Iranian Journal of Mathematical Chemistry, Vol. 1, No. 2, September 2010, pp. 29−36 **IJMC**

On Third Geometric-Arithmetic Index of Graphs

KINKAR CH. DAS[1], IVAN GUTMAN[2,•] AND BORIS FURTULA[2]

[1]*Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
[2]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*

(*Received June 13, 2010*)

ABSTRACT

Continuing the work K. C. Das, I. Gutman, B. Furtula, On second geometric−arithmetic index of graphs, Iran. J. Math Chem., 1 (2010) 17–27, 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.

• Corresponding author (e-mail: gutman@kg.ac.rs).

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.

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

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 ≅ $\boldsymbol{K_{1,n-1}}$ or G ≅ $\boldsymbol{S_{p,m+p-1}}$, 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,

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

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 $S(2r,s)$, $n = 2r + s + 1$. □

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*

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

where $\mathrm{Sz_e(G)}$ 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

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

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

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

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,

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

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]:

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

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:

Corollary2.7. [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, $\bar{\mathrm{p}}$ *and m,* $\bar{\mathrm{m}}$ *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*

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

Acknowledgement. K. C. D. thanks the BK21 Math Modeling HRD Div. Sungkyunkwan University, Suwon, Republic of Korea. I. G. and B. F. thank the Serbian Ministry of Science for support, through Grant no. 144015G.

REFERENCES

1. K. C. Das, I. Gutman, B. Furtula, On second geometric--arithmetic index of graphs, *Iranian J. Math. Chem.* **1** (2010) 17–27.
2. 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.
3. G. Fath−Tabar, B. Furtula, I. Gutman, A new geometric--arithmetic index, *J. Math. Chem.* **47** (2010) 486–477.
4. K. C. Das, On geometric–arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 619−630.
5. M. Mogharrab, G. H. Fath-Tabar, Some bounds on GA_1 index of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 33–38.
6. Y. Yuan, B. Zhou, N. Trinajstić, On geometric–arithmetic index, *J. Math. Chem.* **47** (2010) 833−841.
7. B. Zhou, I. Gutman, B. Furtula, Z. Du, On two types of geometric–arithmetic index, *Chem. Phys. Lett.* **482** (2009) 153−155.
8. I. Gutman, A. R. Ashrafi, The edge version of the Szeged index *Croat. Chem. Acta* **81** (2008) 263–266.
9. P. V. Khadikar, On a novel structural descriptor PI, *Nat. Acad. Sci. Lett.* **23** (2000) 113−118.
10. E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Amer. Math. Monthly* **63** (1956) 175−177.