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On Second Geometric–Arithmetic Index of Graphs

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ABSTRACT

The concept of geometric–arithmetic indices (GA) was put forward in chemical graph theory very recently. In spite of this, several works have already appeared dealing with these indices. In this paper we present lower and upper bounds on the second geometric–arithmetic index (GA_2) and characterize the extremal graphs. Moreover, we establish Nordhaus–Gaddum–type results for GA_2.

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

1 INTRODUCTION

Molecular structure descriptors play a significant role in mathematical chemistry, especially in the QSPR/QSAR investigations. Among them, special place is reserved for so−called topological descriptors. Nowadays, there exists a legion of topological indices that found some applications in chemistry [2−4]. These can be classified by the structural properties of graphs used for their calculation. Hence, probably the best known and widely used Wiener index [5] is based on topological distance of vertices in the respective molecular graph, the Hosoya index [6] is calculated counting of non-incident edges in a graph, the energy [7] and the Estrada index [8] are based on the spectrum of the graph, the Randić connectivity index [9] and the Zagreb group indices [10] are calculated using the degrees of vertices, etc.

Here, a new class of topological descriptors, based on some properties of vertices of graph is presented. These indices are named as "*geometric–arithmetic indices*" ($GA_{general}$) and their definition is as follows [1]:

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$$GA_{general} = GA_{general}(G) = \sum_{ij \in E(G)} \frac{\sqrt{Q_i Q_j}}{\frac{1}{2}(Q_i + Q_j)} \tag{1}$$

where Q_i is some quantity that in a unique manner can be associated with the vertex i of the graph G.

The name of this class of indices is evident from their definition. Namely, indices belonging to this group are calculated as the ratio of geometric and arithmetic means of some properties of adjacent vertices i and j (vertices i and j that are connected by an edge). The summation goes over all edges of the underlying graph G. Three members of GA−type topological indices have been put forward up to now.

The first member [11] and the third member [12] are the so−called *first geometric−arithmetic index* GA_1 and *third geometric−arithmetic index* GA_3, respectively. Mathematical properties for GA_1 and GA_3 are discussed in [13−15] and [12], respectively; see also [16].

Another member of this class we denote by GA_2 and is −tentatively− referred to as the *second geometric−arithmetic index*. Whereas GA_1 is defined so as to be related to the famous Randić index [9], GA_2 is constructed in such a manner that it is related with Szeged [17] and vertex−PI [18,19] indices.

Let G be a connected graph with n vertices and m edges, with vertex set $V(G)$ = {1,2,…,n} and edge set $E(G)$. As usual [20], the distance $d(x,y|G)$ between two vertices $x, y \in V(G)$ is defined as the length (= number of edges) of the shortest path that connects x and y. Let $e=ij$ be an edge of G, connecting the vertices i and j. Define the sets

$$\mathrm{N}(e,i,G) = \{ x \in V(G) \mid d(x,i|G) < d(x,j|G) \}$$
$$\mathrm{N}(e,j,G) = \{ x \in V(G) \mid d(x,i|G) > d(x,j|G) \}$$

consisting, respectively, of vertices of G lying closer to i than to j, and lying closer to j than to i. The number of such vertices is then

$$n_i(e) = n_i(e,G) = |\mathrm{N}(e,i,G)| \qquad \text{and} \qquad n_j(e) = n_j(e) = |\mathrm{N}(e,j,G)|. \tag{2}$$

Note that vertices equidistant to i and j are not included into either $\mathrm{N}(e,i,G)$ or $\mathrm{N}(e,j,G)$. Such vertices exist only if the edge ij belongs to an odd-membered cycle. Hence, in the case of bipartite graphs, $\mathrm{N}(e,i,G) \cup \mathrm{N}(e,j,G) = V(G)$ and, consequently,

$$n_i(e,G) + n_j(e,G) = n \tag{3}$$

for all edges of the graph G.

It is also worth noting that $i \in \mathrm{N}(e,i,G)$ and $j \in \mathrm{N}(e,j,G)$, which implies that $n_i(e) \geq 1$ and $n_j(e) \leq 1$.

Motivated by the expressions for calculation of Szeged (Sz) and recently introduced vertex–PI indices (PI_v), and in view of the general formula (1), the *second geometric–arithmetic index* is defined as

$$GA_2 = GA_2(G) = \sum_{ij\in E(G)} \frac{\sqrt{n_i.n_j}}{\frac{1}{2}[n_i+n_j]}.. \tag{4}$$

This paper is organized as follows. In Section 2, we give lower and upper bounds on $GA_2(G)$ of a connected graph, and characterize graphs for which these bounds are best possible. In Section 3, we present Nordhaus–Gaddum–type results for $GA_2(G)$.

2 BOUNDS ON SECOND GEOMETRIC–ARITHMETIC INDEX

In this section we obtain lower and upper bounds on GA_2 of graphs and trees. 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. Recall that the Szeged index of the graph G is defined as

$$Sz(G) = \sum_{ij\in E(G)} n_i n_j.$$

Now we give lower bound on GA_2.

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

$$GA_2(G) \geq \frac{2m\sqrt{n-2}}{n-1} - 2p\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right). \tag{5}$$

Equality holds in (5) *if and only if* $G \simeq K_{1,n-1}$ *or* $G \simeq K_3$.

Proof: When $G \simeq K_2$, the equality holds in (5). Otherwise, $n \geq 3$. For each edge $ij \in E(G)$, we have

$$1 \leq n_i,\ n_j \leq n-1 \qquad i.e., \quad \frac{1}{n-1} \leq \frac{n_i}{n_j} \leq n-1.$$

From above we get

$$\sqrt{\frac{n_i}{n_j}} - \sqrt{\frac{n_j}{n_i}} \leq \sqrt{n-1} - \sqrt{\frac{1}{n-1}}$$

$$i.e., \quad \sqrt{\frac{n_i}{n_j}} + \sqrt{\frac{n_j}{n_i}} = \sqrt{\left(\sqrt{\frac{n_i}{n_j}} - \sqrt{\frac{n_j}{n_i}}\right)^2 + 4} \leq \sqrt{n-1} + \sqrt{\frac{1}{n-1}}$$

$$i.e., \quad \frac{\sqrt{n_i n_j}}{n_i+n_j} \geq \frac{\sqrt{n-1}}{n}. \tag{6}$$

Moreover, the equality holds in (6) if and only if $n_i = n - 1$ and $n_j = 1$ for $n_i \geq n_j$, that is, if and only if ij is a pendent edge.

For each non–pendent edge $ij \in E(G)$,

$$1 \leq n_i,\ n_j \leq n-2 \qquad i.e., \quad \frac{1}{n-2} \leq \frac{n_i}{n_j} \leq n-2.$$

Similarly,

$$\frac{\sqrt{n_i n_j}}{n_i+n_j} \geq \frac{\sqrt{n-2}}{n-1} \tag{7}$$

Moreover, the equality holds in (7) if and only if $n_i = n - 2$ and $n_j = 1$ for $n_i \geq n_j$.

Since G has p pendent vertices, by (6) and (7) we obtain

$$\begin{aligned} GA_2(G) &= \sum_{ij \in E(G), d_j = 1} \frac{2\sqrt{n_i n_j}}{n_i + n_j} + \sum_{ij \in E(G), d_i, d_j \neq 1} \frac{2\sqrt{n_i n_j}}{n_i + n_j} \\ &\geq \frac{2\sqrt{n-1}}{n}\, p + \frac{2\sqrt{n-2}}{n-1}(m-p). \end{aligned} \tag{8}$$

From (8) we arrive at (5).

Suppose now that equality holds in (5). Then equality holds in (8). We need to consider two cases: (a) $p = 0$ and (b) $p > 0$.

Case (*a*): $p = 0$. In this case all the edges are non–pendent edges. From equality in (7), we have $n_i = n - 2$ and $n_j = 1$ for each edge $ij \in E(G)$ and $n_i \geq n_j$, that is, one vertex is common between vertices i and j, for any edge $ij \in E(G)$.Thus $G \cong K_3$ as G is connected.

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

Next we assume that $p < m$. In this case there is a neighbor of a pendent vertex, say i, adjacent to some non–pendent vertex k. If there is a common neighbor vertex s between vertices i and k, then $n_k + n_s \leq n - 2$ for the non–pendent edge $ks \in E(G)$, as the pendent vertex adjacent to i is at the same shortest distance from vertices k and s, and vertex i is common neighbor of k and s. So, either $n_k \leq n - 3$ or $n_s \leq n - 3$. This is a contradiction because $n_k = n - 2$ or $n_s = n - 2$ for each non–pendent edge $ks \in E(G)$. Otherwise, there is no common neighbor between vertices k and s. Since the vertex k is non–pendent, $n_i \geq 2$ and $n_k \geq 2$, for non-pendent edge $ik \in E(G)$. This is a contradiction, because $n_i = 1$ or $n_k = 1$ for the non–pendent edge $ik \in E(G)$.

Conversely, one can easily see that the equality in (5) holds for the star $K_{1,n-1}$ or the complete graph K_3. □

Corollary 2.2. [1] *Let G be a connected graph of order n with m edges. Then*

$$GA_2(G) \geq \frac{2m\sqrt{n-1}}{n} \tag{9}$$

with equality in (9) if and only if $G \cong K_{1,n-1}$.

Proof: For $G \cong K_2$, the equality holds in (9). Otherwise, $n \geq 3$. We can easily see that

$$\frac{\sqrt{n-2}}{n-1} \geq \frac{\sqrt{n-1}}{n} \qquad for \quad n \geq 3.$$

From this we get the required result (9). Moreover, by Theorem 2.1, the equality holds in (9) if and only if $G \cong K_{1,n-1}$.

Corollary 2.3. [1] *Let G be a connected graph of order n with m edges. Then*

$$GA_2(G) \geq \frac{2}{n}\sqrt{Sz + m(m-1)} \tag{10}$$

where $Sz(G)$ *is the Szeged index of G. Moreover, the equality holds in (10) if and only if* $G \cong K_2$.

Proof: Now we have to show that

$$\frac{2m\sqrt{n-1}}{n} \geq \frac{2}{n}\sqrt{Sz(G) + m(m-1)}$$

that is,

$$Sz(G) \leq m[m(n-2) + 1]$$

which, evidently, is always obeyed as $m \geq n - 1$ and $n_i\, n_j \leq (n-1)(n-2) + 1$ for each edge $ij \in E(G)$. Combining the above result with (9), we obtain (10).

Corollary 2.4. [1] *The star* $K_{1,n-1}$ *is the connected n–vertex graph with minimum second geometric–arithmetic index.*

Proof: Since G is connected, we have $m \geq n-1$ and $p \leq n-1$. Again, since

$$\frac{\sqrt{n-2}}{n-1} \geq \frac{\sqrt{n-1}}{n}$$

from (5) it follows

$$GA_2(G) \geq \frac{2m\sqrt{n-2}}{n-1} - 2p\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right)$$

$$\geq \frac{2(n-1)^{3/2}}{n} \quad as\ m \geq n-1 \ \ and\ p \leq n-1.$$

By Theorem 2.1, $GA_2(G) \geq \frac{2(n-1)^{3/2}}{n}$ with equality if and only if $G \cong k_{1,n-1}$. Hence the result.

Corollary 2.5. [1] *The star $K_{1,n-1}$ is the n–vertex tree with minimum second geometric–arithmetic index.*

Corollary 2.6. *Let T be a tree of order $n > 2$ with p pendent vertices. Then*

$$GA_2(T) \geq 2\sqrt{n-2} - 2p\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right) \tag{11}$$

with equality in (11) if and only if $T \cong K_{1,n-1}$.

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 $v1$ of degree $r + s$ and which has the property $S(2r,s)\backslash\{v_1\}=\underbrace{P_2 \cup P_2 \cup \ldots \cup P_2}_{r} \cup \underbrace{P_1 \cup P_1 \cup \ldots \cup P_1}_{s}$ This tree has $2r + s + 1 = n$ vertices. We say that the starlike tree $S(2r, s)$ has $r+s$ branches, the lengths of which are $\underbrace{2,2,\ldots,2}_{r}$, $\underbrace{1,1,\ldots,1}_{s}$ respectively. Now we give a lower bound on $GA_2(T)$ of any tree T.

Theorem 2.7. *Let T be a tree of order $n > 2$ with p pendent vertices. Then*

$$GA_2(T) \geq \frac{2m\sqrt{2(n-2)}}{n} - \frac{2p}{n}\left(\sqrt{2(n-2)} - \sqrt{n-1}\right) \tag{12}$$

with equality in (12) if and only if $G \cong K_{1,n-1}$ or $G \cong S(2r, s)$, $n = 2r + s + 1$.

Proof: For each edge $ij \in E(T)$, from (6) we have

$$\frac{\sqrt{n_i n_j}}{n_i + n_j} \geq \frac{\sqrt{n-1}}{n}$$

with equality if and only if $n_i = n - 1$ and $n_j = 1$ for $n_i \geq n_j$, that is, if and only if the edge ij is pendent.

For each non–pendent edge $ij \in E(T)$, we have

$$2 \leq n_i, n_j \leq n-2 \quad i.e., \qquad \frac{2}{n-2} \leq \frac{n_i}{n_j} \leq \frac{n-2}{2}$$

We can easily see that for each non–pendent edge $ij \in E(T)$,

$$\frac{\sqrt{n_i n_j}}{n_i + n_j} \geq \frac{\sqrt{2(n-2)}}{n}. \tag{13}$$

Moreover, the equality holds in (13) if and only if $n_i = n - 2$ and $n_j = 2$ for $n_i \geq n_j$.

Since T has p pendent vertices, by (13) we obtain

$$\begin{aligned} GA_2(T) &= \sum_{ij \in E(T),\, d_j = 1} \frac{2\sqrt{n_i n_j}}{n_i + n_j} + \sum_{ij \in E(G),\, d_i, d_{j \neq 1}} \frac{2\sqrt{n_i n_j}}{n_i + n_j} \\ &\geq \frac{2\sqrt{n-1}}{n} p + \frac{2\sqrt{2(n-2)}}{n}(m-p) \end{aligned} \tag{14}$$

From (14) we arrive at (12).

Suppose now that equality holds in (12). Then equality holds in (14). We need to consider two cases: (a) $p = m$ and (b) $p < m$.

Case (a): $p = m$. From equality in (14), we must have $n_i = n - 1$ and $n_j = 1$ for each edge $ij \in E(G)$ and $n_i \geq n_j$, that is, each edge ij must be pendent. Since T is a tree, $T \cong K_{1,n-1}$.

Case (b): $p < m$. In this case the diameter of T is strictly greater than 2. So there is a neighbor of a pendent vertex, say i , adjacent to some non-pendent vertex k . Since $n_i = n - 2$ and $nj = 2$ for each non–pendent edge $ij \in E(T)$, $n_i \geq n_j$, we conclude that the degree of each neighbor of a pendent vertex is two and each such vertex is adjacent to vertex k. In addition, also the remaining pendent vertices are adjacent to vertex k. Hence T is isomorphic to $S(2r, s)$, $n = 2r + s + 1$.

Conversely, one can see easily that the equality in (12) holds for star $K_{1,n-1}$ or $S(2r, s)$, $n = 2r + s + 1$. □

Let Γ_1 be the class of graphs $H_1 = (V_1,E_1)$ such that H_1 is connected graph with $n_i = n_j$ for each edge $ij \in E(H_1)$. For example, $K_{1,n-1}$,$K_n \in \Gamma_1$. Denote by C_n^*, a 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 $n_i = n_j$ for each non-pendent edge $ij \in E(H_2)$. For example, $C_n^* \in \Gamma_2$.

Theorem 2.8. *Let G be a connected graph of order $n > 2$ with m edges and p pendent vertices. Then*

$$GA_2(G) \le \frac{2p\sqrt{n-1}}{n} + m - p \tag{15}$$

Equality in (15) holds 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 $ij \in E(G)$, we have $n_i = 1$ and $n_j = n-1$. Now,

$$GA_2(G) = \frac{2p\sqrt{n-1}}{n} + \sum_{ij \in E(G), d_i, d_j \neq 1} \frac{2\sqrt{n_i n_j}}{n_i + n_j}$$
$$\le \frac{2p\sqrt{n-1}}{n} + m - p.$$

Suppose now that equality holds in (15). Then equality holds in (16). From equality in (16), we get $n_i = n_j$ 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 the edges are non–pendent. We have $n_i = n_j$ for each edge $ij \in E(G)$. Hence $G \in \Gamma_1$.

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

Next we assume that $p < m$. Now we have $n_i = n_j$ for each non–pendent edge $ij \in E(G)$. Hence $G \in \Gamma_2$.

Conversely, one can easily see that the equality in (15) holds for the star $K_{1,n-1}$. Now let $G \in \Gamma_1$. Then $p = 0$ and $GA_2(G) = m$ holds. Finally, let $G \in \Gamma_2$. Then $GA_2(G) = \frac{2p\sqrt{n-1}}{n} + m - p$. □

Corollary 2.9. [1] *Let G be a connected graph with m edges. Then*

$$GA_2(G) \le m \tag{17}$$

with equality in (17) if and only if $G \in \Gamma_1$.

Proof: Since

$$\frac{2\sqrt{n-1}}{n} \le 1 \quad as \ \ n > 2$$

from Theorem 2.8, we get the required result. □

Corollary 2.10. *Let G be a connected graph with m edges. Then* *with equality if and only if* $G \cong K_n$.

Proof: Since G is a connected graph, we have

$$Sz(G) \geq m \qquad i.e., \qquad m \leq \sqrt{mSz(G)}$$

Combining this with (17), we get the required result. Moreover, equality holds in above if and only if $G \cong K_n$. Hence the result. □

Corollary 2.11. *Let G be a connected graph with m edges. Then*

$$GA_2(G) \leq \sqrt{Sz(G) + m(m-1)}$$

with equality if and only if $G \cong K_n$.

Proof: From $Sz(G) \geq m$ it follows

$$m \leq \sqrt{Sz(G) + m(m-1)}$$

which together with (17) yields the required result. Moreover, the equality holds if and only if $G \cong K_n$. □

Remark 2.12. *The upper bounds in Corollaries 2.10 and 2.11 are trivial, because both are greater than or equal to m. On the other hand, because the arithmetic mean is never smaller than the geometric mean,* $GA_2(G) \leq m$ *holds in an evident manner.*

3 Nordhaus–Gaddum–Type Results For The Second Geometric–Arithmetic Index

For a graph G, the chromatic number $\chi(G)$ is the minimum number of colors needed to color the vertices of G in such a way that no two adjacent vertices are assigned the same color. In 1956, Nordhaus and Gaddum [22] gave bounds involving the chromatic number $\chi(G)$ of a graph G and its complement $\bar{G}$:

$$2\sqrt{n} \leq \chi(G) + \chi(\bar{G}) \leq n + 1$$

Motivated by the above results, we now obtain analogous conclusions for the second geometric–arithmetic index.

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

$$GA_2(G) + GA_2(\bar{G}) > \frac{2\sqrt{n-2}}{n-1}\binom{n}{2} - 2(P + \bar{P})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right) \tag{18}$$

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

Proof: We have $\overline{m}$+m =$\binom{n}{2}$ where $\overline{m}$ is the number of edges in $\overline{G}$. Using (5), we get

$$GA_2(G) + GA_2(\bar{G}) \geq \frac{2\sqrt{n-2}}{n-1}(m+\overline{m}) - 2(P+\bar{P})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right)$$
$$= \frac{2\sqrt{n-2}}{n-1}\binom{n}{2} - 2(P+\bar{P})\left(\frac{\sqrt{n-2}}{n-1} - \frac{\sqrt{n-1}}{n}\right) \quad (19)$$

Inequality (18) follows now from Theorem 2.1. □

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

$$GA_2(G) + GA_2(\bar{G}) \leq \binom{n}{2} - (P+\bar{P})\left(1 - \frac{2\sqrt{n-1}}{n}\right) \quad (20)$$

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

Proof: By (15), we get

$$GA_2(G) + GA_2(\bar{G}) \leq \frac{2\sqrt{n-1}}{n}(P+\bar{P}) + (m+\overline{m}) - (P+\bar{P})$$
$$= \binom{n}{2} - (P+\bar{P})\left(1 - \frac{2\sqrt{n-1}}{n}\right)$$

since $m + \overline{m} = \binom{n}{2}$. □

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

$$GA_2(G) + GA_2(\bar{G}) \leq \binom{n}{2} \quad (21)$$

Proof: The proof follows directly from Theorem 3.2. □

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