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On Third Geometric–Arithmetic Index of Graphs

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ABSTRACT

Continuing the work K. C. Das, I. Gutman, B. Furtula, On second geometric−arithmetic index of graphs, Iran. J. Math Chem., 1(2) (2010) 17−28, in this paper we present lower and upper bounds on the third geometric−arithmetic index GA_3 and characterize the extremal graphs. Moreover, we give Nordhaus−Gaddum−type result for GA_3.

Keywords: Graph; Molecular graph; First geometric−arithmetic index; Second geometric−arithmetic index; Third geometric−arithmetic index.

1 INTRODUCTION

In this work we are concerned with the *third geometric—arithmetic index* $GA_3(G)$, associated with the graph G. We use the same notation and terminology as in the preceding paper [1]. Thus, in particular, $V(G)$ and $E(G)$ denote the vertex and edge sets of G. Throughout this paper it is assumed that the graphs considered are connected.

The first and the second geometric−arithmetic index, GA_1 and GA_2 were [3], respectively. Additional mathematical recently put forward in [2] and of GA_1 and GA_2 are discussed in [4,6] and [1,3], respectively.

A further molecular structure descriptor, belonging to the class of GA−indices, is the so−called *third geometric−arithmetic index*, denoted as GA_3 [7]. In order to define it, some preparations need to be done.

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Let $ij \in E(G)$ be an edge of the graph G, connecting the vertices i and j. Let $x \in V(G)$ be any vertex of G. The distance between x and ij is denoted by $d(x,ij|G)$ and is defined as $\min\{d(x,i|G), d(x,j|G)\}$. For $ij \in E(G)$, let

$$m_i = |\{f \in E(G): d(i,f|G) < d(j,f|G\}|.$$

It is immediate to see that in all cases $m_i \geq 0$ and $m_i + m_j \leq m - 1$.

It should be noted that m_i is not a quantity that is in a unique manner associated with the vertex i of the graph G, but that it depends on the edge ij. Yet, this restriction is not relevant for the definition of GA_3.

$$GA_3 = GA_3(G) = \sum_{ij \in E(G)} \frac{\sqrt{m_i m_j}}{\frac{1}{2}[m_i + m_j]} . \tag{1}$$

Then the *third geometric–arithmetic index* is defined as

Similarly to GA_2 (cf. [1]), the GA_3-index is defined so as to be related to the recently conceived edge–Szeged index (Sz_e)[8] and edge–*PI* index (PI_e)[9].

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

Let K_n be the complete graph with n vertices, and let C_n be the cycle of length n. Let $K_{1,n-1}$ and P_n be the star and the path with n vertices, respectively. A tree is said to be starlike if exactly one of its vertices has degree greater than two. By $S(2r,s)$ ($r \geq 1,\ s \geq 1$), we denote the starlike tree with diameter less than or equal to 4, which has a vertex v_1 of degree $r + s$ and which has the property that $S(2r,s) \setminus \{v_1\} = \underbrace{P_2 \cup P_2 \cup \ldots \cup P_2}_{r} \cup \underbrace{P_1 \cup P_1 \cup \ldots \cup P_1}_{s}$. For additional details on $S(2r,s)$ see [1].

For $p,q \geq 2$, by $S_{\{p,q\}}$ we denote the $(p + q)$ – vertex tree formed by adding an edge between the centers of the stars $K_{1,p-1}$ and $K_{1,q-1}$.

This paper is organized as follows. In Section 2, we give lower and upper bounds on $GA_3(G)$ of connected graphs, and characterize the graphs for which these bounds are best possible. In Section 3, we present Nordhaus–Gaddum–type results for GA_3.

2 BOUNDS ON THIRD GEOMETRIC–ARITHMETIC INDEX

In this section we obtain lower and upper bounds on GA_3 of graphs. Recall that the edge–Szeged index of the graph G has been recently defined as [8]

$$Sz_e(G) = \sum_{ij \in E(G)} m_i m_j \ .$$

Recently, in [7], the following lower bound on $GA_3(G)$ was obtained:

$$GA_3(G) \geq \frac{2}{m-1}\sqrt{Sz_e(G)} \tag{2}$$

with equality if and only if G ≅ $K_{1,n-1}$or G ≅ $S_{p,m+p-1}$, 2 ≤ p ≤ $\left\lfloor\frac{(m+1)}{2}\right\rfloor$.

We now offer another lower bound:

Theorem 2.1. *Let G be a connected graph of order n > 2, with m edges edges and p pendent vertices. Then*

$$GA_3(G) \geq \frac{2(m-p)\sqrt{m-2}}{m-1} \tag{3}$$

Equality holds in (3) if and only if G ≅ $K_{1,n-1}$ *or G* ≅ K_3 *or G ≅ S(2r,s), n=2r+s+1.*

Proof: For each pendent edge ij ∈ E(G), it is either $m_i = 0$ or m_j= 0. Thus,

$$\frac{\sqrt{m_i m_j}}{m_i + m_j} = 0. \tag{4}$$

For each non–pendent edge *ij* ∈ *E*(*G*),

$$1 \leq m_i, m_j \leq m-2 \qquad i.e., \qquad \frac{1}{m-2} \leq \frac{m_i}{m_j} \leq m-2\,.$$

One can easily check that

$$\sqrt{\frac{m_i}{m_j}} - \sqrt{\frac{m_j}{m_i}} \leq \sqrt{m-2} - \frac{1}{\sqrt{m-2}}$$

that is,

$$\frac{\sqrt{m_i m_j}}{m_i+m_j} \geq \frac{\sqrt{m-2}}{m-1}. \tag{5}$$

Moreover, the equality holds in (5) if and only if m_i=m–2 and m_j=1 for $m_i \geq m_j$. Since G has *p* pendent vertices, by (4) and(5),

$$GA_2(G) = \sum_{ij\in E(j), d_j=1} \frac{2\sqrt{m_i m_j}}{m_i + m_j} + \sum_{ij\in E(j),\ d_i d_j \neq 1} \frac{2\sqrt{m_i m_j}}{m_i + m_j}$$
$$\geq \frac{2(m-p)\sqrt{m-2}}{m-1}.$$

Suppose now that equality holds in (3). Then all the inequalities in the above argument are equalities. So we must have for each non–pendent edge *ij* ∈ *E*(*G*) , $m_i = m-2$ and $m_j = 1$ for $m_i \geq m_j$. We need to consider two cases: (*a*) *p* = *m* and (*b*) *p* < *m*.

Case (a): p = m. In this case all the edges are pendent and therefore $G \cong K_{1,n-1}$.

Case (b): $p < m$. First we assume that $p = 0$. Thus all edges are non–pendent. Let g denote the girth in G. If $g \geq 5$ then there exists an edge $ij \in E(C_g)$, such that $m_i \geq 2$ and $m_j \geq 2$. This is a contradiction because of $m_i = 1$ or $m_j = 1$. If $g = 4$, then there exists an edge $ij \in E(C_g)$, such that $m_i \in m - 3$ and $m_j \in m - 3$. This again is a contradiction, because $m_i = m - 2$ or $m_j = m - 2$. Remains the case $g = 3$. Since $m_i = m - 2$ and $m_j = 1$, $m_i \geq m_j$, for each edge $ij \in E(G)$, we must have $G \cong K_3$.

Next we assume that $p > 0$. Since G is connected, a neighbor to a pendent vertex, say i, is adjacent to some non–pendent vertex k. Since ik is an non–pendent edge, it must be $m_i = 1$ or $m_k = 1$. Now, we have $d_i \geq 2$ and $d_k \geq 2$. If $d_i = 2$ and $d_k = 2$, then $G \cong P_4$ or $G \cong P_5$ as $m_i = m - 2$ and $m_k = 1$, $m_i \geq m_k$ for each non–pendent edge $ik \in E(G)$. If $d_i \geq 3$ and $d_k \geq 3$, then $m_i > 1$ and $m_k > 1$ for each non–pendent edge $ik \in E(G)$. This is a contradiction because $m_i = 1$ or $m_k = 1$ for any non–pendent edge $ik \in E(G)$. Otherwise, either the vertex i or the vertex k is of degree greater than or equal to 3. If $d_k \geq 3$ and $d_i = 2$, then $m_k = m - 2$ and $m_i = 1$ for the non–pendent edge $ik \in E(G)$. Thus we have the neighbor of a pendent vertex, namely the vertex i, is of degree 2 and adjacent to the vertex k. Similarly, we can show that each neighbor of a pendent vertex is of degree 2 and is adjacent to the vertex k. Also because $m_u = 0$ or $m_v = 0$ for each pendent edge $uv \in E(G)$,the remaining pendent vertices must be adjacent to vertex k. Hence G is isomorphic to a graph $S(2r,s)$, $n = 2r + s + 1$.

The other possible case is $d_k = 2$ and $d_i \geq 3$. Then k must be a neighbor of a pendent vertex and all the remaining pendent vertices are adjacent to vertex i. Hence $G \cong S(2,s)$, $n = s + 3$.

Conversely, one can easily see that equality in (10) holds for the star $K_{1,n-1}$ or the complete graph K_3 or S(2r,s) , n = 2 r + s + 1. □

Directly from Theorem 2.1 we get:

Corollary 2.2. [7] *The star $K_{1,n-1}$ is the connected n–vertex graph with minimum third geometric–arithmetic index.*

Corollary 2.3. *Let T be a tree of order $n > 2$ with p pendent vertices. Then*

$$GA_3(T) \geq \frac{2(n-p-1)\sqrt{n-3}}{n-2} \tag{6}$$

with equality in (6) if and only if $T \cong K_{1,n-1}$ or $T \cong S(2r,s)$, $n = 2r + s + 1$.

Now we give one more lower bound on $GA_3(T)$.

Theorem 2.4. *Let G be a connected graph of order $n > 2$ with m edges, p pendent vertices, and minimum non-pendent vertex degree δ_1. Then*

$$GA_3(T) \geq \frac{2}{m-1}\sqrt{\mathrm{Sz_e(G)} + (\mathrm{m}-\mathrm{p})(\mathrm{m}-\mathrm{p}-1)(\delta_1 - 1)^2} \qquad (7)$$

where $\mathrm{Sz_e}(\mathrm{G})$ is the edge–Szeged index of *G*. Moreover, the equality holds in (7) if and only if $G \cong K_{1,n-1}$ or $G \cong K_3$ or $G \cong S_{p,m+1-p}$, $2 \leq \mathrm{p} \leq \lfloor (m+1)/2 \rfloor$.

Proof: We have

$$GA_3(T) = \sum_{\mathrm{ij} \in \mathrm{E(G)}} \frac{2\sqrt{\mathrm{m_i\ m_j}}}{\mathrm{m_i} + \mathrm{m_j}} = \sum_{\mathrm{ij} \in \mathrm{E(G)},\, \mathrm{d_i},\mathrm{d_j}>1} \frac{2\sqrt{\mathrm{m_i\ m_j}}}{\mathrm{m_i} + \mathrm{m_j}}$$

$$= \sqrt{\sum_{\substack{\mathrm{ij} \in \mathrm{E(G)}, \\ \mathrm{d_i},\mathrm{d_j}>1}} \left[\frac{4\sqrt{\mathrm{m_i\ m_j}}}{(\mathrm{m_i}+\mathrm{m_j})^2}\right] + \sum_{\substack{\mathrm{ij,uv} \in \mathrm{E(G)}, \\ \mathrm{d_i},\mathrm{d_j},\mathrm{d_u},\mathrm{d_v}>1}} \left[\frac{8\sqrt{\mathrm{m_i\ m_j\ m_u\ m_v}}}{(\mathrm{m_i}+\mathrm{m_j})(\mathrm{m_u}+\mathrm{m_v})}\right]}$$

$$\geq \sqrt{4\frac{\mathrm{Sz_e(G)} + (\mathrm{m}-\mathrm{p})(\mathrm{m}-\mathrm{p}-1)(\delta_1-1)^2}{(\mathrm{m}-1)^2}} \qquad (8)$$

Because $m_i + m_j \leq m - 1$ for $ij \in E(G)$ and $m_i \geq \delta_1 - 1$ for all $i \in V(G)$.

Suppose now that equality holds in (7). Then all the inequalities in the above rgument are equalities. We need to consider two cases: (*a*) $p = m$ and (*b*) $p < m$.

Case (a): $p = m$. In this case all edges are pendent. Thus both sides of (7) are equal to zero and hence $\mathrm{G} \cong K_{1,n-1}$.

Case (b): $p < m$. First we assume that $p = 0$. In this case all the edges are non-pendent. From equality in (8) it follows $m_i + m_j = m - 1$ and $m_i = \delta_1 - 1$, $m_j = \delta_1 - 1$ for each edge $ij \in E(G)$. Therefore $\delta_1 = (m+1)/2$. If $n = 3$, then one can easily see that $G \cong K_3$. Otherwise, $n \geq 4$. Now,

$$2\mathrm{m} = \sum_{\mathrm{i}=1}^{\mathrm{n}} \mathrm{d_i} \geq n\delta_1 = \mathrm{n}(\mathrm{m}+1)/2$$

i. e., $4m \geq n(m+1)$, which is a contradiction as $\mathrm{n} \geq 4$.

Next we assume that $m > p > 0$. If there is only one non–pendent edge in *G*, then *G* is isomorphic to $S_{p,m+1-p}$, $2 \leq \mathrm{p} \leq \lfloor (m+1)/2 \rfloor$ and both sides of (7) are equal. Otherwise, *G* has at least two non–pendent edges. Then $m_i + m_j = m - 1$ and $m_i = \delta_1 - 1$, $m_j = \delta_1 - 1$, for each non–pendent edge $ij \in E(G)$. Again we have $\delta_1 = (m+1)/2$ and hence each non–pendent vertex degree is greater than or equal to $(m+1)/2$. Suppose that *ij* is a non-pendent edge of *G*. Then, $d_i, d_j \geq (m+1)/2$.

Since $d_i, d_j = m + 1$, all edges of *G* must be incident either to vertex *i* or to vertex *j* as $ij \in E(G)$. Also we have some common neighbor between vertices *i* and *j*, since there are at least two non–pendent edges. If k is the common neighbor between vertices i and j, then because of $p > 0$ it must be $d_i < (m+1)/2$, which is a contradiction.

Conversely, one can see easily that the equality in (7) holds for $K_{1,n-1}$ or K_3 or $S_{p,m+1-p}$, $2 \leq p \leq \lfloor (m+1)/2 \rfloor$. □

Remark 2.5. The lower bound (7) is better than (2).

Recently the following upper bound on GA_3 was obtained [7]:

$$GA_3(G) \leq \sqrt{\mathrm{Sz_e(G) + m(m-1)}} \tag{9}$$

with equality if and only if G is a triangle or a quadrangle.

Let Γ_1 be the class of graphs $H_1 = (V_1, E_1)$, such that H_1 is connected graph with $m_i = m_j$ for each edge $ij \in E(H_1)$. For example, K_n, $C_n \in \Gamma_1$. Denote by C_n^* , an unicyclic graph of order n and cycle length k, such that each vertex in the cycle is adjacent to one pendent vertex, $n = 2k$. Let Γ_2 be the class of graphs $H_2=(V_2, E_2)$, such that H_2 is connected graph with $m_i = m_j$ for each non–pendent edge $ij \in E(H_2)$. For example, $C_n^* \in \Gamma_2$. Now we are ready to state an upper bound on $GA_3(G)$.

Theorem 2.6. *Let G be a connected graph of order n>2 with m edges and p pendent vertices. Then*

$$GA_3(G) \leq m - p\,. \tag{10}$$

Equality holds in (10) if and only if $G \cong K_{1,n-1}$ *or* $G \in \Gamma_1$ *or* $G \in \Gamma_2$.

Proof: For each pendent edge $ij \in E(G)$ it is $m_i = m - 1$ and $m_j = 0$, $m_i \geq m_j$. For each non–pendent edge $ij \in E(G)$,

$$\frac{2\sqrt{\mathrm{m_i m_j}}}{\mathrm{m_i + m_j}} \leq 1. \tag{11}$$

From (11) inequality (10) follows straightforwardly.

Suppose now that equality holds in (10). From equality in (11), we get that $m_i = m_j$ holds for each non-pendent edge $ij \in E(G)$.

We need to consider two cases: (*a*) $p = 0$ and (*b*) $p > 0$.

Case (a): $p = 0$. In this case all edges are non–pendent. We have $m_i = m_j$ for each edge $ij \in E(G)$. Hence $G \in \Gamma_1$.

Case (b): $p > 0$. First we assume that $p = m$. Then all edges are pendent and hence $G \cong K_{1,n-1}$.

Next we assume that $p < m$. Then $m_i = m_j$ for each non–pendent edge $ij \in E(G)$, implying that $G \in \Gamma_2$.

Conversely, one can easily see that the equality in (10) holds for the star $K_{1,n-1}$. Let $G \in \Gamma_1$. Then p = 0 and $GA_3(G) = m$. Finally, let $G \in \Gamma_2$. Then $GA_3(G) = m - p$. □

Directly from Theorem 2.6 we obtain:

Corollary 2.7. [3] *Let G be a connected graph with m edges. Then*

$$GA_2(T) \leq m . \tag{12}$$

with equality in (*12*) *if and only if* $G \in \Gamma_1$.

Remark 2.8. *The upper bound* (10) *is better than* (9). *This is because*

$$(m-p)^2 \leq Sz_e(G) + m(m-1)$$

which, evidently, is always obeyed since $Sz_e(G) \geq m$.

2 Nordhaus–Gaddum–Type Results for the Third Geometric–Arithmetic Index

In [1] a brief survey can be found on the the work of Nordhaus and Gaddum [10] pertaining to properties of a graph G and its complement $\bar{G}$. This work served as a motivation for obtaining analogous statements for $GA_3(G) + GA_3(\bar{G})$.

Theorem 3.1. *Let G be a connected graph on n vertices with a connected complement* $\bar{G}$. *Then*

$$GA_3(G) + GA_3(\bar{G}) \geq \frac{2(\mathrm{m}-\mathrm{p})\sqrt{\mathrm{m}-2}}{\mathrm{m}-1} + \frac{2(\bar{m}-\bar{p})\sqrt{\bar{m}-2}}{\bar{m}-1}.$$

where p, $\bar{p}$ *and m,* $\bar{m}$ *are the number of pendent vertices and edges in G and* $\bar{G}$*, respectively.*

Proof: Theorem 3.1 is an immediate consequence of inequality (3). □

Theorem 3.2. *Let G be a connected graph on n vertices with a connected complement* $\bar{G}$. *Then*

$$GA_3(G) + GA_3(\bar{G}) \leq \binom{\mathrm{n}}{2} - (\mathrm{p} + \bar{p}) \tag{13}$$

Proof: By (10),

$$GA_3(G) + GA_3(\bar{G}) \le (\mathrm{m} + \bar{m}) - (\mathrm{p} + \bar{p})$$

One arrives at (13) by noting that $\mathrm{m} + \bar{m} = \binom{\mathrm{n}}{2}$. □

Directly from Theorem 3.2. follows:

Corollary 3.3. *Let G be a connected graph on n vertices with a connected complement* $\bar{G}$. *Then*

$$GA_3(G) + GA_3(\bar{G}) \le \binom{\mathrm{n}}{2}. \tag{14}$$

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