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ON ARITHMETIC–GEOMETRIC AND GEOMETRIC–ARITHMETIC INDICES OF GRAPHS

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Abstract. Let G be a connected graph having vertex set $\{v_1,\dots,v_n\}$ and vertex-degree sequence $(d_1,\dots,d_n)$, where d_i represents the degree of the vertex v_i. If the vertices v_i and v_j are adjacent in G, we write $i\sim j$. The arithmetic–geometric index and the geometric–arithmetic index of G are defined as $AG(G)=\sum_{i\sim j}[(d_i+d_j)/(2\sqrt{d_id_j})]$ and $GA(G)=\sum_{i\sim j}[2\sqrt{d_id_j}/(d_i+d_j)]$, respectively. Since $AG(G)$ and $GA(G)$ are closely related quantities, we derive bounds on their addition as well as on their difference, namely on $irr_{AG}(G)=AG(G)-GA(G)$ and $r(G)=AG(G)+GA(G)$. Some new bounds on $AG(G)$ are also obtained.

1. Introduction

For the graph-theoretical concepts that we use in this paper without having defined them here, we refer the readers to the books [4,5]. Throughout this section, it is assumed that G is a connected graph having vertex set $\{v_1,\dots,v_n\}$ and vertex-degree sequence $(d_1,\dots,d_n)$, where d_i represents the degree of the vertex v_i and $n\geqslant 2$. We write $i\sim j$ whenever the vertices v_i and v_j are adjacent in G.

A graph invariant I is a mapping defined on the set of all graphs with the constraint that the equation $I(G_1)=I(G_2)$ holds whenever the graphs G_1 and G_2 are isomorphic. The characteristic polynomial of a graph, the spectrum of a graph, the order of a graph, and the sum of degrees of all vertices of a graph are some examples of graph invariants. In chemical graph theory, the graph invariants that take only numerical values are usually called topological indices [2].

One of the thoroughly studied vertex–degree–based topological indices is the first Zagreb index M_1 [28] introduced in [15]. This index is defined as

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

The general zeroth–order Randić index ${}^0R_\alpha$, a generalization of M_1, was proposed in [16]. It is defined as

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

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which can be written as

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

where α can be any real number. The topological index $^0R_\alpha$ has appeared in the literature with also some other names; for example, the first general Zagreb index [19] and the variable first Zagreb index [20]. Special cases of $^0R_\alpha$ include:

- The inverse degree (ID) index [9], which is obtained from $^0R_\alpha$ by taking $\alpha = -1$, that is

  $$ID(G) = {}^0R_{-1}(G) = \sum_{i=1}^{n}\frac{1}{d_i} = \sum_{i\sim j}\left(\frac{1}{d_i^2} + \frac{1}{d_j^2}\right).$$

  We remark here that $ID(G)$ is also referred to as the modified total adjacency index [28];

- The forgotten (F) topological index [10], which is obtained from $^0R_\alpha$ by taking $\alpha = 3$, that is

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

For additional detail about $^0R_\alpha$, we refer the readers to [1,21].

The general Randić index, devised in [3], is defined as

$$R_\alpha(G) = \sum_{i\sim j}(d_i d_j)^\alpha,$$

where α is an arbitrary real number. Many mathematical properties of this index can be found in the survey [18]. The special cases of the general Randić index R_α include

- The second Zagreb index M_2 [28, 14], which is obtained from R_α by taking $\alpha = 1$;

- The modified second Zagreb index M_2^* [28], which is obtained from R_α by taking $\alpha = -1$ (see also [7,6]).

Another well-studied topological index to which we are concerned in this paper is the harmonic index, first appeared in [9]. The harmonic index is defined as

$$H(G) = \sum_{i\sim j}\frac{2}{d_i + d_j}.$$

A set of 148 novel topological indices was proposed and investigated in [40] (also, see [38]) for chemical applicability. From the aforementioned set of 148 indices, a subset consisting of 20 indices was found useful for predicting certain chemical properties. Two of them are the inverse indeg index, denoted by ISI, and the symmetric division deg index, denoted by SDD. The former index is defined as

$$ISI(G) = \sum_{i\sim j}\frac{d_i d_j}{d_i + d_j}.$$

The $ISI(G)$ is a significant predictor of total surface area for octane isomers. The symmetric division deg index, a significant predictor of total surface area of polychlorobiphenyls, is defined as

$$SDD(G) = \sum_{i\sim j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

The geometric–arithmetic index, $GA(G)$, was conceived in [39] and it is defined as

$$GA(G) = \sum_{i\sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j}.$$

The arithmetic–geometric index (see, for example, [37]), $AG(G)$, is defined as

$$AG(G) = \sum_{i\sim j} \frac{d_i + d_j}{2\sqrt{d_i d_j}}.$$

The following addition and difference of the indices AG and GA

$$irr_{AG}(G) = AG(G) - GA(G) \quad \text{and} \quad r(G) = AG(G) + GA(G),$$

were considered and studied in [37, 13]. Inspired by the results obtained in [37, 13], in this paper we derive several inequalities involving $irr_{AG}(G)$ and $r(G)$. Besides, we obtain some new bounds for $AG(G)$.

2. Preliminaries

This section provides a couple of known inequalities that are frequently used in the remaining sections of this paper.

LEMMA 2.1. (Jensen's Inequality, see [17, 26, 24]) *Let $p = (p_1, \dots, p_n)$ be a sequence of non–negative real numbers and $a = (a_1, \dots, a_n)$ be a sequence of positive real numbers. For any real r satisfying $r \geqslant 1$ or $r \leqslant 0$, the following inequality holds*

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

If $0 \leqslant r \leqslant 1$, the reverse inequality sign in (2.1) holds. Also, the equality sign in (2.1) holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n \neq 0$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = a_{t+2} = \cdots = a_n \neq 0$, or $p_t = p_{t+1} = \cdots = p_n = 0$ and $a_1 = a_2 = \cdots = a_t \neq 0$, for some t satisfying $1 \leqslant t \leqslant n-1$.

LEMMA 2.2. [29] *Let $x = (x_1, \dots, x_n)$ be a sequence of non–negative real numbers and $a = (a_1, \dots, a_n)$ be a sequence of positive real numbers. For any non–negative real r, the following inequality holds*

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

Equality in (2.2) holds if and only if $r = 0$, or $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

REMARK 2.1. The inequality (2.2) is known in the literature as Radon's inequality. Let us note that inequality (2.2) is valid also for $r \leqslant -1$. When $-1 \leqslant r \leqslant 0$, the opposite inequality sign in (2.2) is valid. When $r \leqslant 0$ then the sequence $x = (x_i)$, $i = 1,2,\dots,n$, should be positive real number sequence. Therefore, equality in (2.2) is also attained for $r = -1$.

3. On relations between $AG(G)$ and $GA(G)$

Throughout this section d_i denotes degree of the vertex v_i of a graph G. The set of all different elements of the degree sequence of a graph G is known as the degree set of G. A graph whose degree set consists of only one element or two elements is known as a regular graph or a bidegreed graph, respectively. In the first theorem of this section, we determine an upper bound for the difference $irr_{AG}(G) = AG(G) - GA(G)$ in terms of some other graph invariants and prove that only regular or bidegreed graphs attain this bound.

THEOREM 3.1. *Let G be a connected graph with $n \geqslant 2$ vertices. Then*

$$irr_{AG}(G) = AG(G) - GA(G) \leqslant \frac{1}{2}\sqrt{(n-2H(G))(M_1(G)-4ISI(G))}. \tag{3.1}$$

Equality in (3.1) holds if and only if G is regular or bidegreed graph.

Proof. Let $\{v_1, v_2, \dots, v_n\}$ and $(d_1, d_2, \dots, d_n)$ be the vertex set and vertex-degree sequence of G, where d_i is degree of the vertex v_i. For $r = 2$, $p_i := \frac{(d_i-d_j)^2}{d_i+d_j}$, $a_i := \frac{1}{\sqrt{d_i d_j}}$ with summation performed over all edges of G, the inequality (2.1) becomes

$$\sum_{i\sim j}\frac{(d_i-d_j)^2}{d_i+d_j}\sum_{i\sim j}\frac{(d_i-d_j)^2}{d_id_j(d_i+d_j)} \geqslant \left(\sum_{i\sim j}\frac{(d_i-d_j)^2}{\sqrt{d_id_j}(d_i+d_j)}\right)^2. \tag{3.2}$$

Since

$$irr_{AG}(G) = AG(G) - GA(G) = \frac{1}{2}\sum_{i\sim j}\frac{(d_i-d_j)^2}{\sqrt{d_id_j}(d_i+d_j)}, \tag{3.3}$$

$$\sum_{i\sim j}\frac{(d_i-d_j)^2}{d_i+d_j} = \sum_{i\sim j}\frac{(d_i+d_j)^2-4d_id_j}{d_i+d_j} = M_1(G) - 4ISI(G),$$

$$\sum_{i\sim j}\frac{(d_i-d_j)^2}{d_id_j(d_i+d_j)} = \sum_{i\sim j}\frac{(d_i+d_j)^2-4d_id_j}{d_id_j(d_i+d_j)} = n - 2H(G),$$

from the above identities and (3.2) we obtain

$$4irr_{AG}(G)^2 \leqslant (n-2H(G))(M_1(G)-4ISI(G)),$$

Since $n-2H(G) \geqslant 0$ (see [41]) and $M_1(G)-4ISI(G) \geqslant 0$ (see [33]), from the above inequality we obtain (3.1).

Due to Lemma 2.1, equality in (3.2) holds if and only if the product d_id_j is constant for every pair of adjacent vertices v_i, v_j of G or d_id_j is constant for some pairs of adjacent vertices v_i, v_j and $d_i = d_j$ for all the remaining adjacent vertices. Let v_j and v_k be adjacent to vertex v_i, and $d_i \neq d_k$. Since $d_id_j = d_id_k$, it follows that $d_j = d_k$, meaning that G is bidegreed graph. Hence we conclude that equality in (3.1) holds if and only if G is regular or bidegreed graph. □

REMARK 3.1. Equality in (3.1) is attained for a large number of connected graphs. Figure 1 illustrates some of them for the case $n = 5$.

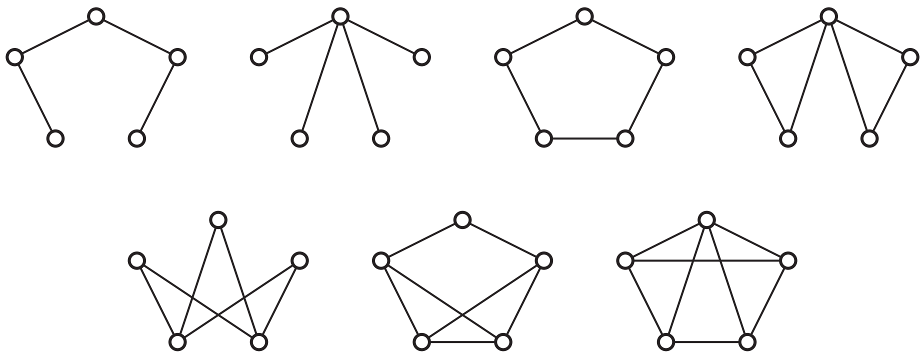

Figure 1: *Some graphs for which the equality in* (3.1) *holds for the case* $n = 5$.

For a graph G, a graph invariant $I(G)$ is said to be a graph irregularity measure if $I(G)$ is non–negative and the equation $I(G) = 0$ holds if and only if G is a regular graph. Detail about some vertex–degree-based irregularity measures can be found in [12, 23, 31, 11, 30].

REMARK 3.2. As mentioned in the proof of Theorem 3.1, the following inequalities are valid

$$irr_1(G) = n-2H(G) \geqslant 0 \quad \text{and} \quad irr_2(G) = M_1(G)-4ISI(G) \geqslant 0,$$

with equalities if and only if G is regular. Having this in mind, the inequality (3.1) can be considered as relationship between irregularity measures $irr_{AG}(G)$, $irr_1(G)$ and $irr_2(G)$, that is the following holds

$$4irr_{AG}(G)^2 \leqslant irr_1(G)irr_2(G),$$

with equality if and only if G is a regular or bidegreed graph.

A non-regular graph G is said to be semiregular bipartite if it is bipartite and all the vertices of every partite set of G have the same degree.

THEOREM 3.2. *Let G be a connected graph with $m \geqslant 1$ edges. Then*

$$irr_{AG}(G) = AG(G) - GA(G) \leqslant \frac{1}{2}\sqrt{(SDD(G)-2m)\left(m - \frac{H(G)^2}{R_{-1}(G)}\right)}. \tag{3.4}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. Let v_i and v_j be two arbitrary adjacent vertices of G. For $r = 2$, $p_i := \frac{(d_i-d_j)^2}{d_id_j}$, $a_i := \frac{\sqrt{d_id_j}}{d_i+d_j}$ with summation performed over all edges of G, the inequality (2.1) becomes

$$\sum_{i\sim j} \frac{(d_i-d_j)^2}{d_id_j} \sum_{i\sim j} \frac{(d_i-d_j)^2}{(d_i+d_j)^2} \geqslant \left(\sum_{i\sim j} \frac{(d_i-d_j)^2}{\sqrt{d_id_j}(d_i+d_j)}\right)^2. \tag{3.5}$$

Since

$$\sum_{i\sim j} \frac{(d_i-d_j)^2}{d_id_j} = \sum_{i\sim j} \frac{d_i^2+d_j^2-2d_id_j}{d_id_j} = SDD(G) - 2m,$$

$$\sum_{i\sim j} \frac{(d_i-d_j)^2}{(d_i+d_j)^2} = \sum_{i\sim j} \frac{(d_i+d_j)^2-4d_id_j}{(d_i+d_j)^2} = m - \sum_{i\sim j} \frac{4d_id_j}{(d_i+d_j)^2},$$

from the above identities, identity (3.3) and inequality (3.5) we obtain

$$4irr_{AG}(G)^2 \leqslant (SDD(G)-2m)\left(m - \sum_{i\sim j} \frac{4d_id_j}{(d_i+d_j)^2}\right). \tag{3.6}$$

On the other hand, for $r = 1$, $x_i := \frac{1}{d_i+d_j}$, $a_i := \frac{1}{d_id_j}$, with summation performed over all edges of G, the inequality (2.2) becomes

$$\sum_{i\sim j} \frac{d_id_j}{(d_i+d_j)^2} = \sum_{i\sim j} \frac{\left(\frac{1}{d_i+d_j}\right)^2}{\frac{1}{d_id_j}} \geqslant \frac{\left(\sum_{i\sim j} \frac{1}{d_i+d_j}\right)^2}{\sum_{i\sim j} \frac{1}{d_id_j}} = \frac{H(G)^2}{4R_{-1}(G)}. \tag{3.7}$$

Now, from the above and (3.6) we obtain

$$4irr_{AG}(G)^2 \leqslant (SDD(G)-2m)\left(m - \frac{H(G)^2}{R_{-1}(G)}\right).$$

Since $SDD(G) - 2m \geqslant 0$ (see [36]), and $m - \frac{H(G)^2}{R_{-1}(G)} \geqslant 0$, from the above inequality we arrive at (3.4).

Equality in (3.7) holds if and only if $\frac{1}{d_i} + \frac{1}{d_j}$ is constant for every pair of adjacent vertices v_i and v_j of G. Suppose vertices v_j and v_k are adjacent to v_i. In that case $\frac{1}{d_i} + \frac{1}{d_j} = \frac{1}{d_i} + \frac{1}{d_k}$, that is $d_j = d_k$. This means that equality in (3.7) holds if and only if G is regular or semiregular bipartite graph. The equality in (3.5) is attained for the same cases, which implies that equality in (3.4) holds if and only if G is regular or semiregular bipartite graph. □

THEOREM 3.3. *Let G be a connected graph with $m \geqslant 1$ edges. Then*

$$irr_{AG}(G) = AG(G) - GA(G) \leqslant \frac{1}{4}(SDD(G) - 2m). \tag{3.8}$$

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

Proof. For every pair of vertices v_i and v_j of G, the following inequality holds because of the arithmetic mean–geometric mean (AM–GM) inequality (see e.g. [25]):

$$d_i + d_j \geqslant 2\sqrt{d_i d_j}. \tag{3.9}$$

From the above inequality and identity (3.3) we obtain that

$$\begin{aligned} irr_{AG}(G) = AG(G) - GA(G) \leqslant \sum_{i\sim j} \frac{(d_i - d_j)^2}{4d_i d_j} &= \frac{1}{4}\sum_{i\sim j}\left(\frac{d_i^2 + d_j^2}{d_i d_j} - 2\right) \\ &= \frac{1}{4}(SDD(G) - 2m), \end{aligned}$$

which is the required inequality.

Equality in (3.9) holds if and only if $d_i = d_j$, which implies that in the above inequality equality sign holds if and only if $d_i = d_j$ for every pair of adjacent vertices v_i and v_j. Thus, since G is connected, equality in (3.8) holds if and only if G is a regular graph. □

REMARK 3.3. As we have mentioned, in [36] it was proven that $SDD(G) \geqslant 2m$ with equality holding if and only if G is regular. Therefore the topological index $irr_3(G) = SDD(G) - 2m$ can be considered as an irregularity measure. Thus, from (3.8) we have that

$$irr_{AG}(G) \leqslant \frac{1}{4} irr_3(G).$$

It is not difficult to observe that

$$\frac{1}{4} irr_3(G) - irr_{AG}(G),$$

is also an irregularity measure.

COROLLARY 3.1. *Let G be a connected graph of order $n \geqslant 2$, size m, and maximum degree Δ. Then*

$$irr_{AG}(G) = AG(G) - GA(G) \leqslant \frac{1}{4}(n\Delta - 2m).$$

The equality sign in the above inequality holds if and only if G is regular.

Proof. In [36] it was proven that

$$SDD(G) \leqslant n\Delta,$$

with equality holding if and only if G is regular. From the above and inequality (3.8) we obtain the required result. □

The next result follows from Corollary 3.1

COROLLARY 3.2. *Let G be a connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$irr_{AG}(G) \leqslant \frac{1}{4}(n(n-1)-2m).$$

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

A unicyclic graph is a connected graph with the same order and size. The next result follows from Corollary 3.1.

COROLLARY 3.3. *Let U be a unicyclic graph of order $n \geqslant 3$ and maximum degree Δ. Then*

$$irr_{AG}(U) = AG(U) - GA(U) \leqslant \frac{n(\Delta-2)}{4}.$$

Equality holds if and only if $U \cong C_n$.

In the next theorem we determine an upper bound on the index $r(G) = AG(G) + GA(G)$.

THEOREM 3.4. *Let G be a connected graph. Then*

$$r(G) \leqslant \frac{1}{2}\sqrt{2R_{-1}(G)(F(G)+6M_2(G))}. \tag{3.10}$$

Equality holds if and only if G is regular.

Proof. Let v_i and v_j be two arbitrary adjacent vertices of G. For $r=2$, $p_i := (d_i+d_j)^2+4d_id_j$, $a_i := \frac{1}{\sqrt{d_id_j}(d_i+d_j)}$, with summation performed over all edges of G, the inequality (2.1) becomes

$$\sum_{i\sim j}((d_i+d_j)^2+4d_id_j)\sum_{i\sim j}\frac{(d_i+d_j)^2+4d_id_j}{d_id_j(d_i+d_j)^2} \geqslant \left(\sum_{i\sim j}\frac{(d_i+d_j)^2+4d_id_j}{\sqrt{d_id_j}(d_i+d_j)}\right)^2. \tag{3.11}$$

Since

$$\begin{aligned} 2r(G) = 2(AG(G)+GA(G)) &= \sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_id_j}} + \sum_{i\sim j}\frac{4\sqrt{d_id_j}}{d_i+d_j} = \\ &= \sum_{i\sim j}\frac{(d_i+d_j)^2+4d_id_j}{\sqrt{d_id_j}(d_i+d_j)}, \end{aligned} \tag{3.12}$$

and

$$\sum_{i\sim j}((d_i+d_j)^2+4d_id_j)=\sum_{i\sim j}(d_i^2+d_j^2+6d_id_j)=F(G)+6M_2(G),$$

from the above identities and inequality (3.11) we obtain

$$4r(G)^2 \leqslant (F(G)+6M_2(G))\sum_{i\sim j}\frac{(d_i+d_j)^2+4d_id_j}{d_id_j(d_i+d_j)^2}. \tag{3.13}$$

On the other hand, from (3.9) we obtain

$$\sum_{i\sim j}\frac{(d_i+d_j)^2+4d_id_j}{d_id_j(d_i+d_j)^2} \leqslant \sum_{i\sim j}\frac{(d_i+d_j)^2+(d_i+d_j)^2}{d_id_j(d_i+d_j)^2}=\sum_{i\sim j}\frac{2}{d_id_j}=2R_{-1}(G).$$

From the above inequality and (3.13) we arrive at (3.10).

Since equality in (3.9) holds if and only if $d_i=d_j$, and since G is connected, it implies that equality in (3.10) holds if and only if G is regular. □

Since $F(G)\geqslant 2M_2(G)$ with equality if and only if G is regular, Theorem 3.4 implies the next result.

COROLLARY 3.4. *Let G be a connected graph. Then*

$$r(G)=AG(G)+GA(G)\leqslant\sqrt{2R_{-1}(G)F(G)}.$$

Equality holds if and only if G is regular.

THEOREM 3.5. *Let G be a connected graph with $n\geqslant 2$ vertices. Then*

$$r(G)=AG(G)+GA(G)\leqslant 2\sqrt{(n-H(G))(M_1(G)-2ISI(G))}. \tag{3.14}$$

Equality holds if and only if G is regular.

Proof. For any two vertices v_i and v_j of G, based on the AM–GM inequality, we have that

$$2d_id_j\leqslant d_i^2+d_j^2. \tag{3.15}$$

From the above inequality and identity (3.12) we have that

$$r(G)=AG(G)+GA(G)=\sum_{i\sim j}\frac{d_i^2+d_j^2+6d_id_j}{2\sqrt{d_id_j}(d_i+d_j)}\leqslant 2\sum_{i\sim j}\frac{d_i^2+d_j^2}{\sqrt{d_id_j}(d_i+d_j)}. \tag{3.16}$$

On the other hand, for $r=\frac{1}{2}$, $p_i:=\frac{d_i^2+d_j^2}{d_i+d_j}$, $a_i:=\frac{1}{d_id_j}$, with summation performed over all edges of G, the inequality (2.1) transforms into

$$\left(\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_i+d_j}\right)^{-1/2}\sum_{i\sim j}\frac{d_i^2+d_j^2}{\sqrt{d_id_j}(d_i+d_j)}\leqslant\left(\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_id_j(d_i+d_j)}\right)^{1/2}. \tag{3.17}$$

Since

$$\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_i+d_j}=\sum_{i\sim j}\frac{(d_i+d_j)^2-2d_id_j}{d_i+d_j}=M_1(G)-2ISI(G)\,,$$

$$\sum_{i\sim j}\frac{d_i^2+d_j^2}{d_id_j(d_i+d_j)}=\sum_{i\sim j}\frac{(d_i+d_j)^2-2d_id_j}{d_id_j(d_i+d_j)}=n-H(G)\,,$$

from the above identities and inequality (3.17) we obtain

$$\sum_{i\sim j}\frac{d_i^2+d_j^2}{\sqrt{d_id_j}(d_i+d_j)}\leqslant\sqrt{(n-H(G))(M_1(G)-2ISI(G))}\,.$$

From the above and (3.16) we obtain (3.14).

Equality in (3.15), and consequently in (3.14), holds if and only if G is a regular graph. □

The proofs of the next two theorems are analogous to that of Theorem 3.5, hence omitted.

THEOREM 3.6. *Let G be a connected graph. Then*

$$r(G)=AG(G)+GA(G)\leqslant\sqrt{F(G)ID(G)}\,.$$

Equality holds if and only if G is regular.

THEOREM 3.7. *Let G be a connected graph with $m\geqslant 1$ edges. Then*

$$r(G)=AG(G)+GA(G)\leqslant\frac{1}{4}(SDD(G)+6m)\,. \tag{3.18}$$

Equality holds if and only if G is regular.

From Theorem 3.7 and the first sentence of Remark 3.3, the next result follows.

COROLLARY 3.5. *Let G be a connected graph. Then*

$$r(G)=AG(G)+GA(G)\leqslant SDD(G)\,.$$

Equality holds if and only if G is regular.

Note that $2m\leqslant n\Delta\leqslant n(n-1)$ for every graph of order n, size m and maximum degree Δ. Hence, from Theorem 3.7 and the first sentence of the proof of Corollary 3.1, the next result follows.

COROLLARY 3.6. *Let G be a connected graph of order $n\geqslant 2$, size m, and maximum degree Δ. Then*

$$r(G)=AG(G)+GA(G)\leqslant\frac{1}{4}(n\Delta+6m)\leqslant n\Delta\leqslant n(n-1)\,.$$

Equalities in the first two inequalities are attained if and only if G is regular, whereas the equality in the third one holds if and only if $G\cong K_n$.

Keeping in mind Theorems 3.3 and 3.7, the first sentence of Remark 3.3 and the first sentence of the proof of Corollary 3.1, we have the next result.

COROLLARY 3.7. *Let G be a connected graph with $n \geqslant 2$ vertices, m edges and maximum degree Δ. Then*

$$AG(G) \leqslant \frac{1}{4}(SDD(G) + 2m) \tag{3.19}$$

$$AG(G) \leqslant \frac{1}{2}SDD(G) \tag{3.20}$$

$$AG(G) \leqslant \frac{n\Delta}{2} \tag{3.21}$$

$$AG(G) \leqslant \frac{n(n-1)}{2}. \tag{3.22}$$

The equality in any of (3.19), (3.20), and (3.21) holds if and only if G is regular. Whereas, the equality in (3.22) holds if and only if $G \cong K_n$.

The inequality (3.19) was proven in [27]. The inequality (3.20) was proven in [8], whereas the inequalities (3.21) and (3.22) were proven in [37].

4. On relations between $AG(G)$ and other topological indices

The next theorem reveals a connection between $AG(G)$ and $M_2(G)$, $F(G)$ and $R_{-1}(G)$.

THEOREM 4.1. *Let G be a connected graph. Then*

$$AG(G) \leqslant \frac{1}{2}\sqrt{R_{-1}(G)(F(G) + 2M_2(G))}. \tag{4.1}$$

Equality holds if and only if G is a regular or semiregular bipartite graph.

Proof. The following identity is valid

$$F(G) + 2M_2(G) = \sum_{i\sim j}(d_i + d_j)^2 = \sum_{i\sim j}\frac{\left(\frac{d_i+d_j}{2\sqrt{d_id_j}}\right)^2}{\frac{1}{4d_id_j}}. \tag{4.2}$$

On the other hand, for $r = 1$, $x_i := \frac{d_i+d_j}{2\sqrt{d_id_j}}$, $a_i := \frac{1}{4d_id_j}$, with summation performed over all edges of G, the inequality (2.2) becomes

$$\sum_{i\sim j}\frac{\left(\frac{d_i+d_j}{2\sqrt{d_id_j}}\right)^2}{\frac{1}{4d_id_j}} \geqslant \frac{\left(\sum_{i\sim j}\frac{d_i+d_j}{2\sqrt{d_id_j}}\right)^2}{\sum_{i\sim j}\frac{1}{4d_id_j}} = \frac{4AG(G)^2}{R_{-1}(G)}. \tag{4.3}$$

From the above inequality and identity (4.2) we obtain (4.1).

Equality in (4.3) holds if and only if $(d_i+d_j)\sqrt{d_id_j}$ is constant for every pair of adjacent vertices v_i and v_j in G. Suppose vertices v_j and v_k are adjacent to vertex v_i. Then

$$(d_i+d_j)\sqrt{d_id_j} = (d_i+d_k)\sqrt{d_id_k},$$

that is

$$\left(\sqrt{d_j}-\sqrt{d_k}\right)\left(d_i+d_j+d_k+\sqrt{d_jd_k}\right)=0,$$

which implies that $d_j = d_k$. Since graph G is connected, it means that it is regular or semiregular bipartite. This implies that equality in (4.1) holds if and only if G is regular of semiregular bipartite graph. □

Since

$$R_{-1}(G) = \sum_{i\sim j}\frac{1}{d_id_j} \leqslant \frac{m}{\delta^2},$$

we have the following corollary of Theorem 4.1.

COROLLARY 4.1. *Let G be a connected graph of size $m \geqslant 1$ and minimum degree δ. Then*

$$AG(G) \leqslant \frac{1}{2\delta}\sqrt{m(F(G)+2M_2(G))}. \tag{4.4}$$

Equality holds if and only if G is regular.

The inequality (4.4) was proven in [8].

Since

$$F(G)+2M_2(G) = \sum_{i\sim j}(d_i+d_j)^2 \leqslant 2\Delta M_1(G),$$

the following result is valid:

COROLLARY 4.2. *Let G be a connected graph of size $m \geqslant 1$, minimum degree δ, and maximum degree Δ. Then*

$$AG(G) \leqslant \frac{1}{2\delta}\sqrt{2m\Delta M_1(G)}.$$

Equality holds if and only if G is regular.

Since

$$M_1(G) = \sum_{i\sim j}(d_i+d_j) \leqslant 2m\Delta,$$

we have the following result:

COROLLARY 4.3. *Let G be a connected graph of size $m \geqslant 1$, minimum degree δ, and maximum degree Δ. Then*

$$AG(G) \leqslant \frac{m\Delta}{\delta}.$$

Equality holds if and only if G is regular.

In the next theorem we determine a relationship between $AG(G)$ and $M_2(G)$, $ID(G)$ and $R_{-1}(G)$.

THEOREM 4.2. *Let G be a connected graph. Then*

$$AG(G) \leqslant \frac{1}{2}\sqrt{M_2(G)(ID(G)+2R_{-1}(G))}\,. \tag{4.5}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. The following identity is valid

$$ID(G)+2R_{-1}(G) = \sum_{i\sim j}\frac{d_i^2+d_j^2}{(d_id_j)^2} + \sum_{i\sim j}\frac{2}{d_id_j} = \sum_{i\sim j}\frac{(d_i+d_j)^2}{(d_id_j)^2}\,. \tag{4.6}$$

On the other hand, for $r=1$, $x_i := \frac{d_i+d_j}{2\sqrt{d_id_j}}$, $a_i := d_id_j$, with summation performed over all edges of G, the inequality (2.2) becomes

$$\sum_{i\sim j}\frac{(d_i+d_j)^2}{4(d_id_j)^2} \geqslant \frac{\left(\sum_{i\sim j}\frac{d_i+d_j}{2\sqrt{d_id_j}}\right)^2}{\sum_{i\sim j}d_id_j}\,,$$

that is

$$\sum_{i\sim j}\frac{(d_i+d_j)^2}{(d_id_j)^2} \geqslant \frac{4AG(G)^2}{M_2(G)}\,. \tag{4.7}$$

From the above inequality and identity (4.6) we arrive at (4.5).

Equality in (4.7) holds if and only if $\frac{d_i+d_j}{(d_id_j)^{3/2}}$ is constant for every pair of adjacent vertices v_i and v_j in G. Now, by a similar arguments as in the case of the proof of Theorem 4.1 we conclude that equality in (4.5) holds if and only if G is regular or semiregular bipartite graph. □

Since

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

we have the following corollary of Theorem 4.2.

COROLLARY 4.4. *Let G be a connected graph of order $n \geqslant 2$ and minimum degree δ. Then*

$$AG(G) \leqslant \sqrt{\frac{nM_2(G)}{2\delta}}\,,$$

with equality if and only if G is regular.

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