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Geometric–Arithmetic Index and Minimum Degree of Connected Graphs

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Abstract

In the present paper, we prove lower and upper bounds for each of the ratios GA/δ, as well as a lower bound on $GA/\sqrt{\delta}$, in terms of the order n, over the class of connected graphs on n vertices, where GA and δ denote the geometric-arithmetic index and the minimum degree, respectively. We also characterize the extremal graphs corresponding to each of those bounds. In order to prove our results, we provide a modified statement of a well-known lower bound on the geometric-arithmetic index in terms of minimum degree.

1 Introduction and definitions

We begin by recalling some definitions. In this paper, we consider only simple, undirected and finite graphs, *i.e*, undirected graphs on a finite number of vertices without multiple edges or loops. A graph is (usually) denoted by $G = G(V, E)$, where V is its vertex set and E its edge set. The *order* of G is the number $n = |V|$ of its vertices and its *size* is the number $m = |E|$ of its edges. For two vertices u and v $(u, v \in V)$, if $uv \in E$, we say u and v are *adjacent* in G. The *degree* of a vertex u, denoted d_u, is the number of vetices adjacent to it in G. A graph G is said to be *regular* of degree d, or d-*regular* if $d_u = d$ for every vertex u in G. The minimum degree in a graph G is denoted by δ. As usual, we denote by S_n the star and by K_n the complete graph, each on n vertices.

Molecular descriptors play a very important role in mathematical chemistry especially in QSAR (quantitative structure-activity relationship) and/or QSPR (quantitative structure-property relationship) related studies. Among those descriptors, a special interest is devoted to so-called topological indices. They are used to understand physicochemical properties of chemical compounds in a simple way, since they sum up some of the properties of a molecule in a single number. During the last decades, a legion of topological indices were introduced and found some applications in chemistry, see *e.g.*, [7, 8, 16]. The study of topological indices goes back to the seminal work by Wiener [18] in which he used the sum of all shortest-path distances, nowadays known as the *Wiener index*, of a (molecular) graph for modeling physical properties of alkanes.

Another very important molecular descriptor, was introduced by Randić [13]. It is called the *Randić (connectivity) index* and defined as

$$Ra = Ra(G) = \sum_{uv\in E} \frac{1}{\sqrt{d_u d_v}}$$

where d_u denotes the degree (number of neighbors) of u in G. The Randić index is probably the most studied molecular descriptor in mathematical chemistry. Actually, there are more than two thousand papers and five books devoted to this index (see, *e.g.*, [6, 9–12] and the references therein).

Motivated by the definition of Randić connectivity index, Vukičević and Furtula [17] proposed the *geometric-arithmetic index*. It is so-called since its definition involves both the geometric and the arithmetic means of the endpoints degrees of the edges in a graph. For a simple graph G, the geometric-arithmetic index $GA(G)$ of a graph G is defined as in [17] by

$$GA = GA(G) = \sum_{uv\in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v} .$$

It is noted in [17] that the predictive power of GA for physico-chemical properties is somewhat better than the predictive power of the Randić connectivity index. In [17], Vukičević and Furtula gave lower and upper bounds for GA, identified the trees with the minimum and the maximum GA indices, which are the star S_n and the path P_n, respectively. In [19] Yuan, Zhou and Trinajsić gave the lower and upper bounds for GA index of molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second, and the third minimum, as

well as the second and the third maximum GA indices. The chemical applicability of the geometric-arithmetic index was highlighted in [3, 5, 17].
Lower and upper bounds on the geometric-arithmetic index in terms of order n, size m, minimum degree δ and/or maximum degree were proved in [14]. Also in [14], GA was compared to other well known topological indices such as the Randić index, the first and second Zagreb indices, the harmonic index and the sum connectivity index. Other lower and upper bounds, on the geometric-arithmetic index, involving the order n the size m, the minimum and the maximum degrees and the second Zagreb index were proved in [2] In [1], several bounds and comparisons, involving the geometric-arithmetic index and several other graph parameters, were proved.

In the present paper we deal with the problem of finding upper and lower bounds, with the charcterization of the corresponding extremal graphs, for the geometric-arithmetic index of a connected graph with given number of vertices n and minimum degree δ. Earlier study of this problem can be found in [4, 15].

2 Main results

In this section, we first prove upper bounds on the ratios GA/δ in terms of the order n, over the class of connected graphs on n vertices. We also charaterize the corresponding extremal graphs. Thereafter, we prove lower bounds on the ratios $GA/\sqrt{\delta}$ and GA/δ in terms of the order n.

To prove our first bound, namely an upper bound on GA/δ, we need the following preliminary result.

Lemma 2.1. *For $n \geq 3$,*

$$\frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n} > \frac{(n-1)(n-2)}{2} .$$

Proof :
Considering the ratio r_n of the left hand side to the right hand side of the inequality we

have

$$\begin{aligned}
r_n &= \left(\frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n}\right) \cdot \left(\frac{2}{(n-1)(n-2)}\right) \\
&= \frac{n-3}{n-1} + \frac{4}{2n-3}\sqrt{\frac{n-2}{n-1}} + \frac{4}{n(n-2)\sqrt{n-1}} \\
&= 1 - \frac{2}{n-1} + \frac{4\sqrt{n-2}}{(2n-3)\sqrt{n-1}} + \frac{4}{n(n-2)\sqrt{n-1}} \\
&= 1 + \frac{2\left(2\sqrt{(n-2)(n-1)} - (2n-3)\right)}{(2n-3)(n-1)} + \frac{4}{n(n-2)\sqrt{n-1}} \\
&= 1 + \frac{2\left(4(n-2)(n-1) - (2n-3)^2\right)}{(2n-3)(n-1)\left(2\sqrt{(n-2)(n-1)} + (2n-3)\right)} + \frac{4}{n(n-2)\sqrt{n-1}} \\
&= 1 - \frac{2}{(2n-3)(n-1)\left(2\sqrt{(n-2)(n-1)} + (2n-3)\right)} + \frac{4}{n(n-2)\sqrt{n-1}} \quad > \quad 1\,.
\end{aligned}$$

This shows the inequality. ■

Theorem 2.2. *For any connected graph on $n \geq 3$ with minimum degree δ and geometric-arithmetic index GA,*

$$\frac{GA}{\delta} \leq \frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n}$$

with equality if and only if G is the kite $Ki_{n,n-1}$.

Proof :

If $\delta = 1$, then the maximum number of edges in G is $(n-1)(n-2)/2+1$ which is attained if and only if G is the kite $Ki_{n,n-1}$. In this case equality holds.

If $\delta = 1$ and the number of edges is not maximum, *i.e.*, $m \leq (n-1)(n-2)/2$, then using Lemma 2.1 and the fact that $GA \leq m$, we have

$$GA \leq \frac{(n-1)(n-2)}{2} < \frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n}\,.$$

Therefore, in this case, the inequality is strict.

If $\delta \geq 2$, then

$$\frac{GA}{\delta} \leq \frac{m}{2} \leq \frac{n(n-1)}{4} < \frac{(n-2)(n-3)}{2} + \frac{2(n-2)\sqrt{(n-1)(n-2)}}{2n-3} + \frac{2\sqrt{n-1}}{n}\,.$$

Therefore, in this case also, the inequality is strict. ■

The following theorem is proved in [14].

Theorem 2.3 ([14]). *Let G be a graph on n vertices with minimum degree δ such that $\delta \geq k \geq 2$, for some integer k.*

(1) If $n \leq 10$, then

$$GA \geq \frac{nk}{2} \,.$$

(2) If $n \geq 11$, then

$$GA \geq \min\left\{\frac{nk}{2}, \frac{(k+1)\sqrt{k}(n-1)^{\frac{3}{2}}}{n-1+k}\right\}.$$

We are going to make a more precise statement of the above theorem. For that purpose, we need the following lemma.

Lemma 2.4. *For an integer $k \geq 4$, let*

$$f_k(t) = \frac{(k+1)\sqrt{k}(t-1)^{\frac{3}{2}}}{t-1+k} - \frac{kt}{2} \qquad \text{for } t \geq k+1.$$

We have

$$f_k(t)\begin{cases} \geq & 0 \qquad \text{if} \quad k+1 \leq t \leq k+8; \\ < & 0 \qquad \text{if} \quad t \geq k+9. \end{cases}$$

Proof :

To do the calculations related to the function in this lemma, we used the software *WolframAlpha* (available at wolframalpha.com).

The second derivative of f_k is

$$f_k''(t) = -\frac{(k+1)\sqrt{k}\,(t^3+(7k-3)t^2+(3k^2-14k+3)t-3k^3-3k^2+7k-1)}{4(t-1+k)^4\sqrt{t-1}}$$

which is negative for all $t \geq k+1$ with $k \geq 4$. Thus the graph of f_k is concave down for all $t \geq k+1$ with $k \geq 4$. Therefore, the equation $f_k(t) = 0$ has at most 2 solutions.

We have $f_k(k+1) = 0$, that is $t_1 = k+1$ is a solution of $f_k(t) = 0$. Also

$$f_k(k+8) = \frac{(k+1)\sqrt{k}(k+7)^{\frac{3}{2}}}{2k+7} - \frac{k(k+8)}{2} \quad > 0 \quad \text{for all } k \geq 4$$

and

$$f_k(k+9) = \frac{(k+1)\sqrt{k}(k+8)^{\frac{3}{2}}}{2k+8} - \frac{k(k+9)}{2} \quad < 0 \quad \text{for all } k \geq 4,$$

that is $f_k(t) = 0$ has a solution t_2 satisfying $k+8 < t_2 < k+9$. ■

In the statement of the above lemma, there is the condition that $k \geq 4$. For $k = 2$ and $k = 3$, the conclusions are slightly different, namely

$$f_2(t) = \frac{3\sqrt{2}(t-1)^{\frac{3}{2}}}{t+1} - t \quad \begin{cases} \geq & 0 \qquad \text{if} \quad 3 \leq t \leq 11; \\ < & 0 \qquad \text{if} \quad t \geq 12; \end{cases}$$

and

$$f_3(t) = \frac{4\sqrt{3}(t-1)^{\frac{3}{2}}}{t+2} - \frac{3t}{2} \begin{cases} \geq \ 0 & \text{if} \quad 3 \leq t \leq 12; \\ < \ 0 & \text{if} \quad t \geq 13. \end{cases}$$

In view of the above lemma and discussion, we can state Theorem 2.3 as follows.

Theorem 2.3′. *Let G be a graph on n vertices with minimum degree δ such that $\delta \geq 2$.*

(1) If $\delta = 2$, then

$$GA \geq \begin{cases} n & \text{if} \quad 3 \leq n \leq 11; \\ \frac{3\sqrt{2}(n-1)^{\frac{3}{2}}}{n+1} & \text{if} \quad n \geq 12. \end{cases}$$

(2) If $\delta = 3$, then

$$GA \geq \begin{cases} \frac{3n}{2} & \text{if} \quad 4 \leq n \leq 12; \\ \frac{4\sqrt{3}(n-1)^{\frac{3}{2}}}{n+2} & \text{if} \quad n \geq 13. \end{cases}$$

(3) If $\delta \geq 4$, then

$$GA \geq \begin{cases} \frac{\delta n}{2} & \text{if} \quad \delta + 1 \leq n \leq \delta + 8; \\ \frac{(\delta+1)\sqrt{\delta}(n-1)^{\frac{3}{2}}}{n+\delta-1} & \text{if} \quad n \geq \delta + 9. \end{cases}$$

Note that the cases $\delta = 2$ and $\delta = 3$ in the above theorem were already stated in [14].

We next prove a lower bound on the ration $GA/\sqrt{\delta}$ and characterize the corresponding extremal graphs.

Proposition 2.5. *For any connected graph on $n \geq 3$ vertices with minimum degree δ and geometric-arithmetic index GA,*

$$\frac{GA}{\sqrt{\delta}} \geq \frac{2(n-1)^{\frac{3}{2}}}{n}$$

with equality if and only if G is the star S_n.

Proof :

If $\delta = 1$, the result is proved in [17].

Assume that $\delta \geq 2$. From Theorem 2.3, we have

$$\frac{GA}{\sqrt{\delta}} \geq \min \left\{ \frac{n\sqrt{\delta}}{2}, \frac{(\delta+1)(n-1)^{\frac{3}{2}}}{(n-1+\delta)} \right\}.$$

First, we compare between

$$\frac{n\sqrt{\delta}}{2} \quad \text{and} \quad \frac{2(n-1)^{\frac{3}{2}}}{n}.$$

We have

$$\frac{n\sqrt{\delta}}{2} - \frac{2(n-1)^{\frac{3}{2}}}{n} \geq \frac{n}{\sqrt{2}} - \frac{2(n-1)^{\frac{3}{2}}}{n} = \frac{n^2 - 2(n-1)^{\frac{3}{2}}}{\sqrt{2}n}.$$

The study of the function

$$f(t) = \frac{t^2 - 2(t-1)^{\frac{3}{2}}}{\sqrt{2}t}$$

shows that $f(t) > 0$ for all $t \geq 1$. Therefore

$$\frac{n\sqrt{\delta}}{2} > \frac{2(n-1)^{\frac{3}{2}}}{n}$$

for all $n \geq \delta + 1 \geq 3$.

Now, we compare between

$$\frac{(\delta+1)(n-1)^{\frac{3}{2}}}{(n-1+\delta)} \quad \text{and} \quad \frac{2(n-1)^{\frac{3}{2}}}{n},$$

or equivalently between

$$\frac{\delta+1}{(n-1+\delta)} \quad \text{and} \quad \frac{2}{n}.$$

We have

$$\begin{aligned}\frac{\delta+1}{(n-1+\delta)} - \frac{2}{n} &= \frac{(\delta+1)n - 2(n-1+\delta)}{n} = \frac{(\delta-1)n - 2(\delta-1)}{n} \\ &= \frac{(\delta-1)(n-2)}{n} > 0 \quad \text{for all } \ n \geq \delta+1 \geq 3.\end{aligned}$$

Thus

$$\frac{\delta+1}{(n-1+\delta)} > \frac{2}{n}$$

for all $n \geq \delta + 1 \geq 3$.

In conclusion

$$\min\left\{\frac{n\sqrt{\delta}}{2}, \frac{(\delta+1)(n-1)^{\frac{3}{2}}}{(n-1+\delta)}\right\} \geq \frac{2(n-1)^{\frac{3}{2}}}{n}$$

for all $n \geq \delta + 1 \geq 3$. This completes the proof. ∎

Under certain conditions, the inequality in the above proposition remains valid if $GA/\sqrt{\delta}$ is replaced by GA/δ, as next stated.

Proposition 2.6. *If G is a connected graph on n vertices with minimum degree δ such that $n \geq \max\left\{13, 2\sqrt{\delta}(\sqrt{\delta}+1)/(\sqrt{\delta}-1)\right\}$, then*

$$\frac{GA}{\delta} \geq \frac{2(n-1)^{\frac{3}{2}}}{n}$$

with equality if and only if G is the star S_n.

Proof :

Again if $\delta = 1$, the result is proved in [17].

Assume that $\delta \geq 2$. In this case, from Theorem 2.3, we have

$$\frac{GA}{\delta} \geq \min\left\{\frac{n}{2}, \frac{(\delta+1)(n-1)^{\frac{3}{2}}}{(n-1+\delta)\sqrt{\delta}}\right\}.$$

First, we compare between

$$\frac{n}{2} \qquad \text{and} \qquad \frac{2(n-1)^{\frac{3}{2}}}{n}.$$

For $t \geq 2$, consider the function

$$f(t) = \frac{t}{2} - \frac{2(t-1)^{\frac{3}{2}}}{t}.$$

This function is continuous and its second derivative is

$$f''(t) = \frac{t(t+4)-8}{2t^3\sqrt{t-1}}.$$

We have $f''(t) > 0$ for all $t \geq 2$ and therefore the function $f(t)$ is concave up for $t \geq 2$. Thus the equation $f(t) = 0$ has (at most) two solutions: one of them is $t_1 = 2$ and the other one, say t_2, satisfies $12 < t_2 < 13$ (since $f(12) < 0$ and $f(13) > 0$). We conclude that $f(t) > 0$, which means

$$\frac{n}{2} > \frac{2(n-1)^{\frac{3}{2}}}{n} \qquad \text{for all } n \geq 13.$$

Now, we compare between

$$\frac{(\delta+1)(n-1)^{\frac{3}{2}}}{(n-1+\delta)\sqrt{\delta}} \qquad \text{and} \qquad \frac{2(n-1)^{\frac{3}{2}}}{n},$$

or equivalently between

$$\frac{\delta+1}{(n-1+\delta)\sqrt{\delta}} \qquad \text{and} \qquad \frac{2}{n}.$$

We have

$$\begin{aligned}
\frac{\delta+1}{(n-1+\delta)\sqrt{\delta}} - \frac{2}{n} &= \frac{(\delta+1)n - 2(n-1+\delta)\sqrt{\delta}}{n(n-1+\delta)\sqrt{\delta}} \\
&= \frac{(\delta - 2\sqrt{\delta}+1)n - 2(\delta-1)\sqrt{\delta}}{n(n-1+\delta)\sqrt{\delta}} \\
&= \frac{(\sqrt{\delta}-1)^2 n - 2(\sqrt{\delta}-1)(\sqrt{\delta}+1)\sqrt{\delta}}{n(n-1+\delta)\sqrt{\delta}} \\
&= \frac{\sqrt{\delta}-1}{n(n-1+\delta)\sqrt{\delta}}\left((\sqrt{\delta}-1)n - 2(\sqrt{\delta}+1)\sqrt{\delta}\right).
\end{aligned}$$

Thus

$$\frac{\delta+1}{(n-1+\delta)\sqrt{\delta}} > \frac{2}{n} \qquad \text{if and only if} \qquad n > \frac{2\sqrt{\delta}(\sqrt{\delta}+1)}{\sqrt{\delta}-1}.$$

The combination of both cases completes the proof. ■

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