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 GA₃ and characterize the extremal graphs. Moreover, we give Nordhaus–Gaddum–type result for GA₃.

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 GA₃(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, GA₁ and GA₂ were [3], respectively. Additional mathematical recently put forward in [2] and of GA₁ and GA₂ 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 GA₃ [7]. In order to define it, some preparations need to be done.
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 \( GA_3 \).

\[
GA_3 = GA_3(G) = \sum_{ij \in E(G)} \frac{\sqrt{m_i m_j}}{2[m_i + m_j]}. 
\] (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 pendant vertex is a vertex of degree one. An edge of a graph is said to be pendant if one of its vertices is a pendant 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 \( S(2r,s) \setminus \{v_1\} = P_2 \cup P_2 \cup ... \cup P_2 \cup P_1 \cup P_1 \cup ... \cup P_1 \). 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:
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\[ GA_3(G) \geq \frac{2}{m-1} \sqrt{S_z(G)} \tag{2} \]

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

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 \( G \cong K_{1,n-1} \) or \( G \cong K_3 \) or \( G \cong S(2r,s), n=2r+s+1 \).

**Proof:** For each pendent edge \( ij \in E(G) \), 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 \( ij \in E(G) \),

\[ 1 \leq m_i, m_j \leq m - 2 \quad i.e., \quad \frac{1}{m - 2} \leq \frac{m_i}{m_j} \leq m - 2. \]

One can easily check that

\[ \frac{\sqrt{m_i m_j}}{m_i + m_j} \geq \frac{\sqrt{m-2}}{m-1} \tag{5} \]

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),

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

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 \( ij \in E(G) \), \( m_i = m-2 \) 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 \( m_j = 1 \), 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 a 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 \( m_k = 1 \), \( m_i = m_k \) 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, $p$ pendant vertices, and minimum non-pendent vertex degree $\delta_1$. Then

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

(7)

where $Sz_e(G)$ 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 $G \cong S_{p,m+1-p}$, $2 \leq p \leq \lfloor (m + 1)/2 \rfloor$.

Proof: We have

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

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

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

(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 argument 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 pendant. Thus both sides of (7) are equal to zero and hence $G \cong K_{1,n-1}$.

Case (b): $p < m$. First we assume that $p = 0$. In this case all the edges are non-pendant. 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,

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

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

Next we assume that $m > p > 0$. If there is only one non-pendent edge in $G$, then $G$ is isomorphic to $S_{p,m+1-p}$, $2 \leq p \leq \lfloor (m + 1)/2 \rfloor$ 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]:

\[
GA_3(G) \leq \sqrt{Sz_e(G)} + m(m - 1)
\]  

(9)

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

Let \( \Gamma_1 \) 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 \( \Gamma_2 \) 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

\[
GA_3(G) \leq m - p.
\]  

(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 \( ij \in E(G) \),

\[
\frac{2\sqrt{m_i m_j}}{m_i + m_j} \leq 1.
\]  

(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

$$GA_2(T) \leq m.$$  

(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

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

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).\[ \square \]

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

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

(13)
Proof: By (10),
\[ GA_3(G) + GA_3(\bar{G}) \leq (m + \bar{m}) - (p + \bar{p}) \]

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

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
\[ GA_3(G) + GA_3(\bar{G}) \leq \binom{n}{2}. \]  

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