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On Upper Bounds for the Geometric–Arithmetic Topological Index

I. Ž. Milovanović, E. I. Milovanović, M. M. Matejić

Faculty of Electronic Engineering, Beogradska 14, P.O.Box 73, 18000 Niš, Serbia

{igor,ema,marjan.matejic}@elfak.ni.ac.rs

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Abstract

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, be a simple connected graph with $n \geq 2$ vertices, and m edges, and let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, be a sequence of its vertex degrees. A vertex-degree-based topological index, called geometric–arithmetic index, is defined as $GA = \sum_{i\sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j}$, where $i \sim j$ denotes adjacency of vertices i and j. We first analyze some upper bounds for GA reported in the literature. The inequality $GA \leq m$, although simple, is very important and can be used to test whether another upper bound, depending on some other parameters, has any sense. We will show that a number of upper bounds for GA reported in the literature are worthless. Namely, if some other upper bound is greater than m, it is obviously useless. Then we determine some new upper bounds for GA in terms of some other vertex-degree-based indices.

1 Introduction

Let G be a simple connected graph with vertex set $V = \{1, 2, \dots, n\}$ and edge set $E = \{e_1, e_2, \dots, e_m\}$. Further, let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, and $d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m)$ be sequences of its vertex and edge degrees, respectively, and $\Delta_{e_1} = d(e_1) + 2$ and $\delta_{e_1} = d(e_m) + 2$. If vertices i and j are adjacent, we write $i \sim j$. As usual $L(G)$ denotes a line graph.

In graph theory, an invariant is a property of graph that depends only on the abstract structure, not on graph representations such as particular labellings or drawings of the graph. Such quantities are also called topological indices. Topological indices represent an important type of molecular descriptors.

The first and second Zagreb indices are vertex–degree–based graph invariants defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j .$$

The quantity M_1 was first time considered in 1972 [17], whereas M_2 in 1975 [18]. These are the oldest and most thoroughly examined vertex–degree–based topological indices. Details of the theory and applications of the two Zagreb indices can be found in surveys [19, 28] and in the references cited therein.

As shown in [28], the first Zagreb index can be also expressed as

$$M_1 = \sum_{i\sim j} (d_i + d_j) .$$

Bearing in mind that for the edge e connecting the vertices i and j,

$$d(e) = d_i + d_j - 2 ,$$

the index M_1 can also be considered as an edge–degree–based topological index [25]

$$M_1 = \sum_{i=1}^{m} (d(e_i) + 2) .$$

A so-called forgotten topological index, F, is defined as [17] (see also [16]):

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

By analogy to M_1, the invariant F can be written in the following way

$$F = \sum_{i=1}^{m} (d(e_i) + 2)^2 - 2M_2 .$$

In [5] a topological index called general Randić index, R_α, was introduced

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

where α is an arbitrary real number. For $\alpha = -1$ the general Randić index R_{-1} is obtained [31], for $\alpha = -1/2$ we have classical Randić (or connectivity) index, $R = R_{-1/2}$ [30], whereas for $\alpha = 1/2$, the reciprocal Randić index [20] is obtained.

The harmonic index, H, was defined in [14] as

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

The sum-connectivity index, SCI, is defined as [43]

$$SCI = SCI(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i + d_j}}\,.$$

Multiplicative versions of the first and the second Zagreb indices, Π_1 and Π_2, were first considered in a paper [39] published in 2011. These indices are defined as:

$$\Pi_1 = \Pi_1(G) = \prod_{i=1}^{n} d_i^2 \quad \text{and} \quad \Pi_2 = \Pi_2(G) = \prod_{i\sim j} d_i d_j.$$

One year later, the multiplicative sum–Zagreb index, Π_1^*, was introduced [13]:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{i\sim j} (d_i + d_j).$$

In analogy to M_1, indices H, SCI and Π_1^* can be considered as edge–degree–based topological indices and written in the following form

$$H = \sum_{i=1}^{m} \frac{2}{d(e_i)+2}, \quad SCI = \sum_{i=1}^{m} \frac{1}{\sqrt{d(e_i)+2}} \quad \text{and} \quad \Pi_1^* = \prod_{i=1}^{m} (d(e_i)+2).$$

The redefined third Zagreb index, ReZ_3, is defined as [31]

$$ReZ_3 = ReZ_3(G) = \sum_{i\sim j} d_i d_j (d_i + d_j).$$

The Albertson index, Alb, used as an irregularity measure of a graph, is defined as [1]

$$Alb = Alb(G) = \sum_{i\sim j} |d_i - d_j|.$$

This index was referred to as the third Zagreb index in [15], and in [41] as missbalance deg index.

A family of Adriatic indices was introduced in [40, 41]. Especially interesting subclass of these descriptors consists of 148 discrete Adriatic indices. A so called inverse sum indeg index, ISI, was selected in [41] as a significant predictor of total surface area of octane isomers. The inverse indeg index is defined as

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

In order to improve predictive power of Randić index, a large number of new topological descriptors resembling the ordinary Randić index was introduced. The (first) geometric–arithmetic index, GA, introduced in [42] is one of the successors of the Randić index. It is defined as

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

In this paper we are concerned with upper bounds for GA. Two basic inequalities involving upper bounds for GA index

$$GA \leq \frac{n(n-1)}{2} \tag{1}$$

and

$$GA \leq m, \tag{2}$$

were established in [42] and [11] (see also [9]), respectively. These bounds, although simple, are very important and, as we shall demonstrate, can be used to test whether another upper bound, depending on some other parameters, has any sense. Namely, if some other upper bound is greater than (1) or (2), it is obviously useless. As we shall illustrate, there are numerous upper bounds for GA reported in the literature after the bounds (1) and (2) had been published, that are more complex and worse than (1) or (2).

2 Preliminaries

In this section we recall some analytical inequalities for real number sequences that will be used in the rest of the paper.

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, m$, be positive real number sequences with the property $0 < r \leq a_i \leq R < +\infty$. In [21] the following inequality was proved

$$\sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} \frac{p_i}{a_i} \leq \frac{1}{4}\left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}}\right)^2 \left(\sum_{i=1}^{m} p_i\right)^2. \tag{3}$$

Let $a = (a_i)$, $i = 1, 2, \ldots, m$, be a positive real number sequence. In [23] (see also [44]) it was proved

$$\begin{aligned} &\sum_{i=1}^{m} a_i + m(m-1)\left(\prod_{i=1}^{m} a_i\right)^{\frac{1}{m}} \leq \left(\sum_{i=1}^{m} \sqrt{a_i}\right)^2 \\ &\leq (m-1)\sum_{i=1}^{m} a_i + m\left(\prod_{i=1}^{m} a_i\right)^{\frac{1}{m}}. \end{aligned} \tag{4}$$

Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, m$, be two positive real number sequences. Then for any $r \geq 0$ holds [29]

$$\sum_{i=1}^{m} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=1}^{m} x_i\right)^{r+1}}{\left(\sum_{i=1}^{m} a_i\right)^{r}}. \tag{5}$$

Let $p = (p_i)$ be a non-negative real number sequence and $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \ldots, m$, real number sequences with the properties

$$0 < r_1 \leq a_i \leq R_1 < +\infty \qquad \text{and} \qquad 0 < r_2 \leq b_i \leq R_2 < +\infty.$$

In [3] the following inequality was proven

$$\left| \sum_{i=1}^{m} p_i \sum_{i=1}^{m} p_i a_i b_i - \sum_{i=1}^{m} p_i a_i \sum_{i=1}^{m} p_i b_i \right| \leq \frac{1}{4}(R_1 - r_1)(R_2 - r_2) \left(\sum_{i=1}^{m} p_i \right)^2. \tag{6}$$

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, m$, be two positive real number sequences with the properties $p_1 + p_2 + \cdots + p_m = 1$ and $0 < r \leq a_i \leq R < +\infty$. The next inequality was proven in [32]

$$\sum_{i=1}^{m} p_i a_i + rR \sum_{i=1}^{m} \frac{p_i}{a_i} \leq r + R. \tag{7}$$

3 Analysis of some known results

In recent years, a plethora of new upper bounds for GA were reported in the literature (see for example [2, 4, 9–11, 24, 27, 33–36, 38, 42]). In the text that follows we outline some of them and compare it with (2). As we shall see, most of them are completely worthless.

The following upper bounds for GA were derived in [38]:

$$GA \leq \frac{M_2}{\delta^2}, \tag{8}$$

$$GA \leq \sqrt{\frac{mM_1}{2\delta}}, \tag{9}$$

$$GA \leq \Delta^2 R_{-1}, \tag{10}$$

$$GA \leq \sqrt{M_2 R_{-1}}, \tag{11}$$

$$GA \leq \sqrt{\Delta m R}, \tag{12}$$

$$GA \leq \frac{\sqrt{(nM_1 + 4M_2 - 4m^2)R_{-1}}}{2}. \tag{13}$$

In [33] the following inequalities were proven:

$$GA \leq \Delta R, \tag{14}$$

$$GA \leq \frac{M_1}{2\delta}, \tag{15}$$

$$GA \leq \Delta H, \tag{16}$$

$$GA \leq \sqrt{\frac{nM_2}{2\delta}}, \tag{17}$$

$$GA \leq \sqrt{2\Delta} SCI. \tag{18}$$

The inequalities (14), (17) and (18) were also proved in [22].

The following upper bounds for GA were established in [34]:

$$GA \leq \frac{\sqrt{nM_1}}{2}, \tag{19}$$

$$GA \leq \frac{\sqrt{M_2 + \delta^2 m(m-1)}}{\delta}, \tag{20}$$

$$GA \leq \Delta\sqrt{mR_{-1}}, \tag{21}$$

$$GA \leq \frac{\sqrt{2\Delta M_1 R_{-1}}}{2}, \tag{22}$$

$$GA \leq \sqrt{R_\alpha R_{-\alpha}}, \tag{23}$$

$$GA \leq \Delta^{-2\alpha+1}\delta^{-1}R_\alpha, \quad \text{if } \alpha \leq \frac{1}{2}, \tag{24}$$

$$GA \leq \delta^{-2\alpha}R_\alpha, \quad \text{if } \alpha \geq \frac{1}{2}, \tag{25}$$

$$GA \leq \Delta^{-2\alpha}R_\alpha, \quad \text{if } \alpha \leq -\frac{1}{2}, \tag{26}$$

$$GA \leq \Delta\delta^{-2\alpha-1}R_\alpha, \quad \text{if } \alpha \geq -\frac{1}{2}. \tag{27}$$

In [35] it was proven that

$$GA \leq 2m\sqrt{\frac{\Delta}{\delta}} - \sqrt{\Delta\delta}H\,, \tag{28}$$

and in [36]

$$GA \leq (n-1)H. \tag{29}$$

In [4] the following upper bounds for GA were obtained:

$$GA \leq (n-1)R, \tag{30}$$

$$GA \leq \delta\left(\frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n}\right), \tag{31}$$

$$GA \leq \frac{\Delta n}{2}. \tag{32}$$

The next inequalities were obtained in [24]:

$$GA \leq 2m - \frac{F}{2\Delta^2}, \tag{33}$$

$$GA \leq \frac{\Delta(\Delta^2+\delta^2)^2 m^2}{4\delta^3 M_2}, \tag{34}$$

$$GA \leq \frac{\sqrt{\Delta}(\Delta+\delta)^3 m^2}{8\delta^{3/2} M_2}. \tag{35}$$

In [11] it was proven

$$GA \leq \sqrt{m\left(m - \frac{F-2M_2}{4\Delta^2}\right)} \leq m \leq \binom{n}{2}. \tag{36}$$

In the sequel, we will prove that the inequalities (8)–(35) are direct consequences of the inequality (2), therefore those have neither theoretical nor practical significance.

Since

$$M_2 = \sum_{i\sim j} d_i d_j \geq m\delta^2, \tag{37}$$

we have that

$$m \leq \frac{M_2}{\delta^2},$$

therefore the inequality (8) is corollary of (2).

Similarly, as

$$M_1 = \sum_{i\sim j}(d_i + d_j) \geq m\delta_{e_1} \geq 2m\delta \geq 2m, \tag{38}$$

it follows

$$m \leq \sqrt{\frac{mM_1}{2\delta}},$$

so the inequality (9) is corollary of inequality (2).

Since

$$R_{-1} = \sum_{i\sim j}\frac{1}{d_i d_j} \geq \frac{m}{\Delta^2} \geq \frac{m}{(n-1)^2}, \tag{39}$$

it follows

$$m \leq \Delta^2 R_{-1},$$

therefore the inequality (10) is corollary of inequality (2).

Since

$$M_2 R_{-1} = \sum_{i\sim j} d_i d_j \sum_{i\sim j}\frac{1}{d_i d_j} \geq m^2, \tag{40}$$

it follows

$$m \leq \sqrt{M_2 R_{-1}}\,.$$

Consequently, the inequality (11) is corollary of inequality (2).

Since

$$R = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}} \geq \frac{m}{\Delta} \geq \frac{m}{n-1}, \tag{41}$$

it follows

$$m \leq \sqrt{m \Delta R}\,.$$

Hence, the inequality (12) is corollary of inequality (2).

Since

$$(F + 2M_2)R_{-1} = \sum_{i \sim j}(d_i + d_j)^2 \sum_{i \sim j} \frac{1}{d_i d_j} \geq 4 \sum_{i \sim j} d_i d_j \sum_{i \sim j} \frac{1}{d_i d_j} \geq 4m^2,$$

it follows

$$m \leq \frac{\sqrt{(F + 2M_2)R_{-1}}}{2}.$$

In [45] it was proven

$$F \leq nM_1 + 2M_2 - 4m^2,$$

therefore

$$m \leq \frac{\sqrt{(nM_1 + 4M_2 - 4m^2)R_{-1}}}{2}.$$

This means that the inequality (13) is corollary of inequality (2).

According to the first inequality in (41) we obtain

$$m \leq \Delta R,$$

so the inequality (14) is corollary of inequality (2).

From the second inequality in (38) we have that

$$m \leq \frac{M_1}{2\delta},$$

so the inequality (15) is corollary of inequality (2).

From the identity

$$H = \sum_{i \sim j} \frac{2}{d_i + d_j} \geq \frac{2m}{\Delta_{e_1}} \geq \frac{m}{\Delta} \geq \frac{n-1}{\Delta},$$

it holds

$$m \leq \Delta H,$$

therefore the inequality (16) is corollary of inequality (2).

According to the inequality (see [8])

$$R_{-1} \leq \frac{n}{2\delta}$$

and the inequality (40) we obtain

$$m \leq \sqrt{\frac{nM_2}{2\delta}}\,.$$

Therefore, the inequality (17) is corollary of inequality (2).

Since

$$SCI = \sum_{i\sim j} \frac{1}{\sqrt{d_i + d_j}} \geq \frac{m}{\sqrt{\Delta_{e_1}}} \geq \frac{m}{\sqrt{2\Delta}},$$

it holds

$$m \leq \sqrt{2\Delta} SCI\,.$$

Hence, the inequality (18) is corollary of (2).

According to the inequality (see [12])

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

we obtain

$$m \leq \frac{\sqrt{nM_1}}{2},$$

so the inequality (19) is corollary of inequality (2).

Since

$$M_2 = \sum_{i\sim j} d_i d_j \geq \delta^2 m = \delta^2 m^2 - \delta^2 m(m-1),$$

we have that

$$m \leq \frac{\sqrt{M_2 + \delta^2 m(m-1)}}{\delta},$$

therefore the inequality (20) is corollary of inequality (2).

According to the first inequality in (39) we have that

$$m \leq \Delta^2 R_{-1},$$

that is

$$m^2 \leq m\Delta^2 R_{-1},$$

therefore

$$m \leq \Delta\sqrt{mR_{-1}},$$

so the inequality (21) is corollary of inequality (2).

Since

$$M_1R_{-1} = \sum_{i\sim j}(d_i+d_j)\sum_{i\sim j}\frac{1}{d_id_j} \geq \frac{2}{\Delta}\sum_{i\sim j}\sqrt{d_id_j}\sum_{i\sim j}\frac{1}{\sqrt{d_id_j}} \geq \frac{2m^2}{\Delta},$$

it follows

$$m \leq \frac{\sqrt{2\Delta M_1R_{-1}}}{2},$$

which means that the inequality (22) is corollary of inequality (2).

Since

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

we have that

$$m \leq \sqrt{R_\alpha R_{-\alpha}}\,,$$

meaning that inequality (23) is corollary of inequality (2).

Let $\alpha \leq 1/2$. Then

$$\begin{aligned}\Delta^{-2\alpha+1}\delta^{-1}R_\alpha &= \Delta^{-2\alpha+1}\delta^{-1}\sum_{i\sim j}(d_id_j)^\alpha = \Delta^{-2\alpha+1}\delta^{-1}\sum_{i\sim j}(d_id_j)^{\alpha-\frac{1}{2}}(d_id_j)^{\frac{1}{2}}\\ &\geq \Delta^{-2\alpha+1}\delta^{-1}\Delta^{2\alpha-1}\delta m = m,\end{aligned}$$

therefore the inequality (24) is corollary of inequality (2).

Let $\alpha \geq 1/2$. Then

$$\delta^{-2\alpha}R_\alpha = \delta^{-2\alpha}\sum_{i\sim j}(d_id_j)^\alpha \geq \delta^{-2\alpha}\delta^{2\alpha}m = m,$$

therefore the inequality (25) is corollary of inequality (2).

Let $\alpha \leq -1/2$. Then

$$\Delta^{-2\alpha}R_\alpha = \Delta^{-2\alpha}\sum_{i\sim j}(d_id_j)^\alpha \geq \Delta^{-2\alpha}\Delta^{2\alpha}m = m,$$

therefore the inequality (26) is corollary of inequality (2).

Let $\alpha \geq -1/2$. Then

$$\begin{aligned}\Delta\delta^{-2\alpha-1}R_\alpha &= \Delta\delta^{-2\alpha-1}\sum_{i\sim j}(d_id_j)^\alpha = \Delta\delta^{-2\alpha-1}\sum_{i\sim j}(d_id_j)^{\alpha+\frac{1}{2}}(d_id_j)^{-\frac{1}{2}}\\ &\geq \Delta\delta^{-2\alpha-1}\Delta^{-1}\delta^{2\alpha+1}m = m,\end{aligned}$$

so the inequality (27) is corollary of inequality (2).

Since

$$\sqrt{\Delta} \geq \sqrt{\delta},$$

$$2\sqrt{\Delta}-\sqrt{\delta}\geq\sqrt{\Delta},$$

$$H=\sum_{i\sim j}\frac{2}{d_i+d_j}\leq\frac{m}{\delta}\leq\frac{m\left(2\sqrt{\Delta}-\sqrt{\delta}\right)}{\delta\sqrt{\Delta}},$$

we have that

$$m\left(2\sqrt{\frac{\Delta}{\delta}}-1\right)\geq\sqrt{\delta\Delta}H,$$

that is

$$m\leq 2m\sqrt{\frac{\Delta}{\delta}}-\sqrt{\delta\Delta}H,$$

therefore the inequality (28) is corollary of inequality (2).

The inequality (29) is corollary of inequality (16), and, consequently, corollary of (2).

The inequality (30) is corollary of inequality (14), and therefore corollary of (2) also.

In [4] it was shown that the right-hand part of inequality (31) is less than m, therefore it is corollary of inequality (2).

Since

$$2m=\sum_{i=1}^{n}d_i\leq n\Delta,$$

we have that

$$m\leq\frac{n\Delta}{2},$$

therefore the inequality (32) is corollary of inequality (2).

Since

$$F=\sum_{i=1}^{n}d_i^3\leq 2\Delta^2 m,$$

it follows

$$\frac{F}{2\Delta^2}\leq m=2m-m,$$

that is

$$m\leq 2m-\frac{F}{2\Delta^2},$$

therefore the inequality (33) is corollary of inequality (2).

Setting $p_i=1$, $a_i:=d_id_j$ in (3), we obtain

$$\frac{m}{\Delta^2}M_2\leq\sum_{i\sim j}d_id_j\sum_{i\sim j}\frac{1}{d_id_j}\leq\frac{m^2}{4}\left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right)^2,$$

i.e.

$$m\leq\frac{m^2(\delta^2+\Delta^2)^2}{4\delta^2M_2}.$$

Since

$$m \leq \frac{m^2(\delta^2+\Delta^2)^2}{4\delta^2 M_2} \leq \frac{m^2\Delta(\delta^2+\Delta^2)^2}{4\delta^3 M_2},$$

the inequality (34) is corollary of inequality (2).

Since

$$M_2 = \sum_{i\sim j} d_i d_j \leq m\Delta^2,$$

we have that

$$\frac{\sqrt{\Delta}(\Delta+\delta)^3 m^2}{8\delta^{3/2} M_2} \geq \frac{\sqrt{\Delta}(\Delta+\delta)^3 m^2}{8\delta^{3/2}\Delta^2 m} = \frac{m}{8}\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)^3 \geq m\,,$$

so the inequality (35) is corollary of (2).

Although the inequalities (8)–(35) are all correct, these are worthless and have no significance since all were published many years after the bound (2) has been established and are worse than it.

On the other hand, the inequality (36) is stronger than (2), and as such is noteworthy. Inspired by it, we determine some new upper bounds for GA presented in the next section.

4 New upper bounds for GA

In the next theorem we determine upper bound for GA in terms of graph parameters m, Δ_{e_1}, δ_{e_1} and invariants M_2, Π_2 and Π_1^*.

Theorem 1. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$GA \leq \frac{(\Delta_{e_1}+\delta_{e_1})^2}{2\Delta_{e_1}\delta_{e_1}} \frac{(m-1)M_2 + m\,(\Pi_2)^{\frac{1}{m}}}{m\,(\Pi_2)^{\frac{1}{2m}}\,(\Pi_1^*)^{\frac{1}{m}}}. \tag{42}$$

Equality holds if and only if $L(G)$ is a regular graph.

Proof. For $p_i := \sqrt{d_i d_j}$, $a_i := d_i + d_j$, $r = \delta_{e_1}$, $R = \Delta_{e_1}$, where summation goes over all adjacent vertices i and j of G, i.e. over all edges, the inequality (3) becomes

$$\sum_{i\sim j}\sqrt{d_i d_j}(d_i+d_j)\sum_{i\sim j}\frac{\sqrt{d_i d_j}}{d_i+d_j} \leq \frac{(\Delta_{e_1}+\delta_{e_1})^2}{4\Delta_{e_1}\delta_{e_1}}\left(\sum_{i\sim j}\sqrt{d_i d_j}\right)^2,$$

i.e.

$$\frac{1}{2}GA\sum_{i\sim j}\sqrt{d_i d_j}(d_i+d_j) \leq \frac{(\Delta_{e_1}+\delta_{e_1})^2}{4\Delta_{e_1}\delta_{e_1}}\left(\sum_{i\sim j}\sqrt{d_i d_j}\right)^2. \tag{43}$$

According to the arithmetic-geometric mean inequality (see e.g. [26]), we have

$$\sum_{i\sim j}\sqrt{d_id_j}(d_i+d_j)\geq m\left(\prod_{i\sim j}\sqrt{d_id_j}(d_i+d_j)\right)^{\frac{1}{m}},$$

i.e.

$$\sum_{i\sim j}\sqrt{d_id_j}(d_i+d_j)\geq m\,(\Pi_2)^{\frac{1}{2m}}\,(\Pi_1^*)^{\frac{1}{m}}\,. \tag{44}$$

For $a_i := d_id_j$ right part of inequality (4) becomes

$$\left(\sum_{i\sim j}\sqrt{d_id_j}\right)^2\leq(m-1)\sum_{i\sim j}d_id_j+m\left(\prod_{i\sim j}d_id_j\right)^{\frac{1}{m}},$$

that is

$$\left(\sum_{i\sim j}\sqrt{d_id_j}\right)^2\leq(m-1)M_2+m\,(\Pi_2)^{\frac{1}{m}}\,. \tag{45}$$

According to (43), (44) and (45) we obtain (42).

Equality in (43) holds if and only if $d_i + d_j$ is a constant for each pair of adjacent vertices i and j. Equality in (44) is attained if and only if $\sqrt{d_id_j}(d_i+d_j)$ is a constant for each pair of adjacent vertices i and j. Equality in (45) holds if and only if d_id_j is a constant for each pair of adjacent vertices i and j. Finally, these three conditions together give that equality in (42) holds if and only if $L(G)$ is a regular graph. ■

According to (42) we get the following result.

Theorem 2. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$GA\leq\frac{(\Delta_{e_1}+\delta_{e_1})^2}{2\Delta_{e_1}\delta_{e_1}}\frac{(m-1)M_2+m\,(\Pi_2)^{\frac{1}{m}}}{ReZ_3}$$

and

$$GA\leq\frac{(\Delta_{e_1}+\delta_{e_1})^2}{2\Delta_{e_1}\delta_{e_1}}\frac{RR^2}{ReZ_3}.$$

Equalities hold if and only if $L(G)$ is a regular graph.

Since $2\delta\leq\delta_{e_1}\leq\Delta_{e_1}\leq2\Delta$, we obtain the following corollaries of Theorems 1 and 2.

Corollary 1. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$GA\leq\frac{\left(\Delta_{e_1}+\delta_{e_1}\right)^2(RR)^2}{2m\Delta_{e_1}\delta_{e_1}\left(\Pi_2\right)^{\frac{1}{2m}}\left(\Pi_1^*\right)^{\frac{1}{m}}},$$

and

$$GA\leq\frac{\left(\Delta_{e_1}+\delta_{e_1}\right)^2RR}{2\delta_{e_1}^2\Delta_{e_1}}.$$

Equalities hold if and only if $L(G)$ is a regular graph.

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

$$GA \leq \frac{(\Delta+\delta)^2}{2\Delta\delta} \frac{(m-1)M_2 + m\,(\Pi_2)^{\frac{1}{m}}}{m\,(\Pi_2)^{\frac{1}{2m}}\,(\Pi_1^*)^{\frac{1}{m}}},$$

$$GA \leq \frac{(\Delta+\delta)^2}{2\Delta\delta} \frac{(m-1)M_2 + m\,(\Pi_2)^{\frac{1}{m}}}{ReZ_3},$$

$$GA \leq \frac{(\Delta+\delta)^2}{2\Delta\delta} \frac{RR^2}{ReZ_3}.$$

Equalities hold if and only if G is a regular graph.

In the next theorem we establish upper bound for GA in terms of indices H and ISI.

Theorem 3. *Let G be a simple connected graph with $m \geq 1$ edges. Then*

$$GA \leq \sqrt{2H \cdot ISI}.$$

Equality holds if and only if $L(G)$ is a regular graph.

Proof. For $r = 1$, $x_i := \frac{\sqrt{d_i d_j}}{d_i + d_j}$, $a_i := \frac{1}{d_i + d_j}$, where summation goes over all adjacent vertices i and j of G, i.e. over all edges, the inequality (5) becomes

$$\sum_{i \sim j} \frac{d_i d_j}{d_i + d_j} \geq \frac{\left(\sum_{i \sim j} \frac{\sqrt{d_i d_j}}{d_i + d_j} \right)^2}{\sum_{i \sim j} \frac{1}{d_i + d_j}},$$

i.e.

$$ISI \geq \frac{(GA)^2}{2H},$$

which completes the proof. ∎

Theorem 4. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$GA \leq \frac{2(m-1)ISI}{RR} + \frac{2m\,(\Pi_2)^{\frac{1}{m}}}{RR\,(\Pi_1^*)^{\frac{1}{m}}} + \frac{\left(\sqrt{\Delta_{e_1}} - \sqrt{\delta_{e_1}}\right)^2 RR}{2\Delta_{e_1}\delta_{e_1}}. \qquad (46)$$

Equality holds if and only if $L(G)$ is a regular graph.

Proof. For $p_i := \sqrt{d_i d_j}$, $a_i = b_i := \frac{1}{\sqrt{d_i + d_j}}$, $r = \frac{1}{\sqrt{\Delta_{e_1}}}$, $R = \frac{1}{\sqrt{\delta_{e_1}}}$, where summation goes over all adjacent vertices of G, i.e. over all edges, the inequality (6) becomes

$$\sum_{i \sim j} \sqrt{d_i d_j} \sum_{i \sim j} \frac{\sqrt{d_i d_j}}{d_i + d_j} - \left(\sum_{i \sim j} \frac{\sqrt{d_i d_j}}{\sqrt{d_i + d_j}} \right)^2$$
$$\leq \frac{1}{4} \left(\frac{1}{\sqrt{\delta_{e_1}}} - \frac{1}{\sqrt{\Delta_{e_1}}} \right)^2 \left(\sum_{i \sim j} \sqrt{d_i d_j} \right)^2,$$

that is

$$\frac{1}{2}RR \cdot GA \le \left(\sum_{i\sim j}\sqrt{\frac{d_id_j}{d_i+d_j}}\right)^2 + \frac{\left(\sqrt{\Delta_{e_1}}-\sqrt{\delta_{e_1}}\right)^2 (RR)^2}{4\Delta_{e_1}\delta_{e_1}}. \tag{47}$$

For $a_i := \frac{d_id_j}{d_i+d_j}$ the right-hand part of inequality (4) becomes

$$\left(\sum_{i\sim j}\sqrt{\frac{d_id_j}{d_i+d_j}}\right)^2 \le (m-1)\sum_{i\sim j}\frac{d_id_j}{d_i+d_j} + m\left(\prod_{i\sim j}\frac{d_id_j}{d_i+d_j}\right)^{\frac{1}{m}},$$

i.e.

$$\left(\sum_{i\sim j}\sqrt{\frac{d_id_j}{d_i+d_j}}\right)^2 \le (m-1)ISI + m\frac{(\Pi_2)^{\frac{1}{m}}}{(\Pi_1^*)^{\frac{1}{m}}}. \tag{48}$$

Finally, from (47) and (48) we arrive at (46). ∎

Theorem 5. *Let G be a simple connected graph with $m \ge 2$ edges. Then*

$$GA \le \frac{2}{\Delta_{e_1}\delta_{e_1}}\left((\Delta_{e_1}+\delta_{e_1})\sqrt{(m-1)M_2 + m\,(\Pi_2)^{\frac{1}{m}}} - m\,(\Pi_2)^{\frac{1}{2m}}\,(\Pi_1^*)^{\frac{1}{m}}\right). \tag{49}$$

Equality holds if and only if $L(G)$ is regular.

Proof. For $p_i := \frac{\sqrt{d_id_j}}{\sum_{i\sim j}\sqrt{d_id_j}}$, $a_i := d_i + d_j$, $r = \delta_{e_1}$, $R = \Delta_{e_1}$, the inequality (7) transforms into

$$\sum_{i\sim j}\sqrt{d_id_j}(d_i+d_j) + \Delta_{e_1}\delta_{e_1}\sum_{i\sim j}\frac{\sqrt{d_id_j}}{d_i+d_j} \le (\Delta_{e_1}+\delta_{e_1})\sum_{i\sim j}\sqrt{d_id_j},$$

i.e.

$$\sum_{i\sim j}\sqrt{d_id_j}(d_i+d_j) + \frac{\Delta_{e_1}\delta_{e_1}}{2}GA \le (\Delta_{e_1}+\delta_{e_1})\sum_{i\sim j}\sqrt{d_id_j}. \tag{50}$$

Now, according to (44), (45) and (50) we obtain (49). ∎

Since $\sum_{i\sim j}\sqrt{d_id_j}(d_i+d_j) \ge \delta_{e_1}RR$, we get the next corollary of Theorem 5.

Corollary 3. *Let G be a simple connected graph with $m \ge 2$ edges. Then*

$$GA \le \frac{2RR}{\delta_{e_1}}.$$

Equality holds if and only if $L(G)$ is regular.

In the following theorem we establish an upper bound for GA in terms of m, M_2, F and Alb.

Theorem 6. *Let G be a simple connected graph with m edges. Then*

$$GA \leq \sqrt{m\left(m - \frac{(Alb)^2}{F + 2M_2}\right)}.$$

Equality holds if and only if $L(G)$ is a regular graph.

Proof. The following is valid

$$\begin{aligned} m^2 - (GA)^2 &= m^2 - \left(\sum_{i\sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j}\right)^2 \geq m^2 - m\sum_{i\sim j} \frac{4d_i d_j}{(d_i + d_j)^2} \\ &= m\sum_{i\sim j} \frac{(d_i - d_j)^2}{(d_i + d_j)^2}. \end{aligned} \tag{51}$$

For $r = 1$, $x_i := |d_i - d_j|$, $a_i := (d_i + d_j)^2$, from (5) we obtain

$$\sum_{i\sim j} \frac{(d_i - d_j)^2}{(d_i + d_j)^2} \geq \frac{\left(\sum_{i\sim j} |d_i - d_j|\right)^2}{\sum_{i\sim j} (d_i + d_j)^2},$$

i.e.

$$\sum_{i\sim j} \frac{(d_i - d_j)^2}{(d_i + d_j)^2} \geq \frac{(Alb)^2}{F + 2M_2}. \tag{52}$$

From (51) and (52) follows

$$m^2 - (GA)^2 \geq m\frac{(Alb)^2}{F + 2M_2},$$

wherefrom we obtain the desired result. ■

Since $d_i + d_j \leq \Delta_{e_1}$, we have the next corollary of Theorem 6.

Corollary 4. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$GA \leq \sqrt{m\left(m - \frac{F - 2M_2}{\Delta_{e_1}^2}\right)}. \tag{53}$$

Equality holds if and only if $L(G)$ is a regular graph.

Since $\Delta_{e_1} \leq 2\Delta$, according to (53) we get inequality (36).

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