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# On the first geometric–arithmetic index of graphs

K.Ch. Das [a], I. Gutman [b,*], B. Furtula [b]

[a] *Department of Mathematics, Sungkyunkwan University, Suwon, Republic of Korea*

[b] *Faculty of Science, University of Kragujevac, Kragujevac, Serbia*

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ABSTRACT

Let $G$ be a simple connected graph and $d_i$ be the degree of its $i$th vertex. In a recent paper [D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem. 46 (2009) 1369–1376] the "first geometric–arithmetic index" of a graph $G$ was defined as

$$GA_1 = \sum \frac{\sqrt{d_i\, d_j}}{(d_i + d_j)/2}$$

with summation going over all pairs of adjacent vertices. We obtain lower and upper bounds on $GA_1$ and characterize graphs for which these bounds are best possible. Moreover, we discuss the effect on $GA_1$ of inserting an edge into a graph.



## 1. Introduction

In the last few years, a large number of mathematical investigations were reported on graph invariants whose origin is from chemistry, and which are claimed to have chemical applications (see the books [9,14], the recent papers [1,2,6,4,11,16], and the references quoted therein). Quite a few of these graph invariants are based on vertex degrees (see e.g., [3,7,10,13]). A whole class of newly studied graph invariants are the "*geometric–arithmetic indices*" whose general definition is

$$GA_{general} = GA_{general}(G) = \sum_{v_i v_j \in E(G)} \frac{\sqrt{\mathcal{Q}_i \mathcal{Q}_j}}{\frac{1}{2}(\mathcal{Q}_i + \mathcal{Q}_j)} \tag{1}$$

where $\mathcal{Q}_i$ is some quantity that in a unique manner can be associated with the vertex $v_i$ of the graph $G$.

The name of this class of indices is evident from their definition. Namely, these are obtained from the ratio of geometric and arithmetic means of some properties of adjacent vertices.

The first $GA$-index was proposed by Vukičević and one of the present authors [15], and was simply named "*geometric–arithmetic index*". Since in the meantime at least two additional $GA$-indices were conceived, we now refer to the original $GA$-index as the "*first geometric–arithmetic index*" and denote it by $GA_1 = GA_1(G)$. It is defined as follows [15]:

$$GA_1 = GA_1(G) = \sum_{v_i v_j \in E(G)} \frac{\sqrt{d_i d_j}}{\frac{1}{2}(d_i + d_j)} \tag{2}$$

where $v_i v_j$ is an edge of the graph $G$ connecting the vertices $v_i$ and $v_j$, where $d_i$ stands for the degree of the vertex $v_i$, and where the summation goes over all edges of $G$. Needless to say that $GA_1$ is one more vertex-degree-based graph invariant.

* Corresponding author. Fax: +381 34335040.
*E-mail address:* gutman@kg.ac.rs (I. Gutman).

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The chemical applicability of the $GA_1$ index was examined and documented in detail in the paper [15] and the reviews [8,5].

This paper is organized as follows. In Section 2, we specify the notation used and provide the necessary definitions. In Section 3, we give lower and upper bounds on the $GA_1$ index of a connected graph, and characterize graphs for which these bounds are best possible. In Section 4, we discuss the change on $GA_1$ when an edge is inserted into the graph.

## 2. Preparations

Let $G = (V, E)$ be a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$, $|V(G)| = n$, and $|E(G)| = m$. Let $d_i$ be the degree of vertex $v_i$ for $i = 1, 2, \ldots, n$. The maximum vertex degree is denoted by $\Delta$, the minimum by $\delta$ and the minimum non-pendent vertex degree by $\delta_1$. The second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying graph $G$, that is, $M_2(G) = \sum_{v_iv_j\in E(G)} d_id_j$.

If the vertex set $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$, such that every vertex in $V_1(G)$ has degree $r$ and every vertex in $V_2(G)$ has degree $s \neq r$, then $G$ is said to be $(r, s)$-semiregular. When $r = s$, then $G$ is a regular graph (of degree $r$).

A vertex of a graph is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its vertices is a pendent vertex.

As usual, we denote by $K_n$ and $K_{a,b}$ the complete graph on $n$ vertices and the complete bipartite graph on $a + b$ vertices, with parts of size $a$ and $b$. In particular, $K_{1,n-1}$ the $n$-vertex star; all its edges are pendent.

## 3. Bounds on geometric–arithmetic index

In this section we establish lower bounds on $GA_1(G)$ of a graph $G$ in terms of number of vertices $n$, number of edges $m$, maximum vertex degree $\Delta$, minimum non-pendent vertex degree $\delta_1$, number of pendent vertices $p$, and the second Zagreb index $M_2$.

**Theorem 1.** *Let $G$ be a simple connected graph of order $n$ with $m$ edges, maximum degree $\Delta$, and minimum non-pendent vertex degree $\delta_1$. Then*

$$GA_1(G) \geq \frac{2p\sqrt{\Delta}}{\Delta+1} + \frac{1}{\Delta}\sqrt{M_2 - p\Delta + (m-p)(m-p-1)\delta_1^2}. \tag{3}$$

*The equality holds in (3) if and only if $G \cong K_{1,n-1}$ or $G$ is isomorphic to a regular graph or $G$ is isomorphic to a $(\Delta, 1)$-semiregular graph.*

**Proof.** For brevity write

$$\Xi_1 = \sum_{v_iv_j\in E(G),\ d_i,d_j>1} \frac{4d_id_j}{(d_i+d_j)^2}$$

$$\Xi_2 = \sum_{v_iv_j,v_kv_\ell\in E(G),\ d_i,d_j,d_k,d_\ell>1} \frac{4\sqrt{d_id_jd_kd_\ell}}{(d_i+d_j)(d_k+d_\ell)}$$

$$\Xi_3 = \sum_{v_iv_j\in E(G),\ d_i,d_j>1} d_id_j$$

$$\Xi_4 = \sum_{v_iv_j,v_kv_\ell\in E(G),\ d_i,d_j,d_k,d_\ell>1} \sqrt{d_id_jd_kd_\ell}.$$

Then we have

$$GA_1(G) = \sum_{v_iv_j\in E(G)} \frac{2\sqrt{d_id_j}}{d_i+d_j} \tag{4}$$

$$= \sum_{v_iv_j\in E(G),\ d_j=1} \frac{2\sqrt{d_id_j}}{d_i+d_j} + \sum_{v_iv_j\in E(G),\ d_i,d_j>1} \frac{2\sqrt{d_id_j}}{d_i+d_j}$$

$$\geq \frac{2p\sqrt{\Delta}}{\Delta+1} + \sqrt{\Xi_1 + 2\Xi_2} \quad \text{as } d_i \leq \Delta \tag{5}$$

$$\geq \frac{2p\sqrt{\Delta}}{\Delta+1} + \frac{1}{\Delta}\sqrt{\Xi_3 + 2\Xi_4} \tag{6}$$

$$\geq \frac{2p\sqrt{\Delta}}{\Delta+1} + \frac{1}{\Delta}\sqrt{M_2 - p\Delta + (m-p)(m-p-1)\delta_1^2} \quad \text{as } 1 \neq d_i \geq \delta_1. \tag{7}$$

Suppose now that equality holds in (3). Then all inequalities in the above argument must be equalities. In particular, from equality in (5), we get that $d_i = \Delta$ and $d_j = 1$ for each pendent edge $v_iv_j \in E(G)$.

Analogously, from equality in (6) it follows that $d_i = \Delta$ for each non-pendent vertex $v_i \in V(G)$, whereas equality in (7) implies that $d_i = \delta_1$ for each non-pendent vertex $v_i \in V(G)$.

We now need to distinguish between two cases (a) $m = p$ and (b) $m > p$.

*Case* (a): $m = p$, i.e., all the edges are pendent. Hence $G$ is isomorphic to the star $K_{1,n-1}$ as $G$ is assumed to be connected.

*Case* (b): $m > p$. If $p = 0$, then we have $\Delta = \delta_1$ and hence $G$ is isomorphic to a regular graph. Otherwise, $m > p > 0$. In this case we have $d_i = \Delta = \delta_1$ for non-pendent vertex $v_i \in V(G)$. Hence $G$ is isomorphic to a $(\Delta, 1)$-semiregular graph.

Conversely, one can easily see that the equality holds in (3) for the star $K_{1,n-1}$ or a regular graph or a $(\Delta, 1)$-semiregular graph. □

If in inequality (3), $\delta_1$ is replaced by $\delta$, then it holds as equality for the two-vertex graph $K_2$. In addition, by setting $p = 0$ into (3) and bearing in mind that $\delta \leq \delta_1$, we obtain the following.

**Corollary 2.** *Let G be a simple connected graph of order n with m edges, maximum degree $\Delta$, and minimum degree $\delta$. Then*

$$GA_1(G) \geq \frac{1}{\Delta}\sqrt{M_2 + m(m-1)\delta^2}$$

*with equality if and only if G is isomorphic to a regular graph.*

**Lemma 3** ([12]). *Let $(a_1, a_2, \ldots, a_n)$ be positive n-tuples such that there exist positive numbers A and a satisfying*

$$0 < a \leq a_i \leq A.$$

*Then*

$$\frac{n\sum_{i=1}^{n} a_i^2}{\left(\sum_{i=1}^{n} a_i\right)^2} \leq \frac{1}{4}\left(\sqrt{\frac{A}{a}} + \sqrt{\frac{a}{A}}\right)^2. \tag{8}$$

*The inequality becomes an equality if and only if $a = A$ or*

$$q = \frac{A/a}{A/a+1} n$$

*is an integer and q of the numbers $a_i$ coincide with a and the remaining $n - q$ of the $a_i$'s coincide with $A(\neq a)$.*

**Theorem 4.** *Let G be a simple connected graph of order $n(n > 2)$, with degree sequences $d_1, d_2, \ldots, d_n$. Then*

$$GA_1(G) \geq \frac{2p\sqrt{\Delta}}{\Delta+1} + \frac{\sqrt{8(\Delta+\delta_1)\sqrt{\Delta\delta_1}}}{(\sqrt{\Delta}+\sqrt{\delta_1})^2}\sqrt{(m-p)^2 - \frac{m-p}{4\delta_1^2}\left[\sum_{i=1}^{n} d_i^3 - 2M_2 - p(\delta_1 - 1)^2\right]}. \tag{9}$$

*The equality holds in (9) if and only if $G \cong K_{1,n-1}$ or G is isomorphic to a regular graph or G is isomorphic to a $(\Delta, 1)$-semiregular graph.*

**Proof.** For $\delta_1 \leq d_i, d_j \leq \Delta$, we have $\frac{\Delta}{\delta_1} \geq \frac{d_i}{d_j} \geq \frac{\delta_1}{\Delta}$ and thus

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{\frac{\Delta}{\delta_1}} - \sqrt{\frac{\delta_1}{\Delta}}.$$

This implies

$$\left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}\right)^2 = \left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}}\right)^2 + 4$$

$$\leq \left(\sqrt{\frac{\Delta}{\delta_1}} - \sqrt{\frac{\delta_1}{\Delta}}\right)^2 + 4 = \left(\sqrt{\frac{\Delta}{\delta_1}} + \sqrt{\frac{\delta_1}{\Delta}}\right)^2$$

and finally we get

$$\frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1} \leq \frac{2\sqrt{d_i d_j}}{d_i+d_j} \leq 1. \tag{10}$$

Now, since

$$\frac{2\sqrt{d_i d_j}}{d_i+d_j} = \sqrt{1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2}$$

and $m-p$ is the number of non-pendent edges in $G$, using (8) and (10) we get

$$\left(\sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1} \frac{2\sqrt{d_i d_j}}{d_i+d_j}\right)^2 \geq \frac{8(m-p)(\Delta+\delta_1)\sqrt{\Delta\delta_1}}{(\sqrt{\Delta}+\sqrt{\delta_1})^4} \sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1} \left[1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2\right]. \tag{11}$$

Now,

$$\begin{aligned}\sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1}(d_i-d_j)^2 &= \sum_{v_iv_j\in E(G)}(d_i-d_j)^2 - \sum_{v_iv_j\in E(G), d_j=1}(d_i-1)^2\\ &= \sum_{i=1}^n d_i^3 - 2\sum_{v_iv_j\in E(G)} d_id_j - \sum_{v_iv_j\in E(G), d_j=1}(d_i-1)^2\\ &\leq \sum_{i=1}^n d_i^3 - 2M_2(G) - p(\delta_1-1)^2\end{aligned}$$

and therefore,

$$\begin{aligned}\sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1}\left[1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2\right] &\geq m-p-\frac{1}{4\delta_1^2}\sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1}(d_i-d_j)^2\\ &\geq m-p-\frac{1}{4\delta_1^2}\left[\sum_{i=1}^n d_i^3 - 2M_2 - p(\delta_1-1)^2\right].\end{aligned} \tag{12}$$

Combining (12) with (11), we get

$$\sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1} \frac{2\sqrt{d_id_j}}{d_i+d_j} \geq \frac{\sqrt{8(\Delta+\delta_1)\sqrt{\Delta\delta_1}}}{(\sqrt{\Delta}+\sqrt{\delta_1})^2}\sqrt{(m-p)^2-\frac{m-p}{4\delta_1^2}\left[\sum_{i=1}^n d_i^3 - 2M_2 - p(\delta_1-1)^2\right]} \tag{13}$$

which implies

$$GA_1(G) = \sum_{v_iv_j\in E(G),\ d_i=1}\frac{2\sqrt{d_j}}{d_j+1} + \sum_{v_iv_j\in E(G),\ d_i,d_j\neq 1}\frac{2\sqrt{d_id_j}}{d_i+d_j}. \tag{14}$$

For $2 \leq d_j \leq \Delta$, we have

$$\frac{\sqrt{d_j}}{d_j+1} \geq \frac{\sqrt{\Delta}}{\Delta+1}.$$

By (13) and using (14), we get the required result (9).

Suppose now that equality holds in (9). Then all inequalities in the above argument must be equalities. In particular, from (12),

$$d_i = d_j = \delta_1 \quad \text{for any } v_iv_j \in E(G), d_i, d_j \neq 1, m-p > 0.$$

Also, we have

$$d_j = \Delta \quad \text{for } v_iv_j \in E(G), d_i = 1.$$

If $m = p$, then $n-1 \leq m = p \leq n-1$, as $G$ is connected. Hence $G$ is isomorphic to the star $K_{1,n-1}$. Otherwise, $m > p$. When $p = 0$, then $G$ is isomorphic to a regular graph. When $p \neq 0$, then $G$ is isomorphic to a $(\Delta, 1)$-semiregular graph, as $G$ is connected.

Conversely, one can easily see that the equality holds in (9) for the star $K_{1,n-1}$ or a $(\Delta, 1)$-semiregular graph or a regular graph. □

**Corollary 5.** *Let G be same as in Theorem 4, except that it has no pendent vertices. Then,*

$$GA_1(G) \geq \frac{\sqrt{8m(\Delta+\delta)\sqrt{\Delta\delta}}}{(\sqrt{\Delta}+\sqrt{\delta})^2}\sqrt{m-\frac{1}{4\delta^2}\left(\sum_{i=1}^{n} d_i^3-2M_2\right)}. \tag{15}$$

*Moreover, the equality holds in (15) if and only if G is isomorphic to a regular graph.*

**Proof.** The proof follows directly from Theorem 4. □

Note that if we permit pendent vertices, then in the case of the two-vertex graph $K_2$, formula (15) holds as equality.

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

$$GA_1(G) \geq \frac{2m\sqrt{2(n-1)}}{n+1} - 2p\left(\frac{\sqrt{2(n-1)}}{n+1} - \frac{\sqrt{n-1}}{n}\right). \tag{16}$$

*The equality holds in (16) if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$.*

**Proof.** For each pendent edge $v_iv_j \in E(G)$, we have either $d_i = 1$ or $d_j = 1$. Thus,

$$\frac{1}{n-1} \leq \frac{d_i}{d_j} \leq n-1$$

which implies

$$\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}} \leq \sqrt{n-1} - \sqrt{\frac{1}{n-1}}$$

$$\text{i.e., } \sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} = \sqrt{\left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}}\right)^2 + 4} \leq \sqrt{n-1} + \sqrt{\frac{1}{n-1}}$$

$$\text{i.e., } \frac{\sqrt{d_id_j}}{d_i+d_j} \geq \frac{\sqrt{n-1}}{n}. \tag{17}$$

Moreover, the equality holds in (17) if and only if $d_i = n-1$ and $d_j = 1$ for $d_i \geq d_j$.

For each non-pendent edge $v_iv_j \in E(G)$, we have

$$2 \leq d_i, d_j \leq n-1 \quad \text{i.e.,} \quad \frac{2}{n-1} \leq \frac{d_i}{d_j} \leq \frac{n-1}{2}.$$

Similarly as before we get

$$\frac{\sqrt{d_id_j}}{d_i+d_j} \geq \frac{\sqrt{2(n-1)}}{n+1}. \tag{18}$$

Moreover, the equality holds in (18) if and only if $d_i = n-1$ and $d_j = 2$ for $d_i \geq d_j$.

Since $G$ has $p$ pendent vertices, by (17) and (18), we obtain

$$\begin{aligned} GA_1(G) &= \sum_{v_iv_j \in E(G),\ d_j=1} \frac{2\sqrt{d_i\,d_j}}{d_i+d_j} + \sum_{v_iv_j \in E(G),\ d_i,d_j \neq 1} \frac{2\sqrt{d_id_j}}{d_i+d_j} \\ &\geq \frac{2\sqrt{n-1}}{n}p + \frac{2\sqrt{2(n-1)}}{n+1}(m-p). \end{aligned} \tag{19}$$

From (19) we arrive at (16).

Suppose now that equality holds in (16). Then equality holds in (19). If $p = 0$, then all the edges are non-pendent. From equality in (18), we have $d_i = n-1$ and $d_j = 2$ for each edge $v_iv_j \in E(G)$ and $d_i \geq d_j$, that is, there is a common neighbor between the vertices $v_i$ and $v_j$, for any edge $v_iv_j \in E(G)$. Thus $G$ is isomorphic to the complete graph $K_3$ as $G$ is connected.

Otherwise, $p > 0$. First we assume that $m = p$. Thus all the edges are pendent, and hence $G$ is isomorphic to the star $K_{1,n-1}$ as $G$ is connected. Next, assume that $m > p > 0$. In this case, the maximum degree vertex, say $v_i$, by equality in (17) has degree $n-1$. Thus $G$ is a supergraph of the star $K_{1,n-1}$. Since $m > p$, there exists at least one non-pendent edge in $G$, and hence two vertices, say, $v_j$ and $v_k$ adjacent to vertex $v_i$, are adjacent. By equality in (18), for the non-pendent edge $v_jv_k \in E(G)$, either $d_j = n-1$ or $d_k = n-1$. Thus we do not have any pendent vertex in $G$ as $d_i = n-1$, a contradiction.

Conversely, one can see easily that the equality holds in (16) for the star $K_{1,n-1}$ or the complete graph $K_3$. □

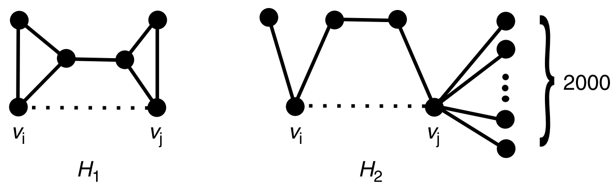


**Fig. 1.** By joining the vertices $v_i$ and $v_j$ by a new edge, in the case of $H_1$ the $GA_1$ index increases (from 6.919 to 7.919), whereas in the case of $H_2$ it decreases (from 92.38 to 92.34).

**Theorem 7.** *Let G be a simple connected graph. Then*

$$\frac{1}{\Delta}\sqrt{M_2+m(m-1)\delta^2} \le GA_1(G) \le \frac{1}{\delta}\sqrt{M_2+m(m-1)\Delta^2}. \tag{20}$$

*Moreover, the equality holds on both sides if and only if G is a regular graph.*

**Proof.** We have

$$[GA_1(G)]^2 = \sum_{v_iv_j\in E(G)} \frac{4d_id_j}{(d_i+d_j)^2} + 2\sum_{v_iv_j\neq v_kv_\ell} \frac{2\sqrt{d_id_j}}{d_i+d_j}\cdot\frac{2\sqrt{d_kd_\ell}}{d_k+d_\ell}. \tag{21}$$

Since $2\delta \le d_i+d_j \le 2\Delta$ for each edge $v_iv_j \in E(G)$, and $\delta \le d_i \le \Delta$ for each vertex $v_i \in V(G)$, (20) follows from (21).

Moreover, equality on the both sides of (20) holds if and only if $G$ is isomorphic to a regular graph. □

We now give an upper bound on the $GA_1$ index.

**Theorem 8.** *Let G be a simple connected graph with m edges and with minimum degree δ. Then*

$$GA_1(G) \le \frac{\sqrt{mM_2}}{\delta}. \tag{22}$$

*The equality holds in (22) if and only if G is isomorphic to a regular graph.*

**Proof.** By the Cauchy–Schwarz inequality,

$$\sum_{v_iv_j\in E(G)} \frac{2\sqrt{d_id_j}}{d_i+d_j} \le \sqrt{\sum_{v_iv_j\in E(G)} 4d_id_j \sum_{v_iv_j\in E(G)} \frac{1}{(d_i+d_j)^2}} \le \sqrt{\frac{mM_2}{\delta^2}}. \tag{23}$$

Moreover, equality holds in (23) if and only if $d_i = \delta$ for all $v_i \in V(G)$. Hence equality holds in (22) if and only if $G$ is isomorphic to a regular graph. □

## 4. Effect on $GA_1$ index of inserting an edge into the graph $G$

In this section we consider the change of the $GA_1$ index when a new edge is inserted into the underlying graph. Suppose that the vertices $v_i$ and $v_j$ of the graph $G$ are not adjacent, and insert a new edge $v_iv_j$ into $G$ to obtain the graph $G+\{v_iv_j\}$. In the general case, the transformation $G \to G+\{v_iv_j\}$ may either increase or decrease the $GA_1$-value.

In Fig. 1 are given two examples: in one the $GA_1$ index increases, whereas in the other it decreases when two nonadjacent vertices are joined by a new edge.

Theorem 10 provides a partial characterization of the graphs for which $GA_1(G+\{v_iv_j\}) > GA_1(G)$. The general solution of this problem remains open.

We first state the following elementary lemma.

**Lemma 9.** *Let*

$$f(x) = \frac{\sqrt{x}}{\sqrt{k+6x}}, \quad k > 0.$$

*Then $f(x)$ is an increasing function for $x > 0$.*

Now we are ready to prove the theorem.

**Theorem 10.** *Let G be a simple graph with nonadjacent vertices $v_i$ and $v_j$. Let $d_r = \max\{d_k \mid v_iv_k \in E(G)\}$ and $d_s = \max\{d_k \mid v_jv_k \in E(G)\}$. If*

$$\frac{d_i}{d_j} \le \min\left\{\frac{d_i}{d_r}, \frac{d_j}{d_s}\right\}$$

*then $GA_1(G+\{v_iv_j\}) > GA_1(G)$.*

**Proof.** We start by observing that

$$GA_1(G+\{v_iv_j\}) - GA_1(G) = 2\sum_{v_k\in N_i}\left[\frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1} - \frac{\sqrt{d_id_k}}{d_i+d_k}\right] + 2\sum_{v_k\in N_j}\left[\frac{\sqrt{(d_j+1)d_k}}{d_j+d_k+1} - \frac{\sqrt{d_jd_k}}{d_j+d_k}\right] + \frac{2\sqrt{(d_i+1)(d_j+1)}}{d_i+d_j+2} \tag{24}$$

where $N_i$ denotes the set of first neighbors of the vertex $v_i$.

Since

$$\sqrt{d_i+1} = \sqrt{d_i}\sqrt{1+\frac{1}{d_i}} \ge \sqrt{d_i}\left(1+\frac{1}{2d_i}-\frac{1}{8d_i^2}\right) = \sqrt{d_i}+\frac{1}{2\sqrt{d_i}}-\frac{1}{8d_i^{3/2}}$$

we have

$$\frac{\sqrt{d_id_k}}{d_i+d_k} - \frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1} \le \frac{\sqrt{d_i}(d_i+d_k+1)-(d_i+d_k)\left(\sqrt{d_i}+\frac{1}{2\sqrt{d_i}}-\frac{1}{8d_i^{3/2}}\right)}{(d_i+d_k)(d_i+d_k+1)}\sqrt{d_k}$$

$$= \frac{\left(d_i-d_k+\frac{d_i+d_k}{4d_i}\right)\sqrt{d_k}}{2\sqrt{d_i}(d_i+d_k)(d_i+d_k+1)}. \tag{25}$$

For $d_i \ge d_k$, we have to show that

$$\frac{\left(d_i-d_k+\frac{d_i+d_k}{4d_i}\right)\sqrt{d_k}}{2\sqrt{d_i}(d_i+d_k)(d_i+d_k+1)} < \frac{\sqrt{d_k}}{2d_i\sqrt{d_i+6d_k}}$$

that is,

$$\sqrt{(d_i+3d_k)^2-9d_k^2}\left(d_i-d_k+\frac{d_i+d_k}{4d_i}\right) < (d_i+d_k)(d_i+d_k+1)$$

that is,

$$\sqrt{(d_i+3d_k)^2-9d_k^2}\left(d_i-d_k+\frac{d_i+d_k}{4d_i}\right) < (d_i+3d_k)\left(d_i-d_k+\frac{d_i+d_k}{4d_i}\right) < (d_i+d_k)(d_i+d_k+1)$$

which, evidently, is always obeyed as $d_i \ge d_k$. For $d_i \ge d_k$, by Lemma 9 we have

$$\frac{\sqrt{d_id_k}}{d_i+d_k} - \frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1} < \frac{\sqrt{d_k}}{2d_i\sqrt{d_i+6d_k}} \le \frac{\sqrt{d_r}}{2d_i\sqrt{d_i+6d_r}}$$

as $d_r \ge d_k$ for all $v_k$ such that $v_iv_k \in E(G)$. Moreover, one can easily see that

$$\frac{\sqrt{d_id_k}}{d_i+d_k} - \frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1} < 0 \quad \text{for } d_k > d_i.$$

Thus,

$$\frac{\sqrt{d_id_k}}{d_i+d_k} - \frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1} < \frac{\sqrt{d_r}}{2d_i\sqrt{d_i+6d_r}}. \tag{26}$$

Let $t_1 = d_i/d_j$, $t_2 = d_i/d_r$, and $t_3 = d_j/d_s$. Then from (26) it follows

$$\sum_{v_k\in N_i}\left[\frac{\sqrt{d_jd_k}}{d_j+d_k} - \frac{\sqrt{(d_j+1)d_k}}{d_j+d_k+1}\right] < \frac{\sqrt{d_r}}{2\sqrt{d_i+6d_r}} = \frac{1}{2\sqrt{t_2+6}}. \tag{27}$$

Similarly,

$$\sum_{v_k\in N_i}\left[\frac{\sqrt{d_jd_k}}{d_j+d_k} - \frac{\sqrt{(d_j+1)d_k}}{d_j+d_k+1}\right] \le \frac{1}{2\sqrt{t_3+6}}. \tag{28}$$

Without loss of generality, we can assume that $t_2 \leq t_3$. Then,

$$\frac{1}{2\sqrt{t_2+6}} + \frac{1}{2\sqrt{t_3+6}} \leq \frac{1}{\sqrt{t_2+6}}. \tag{29}$$

By simple calculation, using $t_2 \geq t_1$, we get

$$\frac{1}{\sqrt{t_2+6}} < \frac{\sqrt{\left(t_1+\frac{1}{d_j}\right)\left(1+\frac{1}{d_j}\right)}}{t_1+1+2/d_j} = \frac{\sqrt{(d_i+1)(d_j+1)}}{d_i+d_j+2}. \tag{30}$$

Using (27)–(30), we get

$$\sum_{v_k\in N_i}\left[\frac{\sqrt{d_i d_k}}{d_i+d_k} - \frac{\sqrt{(d_i+1)d_k}}{d_i+d_k+1}\right] + \sum_{v_k\in N_j}\left[\frac{\sqrt{d_j d_k}}{d_j+d_k} - \frac{\sqrt{(d_j+1)d_k}}{d_j+d_k+1}\right] < \frac{\sqrt{(d_i+1)(d_j+1)}}{d_i+d_j+2}.$$

Combining the above inequality with Eq. (24) we arrive at Theorem 10. □

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## References

[1] X. Cai, B. Zhou, Reciprocal complementary Wiener numbers of trees, unicyclic graphs and bicyclic graphs, Discrete Appl. Math. 157 (2009) 3046–3054.
[2] P. Dankelmann, I. Gutman, S. Mukwembi, H.C. Swart, On the degree distance of a graph, Discrete Appl. Math. 157 (2009) 2773–2777.
[3] K.C. Das, Atom–bond connectivity index of graphs, Discrete Appl. Math. 158 (2010) 1181–1188.
[4] K.C. Das, I. Gutman, Estimating the Wiener index by means of number of vertices, number of edges, and diameter, MATCH Commun. Math. Comput. Chem. 64 (2010) 647–660.
[5] K.C. Das, I. Gutman, B. Furtula, Survey on geometric–arithmetic indices of graphs, MATCH Commun. Math. Comput. Chem. 65 (2011) 595–644.
[6] A. Dolati, I. Motevalian, A. Ehyaee, Szeged index, edge Szeged index, and semi-star trees, Discrete Appl. Math. 158 (2010) 876–881.
[7] B. Furtula, A. Graovac, D. Vukičević, Atom–bond connectivity index of trees, Discrete Appl. Math. 157 (2009) 2828–2835.
[8] B. Furtula, I. Gutman, in: I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors—Theory and Applications, vol. I, Univ. Kragujevac, Kragujevac, 2010, pp. 137–172.
[9] I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors—Theory and Applications vols. I–II, Univ. Kragujevac, Kragujevac, 2010.
[10] B. Horoldagva, S.G. Lee, Comparing Zagreb indices for connected graphs, Discrete Appl. Math. 158 (2010) 1073–1078.
[11] T. Pisanski, M. Randić, Use of the Szeged index and the revised Szeged index for measuring network bipartivity, Discrete Appl. Math. 158 (2010) 1936–1944.
[12] G. Pólya, G. Szegö, Probelms and Theorems in Analysis, in: Series, Integral Calculus, Theory of Functions, vol. I, Springer-Verlag, Berlin, 1972.
[13] L. Sun, T. Chen, Comparing the Zagreb indices for graphs with small difference between the maximum and minimum degrees, Discrete Appl. Math. 157 (2009) 1650–1654.
[14] R. Todeschini, V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley–VCH, Weinheim, 2009.
[15] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem. 46 (2009) 1369–1376.
[16] H. Zhang, Y. Yang, C. Li, Kirchhoff index of composite graphs, Discrete Appl. Math. 157 (2009) 2918–2927.