mk-n\delta_I)^{\alpha-2}} \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} S_{\alpha,k}(G) &\leq \Delta_I S_{\alpha-1,k}(G) \\ &- \frac{k^{\alpha-2}\binom{n-1}{k-1}(2m((n-1)\Delta_I-2m(k-1))-(n-k)M_1(G))^{\alpha-1}}{(n-1)^{\alpha-1}(n\Delta_I-2mk)^{\alpha-2}}. \end{aligned} \tag{3.2}$$

When $1 \leq \alpha \leq 2$, the opposite inequalities are valid. Equalities hold if and only if either $\alpha = 1$, or $\alpha = 2$, or $d_I \in \{\delta_I, \Delta_I\}$, $\Delta_I \neq \delta_I$, for every k-tuple I, $I \in J$.

Proof. First, we have that

$$\sum_{I\in J} 1 = \binom{n}{k}, \tag{3.3}$$

$$\sum_{I\in J} d_I = \binom{n-1}{k-1}\sum_{i=1}^{n} d_i = 2m\binom{n-1}{k-1}, \tag{3.4}$$

$$\begin{aligned} \sum_{I\in J} d_I^2 &= \binom{n-2}{k-1}\sum_{i=1}^{n} d_i^2 + \binom{n-2}{k-2}\left(\sum_{i=1}^{n} d_i\right)^2 = \\ &= \frac{\binom{n-1}{k-1}}{n-1}\left((n-k)M_1(G)+2m(k-1)\right), \end{aligned} \tag{3.5}$$

$$S_{\alpha,k}(G) - \delta_I S_{\alpha-1,k}(G) = \sum_{I\in J}(d_I-\delta_I)d_I^{\alpha-1}. \tag{3.6}$$

On the other hand, for $n := \binom{n}{k}$, $p_i := d_I - \delta_I$, $a_i := d_I$, $r = \alpha - 1$, $\alpha \leq 1$ or $\alpha \geq 2$, where summation is performed over all k-tuples I, $I \in J$, the inequality (2.1) becomes

$$\left(\sum_{I\in J}(d_I-\delta_I)\right)^{\alpha-2}\sum_{I\in J}(d_I-\delta_I)d_I^{\alpha-1} \geq \left(\sum_{I\in J}(d_I-\delta_I)d_I\right)^{\alpha-1}.$$

If G is regular, then in the above inequality holds equality. Without affecting generality, let us assume that G is not regular. Then $\sum_{I\in J}(d_I-\delta_I) \neq 0$, therefore we have

$$\sum_{I\in J}(d_I-\delta_I)d_I^{\alpha-1} \geq \frac{\left(\sum_{I\in J}(d_I-\delta_I)d_I\right)^{\alpha-1}}{\left(\sum_{I\in J}(d_I-\delta_I)\right)^{\alpha-2}}. \tag{3.7}$$

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By combining (3.3), (3.4), (3.5), (3.6) and (3.7) we arrive at (3.1).

Similarly, the opposite inequality in (3.1) is obtained when $1 \leq \alpha \leq 2$.

Equality in (3.7), and consequently in (3.1), holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $d_I \in \{\delta_I, \Delta_I\}$, $\Delta_I \neq \delta_I$, for every I, $I \in J$.

Now, for $n := \binom{n}{k}$, $p_i := \Delta_I - d_I$, $a_i := d_I$, $r = \alpha - 1$, $\alpha \leq 1$ or $\alpha \geq 2$, where summation is performed over all k-tuples I, $I \in J$, the inequality (2.1) transform into

$$\left(\sum_{I\in J}(\Delta_I - d_I)\right)^{\alpha-2} \sum_{I\in J}(\Delta_I - d_I)d_I^{\alpha-1} \geq \left(\sum_{I\in J}(\Delta_I - d_I)d_I\right)^{\alpha-1}.$$

Suppose that G is not regular. Then $\sum_{I\in J}(\Delta_I - d_I) \neq 0$, and from the above it follows

$$\sum_{I\in J}(\Delta_I - d_I)d_I^{\alpha-1} \geq \frac{\left(\sum_{I\in J}(\Delta_I - d_I)d_I\right)^{\alpha-1}}{\left(\sum_{I\in J}(\Delta_I - d_I)\right)^{\alpha-2}}. \tag{3.8}$$

Also, the following identity holds

$$\Delta_I S_{\alpha-1,k}(G) - S_{\alpha,k}(G) = \sum_{I\in J}(\Delta_I - d_I)d_I^{\alpha-1}. \tag{3.9}$$

From (3.3), (3.4), (3.5), (3.8) and (3.9) we get (3.2).

By a similar procedure we prove that opposite inequality holds in (3.2) when $1 \leq \alpha \leq 2$.

Equality in (3.8), and consequently in (3.2), holds if and only if either $\alpha = 1$, or $\alpha = 2$, or $d_I \in \{\delta_I, \Delta_I\}$, $\Delta_I \neq \delta_I$, for every I, $I \in J$. □

In [4] it was proven that

$$M_1(G) \geq \frac{4m^2}{n},$$

with equality holding if and only if G is regular. Based on this inequality the following corollaries of Theorem 3.1 are obtained.

Corollary 3.2. *Let G be a simple graph with $n \geq 3$ vertices and m edges. Then, for any real α, $\alpha \geq 2$, holds*

$$S_{\alpha,k}(G) \geq \delta_I S_{\alpha-1,k}(G) + \frac{k^{\alpha-2}(2m)^{\alpha-1}(2mk - n\delta_I)\binom{n-1}{k-1}}{n^{\alpha-1}}.$$

Equality holds if and only if G is regular.

For $k = 1$ we have the following corollaries of Theorem 3.1.

Corollary 3.3. *Let G be a simple non-regular graph of order $n \geq 3$ and size m without isolated vertices. Then, for any real α, $\alpha \leq 1$ or $\alpha \geq 2$, holds*

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

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and

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

When $1 \le \alpha \le 2$, the opposite inequalities hold. Equalities hold if and only if $\alpha = 1$, or $\alpha = 2$, or $d_i \in \{\delta, \Delta\}$, $\Delta \ne \delta$, for every $i = 1, 2, \ldots, n$.

Corollary 3.4. *Let G be a simple non-regular graph with $n \ge 3$ vertices, m edges. Then*

$$F(G) \ge \delta M_1(G) + \frac{(M_1(G) - 2m\delta)^2}{2m - n\delta}$$

and

$$F(G) \le \Delta M_1(G) - \frac{(2m\Delta - M_1(G))^2}{n\Delta - 2m}.$$

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

By the similar arguments as in case of Theorem 3.1, the following results can be proven.

Theorem 3.5. *Let G be a simple graph of order $n \ge 2$ and size m without isolated vertices. Then for any real α, $\alpha \le 0$ or $\alpha \ge 1$, holds*

$$S_{\alpha,k}(G) \ge \frac{k^{\alpha-1}(2m)^\alpha \binom{n-1}{k-1}}{n^{\alpha-1}}.$$

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

Theorem 3.6. *Let G be a simple graph of order $n \ge 2$ and size m without isolated vertices. Then for any real α, $\alpha \le 1$ or $\alpha \ge 2$, holds*

$$S_{\alpha,k}(G) \ge \frac{\binom{n-1}{k-1}\left((n-k)M_1(G) + 2m(k-1)\right)^{\alpha-1}}{(2m)^{\alpha-2}(n-1)^{\alpha-1}}.$$

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

For $k = 1$ we have the following corollaries of Theorem 3.5 and 3.6.

Corollary 3.7. *Let G be a simple graph of order $n \ge 2$ and size m without isolated vertices. Then, for any real α, $\alpha \le 1$ or $\alpha \ge 2$, holds*

$$^0R_\alpha(G) \ge \frac{M_1(G)^{\alpha-1}}{(2m)^{\alpha-2}}. \tag{3.10}$$

If $1 \le \alpha \le 2$, then the opposite inequality holds.

If $\alpha \le 0$ or $\alpha \ge 1$, then

$$^0R_\alpha(G) \ge \frac{(2m)^\alpha}{n^{\alpha-1}}. \tag{3.11}$$

If $0 \le \alpha \le 1$, then the opposite inequality holds. Equality in (3.10) holds if and only if either $\alpha = 1$, or $\alpha = 2$, or G is regular.

Equality in (3.11) holds if and only if $\alpha = 0$, or $\alpha = 1$, or G is regular.

The inequality (3.10) was proven in [19], whereas (3.11) in [13].

Corollary 3.8. *Let G be a simple graph with $n \geq 2$ vertices and m edges. Then*

$$F(G) \geq \frac{M_1(G)^2}{2m}, \tag{3.12}$$

$$F(G) \geq \frac{8m^3}{n^2}. \tag{3.13}$$

If G has no isolated vertices, then

$$ID(G) \geq \frac{n^2}{2m}. \tag{3.14}$$

The inequality (3.12) was proven in [7], the inequality (3.13) in [13], while (3.14) in [2].

In the next theorem we prove an inequality that establishes relation between $S_{\alpha+1,k}(G)$, $S_{\alpha,k}(G)$ and $S_{\alpha-1,k}(G)$, where α is an arbitrary real number.

Theorem 3.9. *Let G be a simple graph of order $n \geq 3$ without isolated vertices. Then for every real α holds*

$$S_{\alpha+1,k}(G) + \Delta_I \delta_I S_{\alpha-1,k}(G) \leq (\Delta_I + \delta_I) S_{\alpha,k}(G). \tag{3.15}$$

Equality holds if and only if $d_I \in \{\delta_I, \Delta_I\}$, for every I, $I \in J$.

Proof. For every k-tuple I, $I \in J$, we have that

$$(d_I - \Delta_I)(d_I - \delta_I) \leq 0,$$

i.e.

$$d_I^2 + \Delta_I \delta_I \leq (\Delta_I + \delta_I) d_I. \tag{3.16}$$

After multiplying (3.16) by $d_I^{\alpha-1}$ and summation over I, $I \in J$, we get

$$\sum_{I \in J} d_I^{\alpha+1} + \Delta_I \delta_I \sum_{I \in J} d_I^{\alpha-1} \leq (\Delta_I + \delta_I) \sum_{I \in J} d_I^{\alpha},$$

from which (3.15) is obtained.

Equality in (3.16), and consequently in (3.15), holds if and only if $d_I \in \{\delta_I, \Delta_I\}$, for every I, $I \in J$. □

Corollary 3.10. *Let G be a simple graph of order $n \geq 3$ without isolated vertices. Then, for any real α holds*

$$S_{\alpha+1,k}(G) \leq \frac{S_{\alpha,k}(G)}{S_{\alpha-1,k}(G)} \left(\sqrt{\frac{\Delta_I}{\delta_I}} + \sqrt{\frac{\delta_I}{\Delta_I}} \right)^2. \tag{3.17}$$

Equality holds if and only if G is a regular graph.

Proof. By applying the arithmetic–geometric mean inequality for real numbers (see e.g. [22]) to (3.15), we get

$$2\sqrt{\Delta_I \delta_I S_{\alpha+1,k}(G) S_{\alpha-1,k}(G)} \le (\Delta_I + \delta_I)\, S_{\alpha,k}(G),$$

from which (3.17) follows. □

For $k = 1$ the following corollaries of Theorem 3.9 and Corollary 3.10 are obtained.

Corollary 3.11. *Let G be a simple graph of oreder $n \ge 2$ without isolated vertices. Then for any real α holds*

$$ {}^0R_{\alpha+1}(G) - (\Delta + \delta)\, {}^0R_\alpha(G) + \Delta\delta\, {}^0R_{\alpha-1}(G) \le 0 \tag{3.18}$$

and

$$ {}^0R_{\alpha+1}(G) \le \frac{{}^0R_\alpha(G)^2}{4\, {}^0R_{\alpha-1}(G)} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 . \tag{3.19}$$

Equality in (3.18) is attained if and only if $d_i \in \{\delta, \Delta\}$, for every $i = 1, 2, \ldots, n$, whereas in (3.19) if and only if G is regular.

The inequalities (3.18) and (3.19) were proven in [20].

Corollary 3.12. *Let G be a simple graph of order $n \ge 2$ and size m without isolated vertices. Then*

$$M_1(G) \le 2m(\Delta + \delta) - n\Delta\delta, \tag{3.20}$$

$$M_1(G) \le \frac{m^2}{n} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 , \tag{3.21}$$

$$F(G) \le (\Delta + \delta) M_1(G) - 2m\Delta\delta, \tag{3.22}$$

$$F(G) \le \frac{M_1(G)^2}{8m} \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 , \tag{3.23}$$

Equalities in (3.20) and (3.22) are attained if and only if $d_i \in \{\delta, \Delta\}$, for every $i = 1, 2, \ldots, n$, whereas in (3.21) and (3.23) if and only if G is regular.

The inequality (3.20) was proven in [3] (see also [9, 16]), (3.21) in [17] (see also [6, 11, 24]), the inequality (3.22) in [12], whereas (3.23) in [20].

In the next theorem we determine relation between $S_{\alpha,k}(G)$ and $S_{2\alpha-1,k}(G)$.

Theorem 3.13. *Let G be a simple graph with $n \ge 3$ vertices, m edges and without isolated vertices. Then, for every real number α holds*

$$S_{\alpha,k}(G) \le \sqrt{2m \binom{n-1}{k-1} S_{2\alpha-1,k}(G)}. \tag{3.24}$$

Equality holds if and only if $\alpha = 1$ or G is regular.

Proof. For every real number α we have that

$$S_{2\alpha-1,k}(G) = \sum_{I\in J} d_I^{2\alpha-1} = \sum_{I\in J} \frac{(d_I^\alpha)^2}{d_I}. \tag{3.25}$$

On the other hand, for $r=1$, $x_i := d_I^\alpha$, $a_i := d_I$, where summation is performed over all k-tuples I, $I\in J$, the inequality (2.2) transform into

$$\sum_{I\in J} \frac{(d_I^\alpha)^2}{d_I} \ge \frac{\left(\sum_{I\in J} d_I^\alpha\right)^2}{\sum_{I\in J} d_I} = \frac{S_{\alpha,k}(G)^2}{2m\binom{n-1}{k-1}}. \tag{3.26}$$

From the above and (3.25) we arrive at (3.24).

Equality in (3.26), and consequently in (3.24), holds if and only if $\alpha = 1$ or d_I is constant for every k-tuple I, $I\in J$, i.e. if and only if $\alpha=1$ or G is regular. □

Corollary 3.14. *Let G be a simple graph oforder $n\ge 2$ and size m without isolated vertices. Then for any real α holds*

$${}^0R_\alpha(G) \le \sqrt{2m\,{}^0R_{2\alpha-1}(G)}.$$

Equality holds if and only if $\alpha = 1$ or G is regular graph.

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