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Geometric–arithmetic index and degrees 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, $GA/\overline{d}$ and Δ, in terms of the order n, over the class of connected graphs on n vertices, where GA, δ, $\overline{d}$ and Δ denote the geometric–arithmetic index and the minimum, the average and the maximum degrees, respectively. We also characterize the extremal graphs corresponding to each of those bounds. We also prove bounds where, in addition to the geometric–arithmetic index GA, the Randić index Ra and the maximum degree Δ are involved.

Keywords: Graph, geometric–arithmetic index, degree, Randić index, conjecture

Résumé : Dans le présent article, nous démontrons des bornes inférieure et supérieure sur chacun des rapports GA/δ, $GA/\overline{d}$ et Δ, en fonction de l'ordre n, sur l'ensemble de tous les graphes connexes avec n sommets, où GA, δ, $\overline{d}$ et Δ désignent l'indice géométrique–arithmétique et les degrés minimum, moyen et maximum, respectivement. Nous caractérisons, les graphes extrémaux correspondant à chacune de ces bornes. Nous démontrons aussi des bornes o, en plus de l'indice géométrique–arithmétique, l'indice de Randić Ra et le degré maximum sont utilisés.

Mots clés : Graphe, indice géométrique–arithmétique, degré, conjecture

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 vertices adjacent to it in G. A graph G is said to be *regular* of degree d, or d-*regular* if $d_u = d$ for everey vertex u in G. The minimum, average and maximum degrees in a graph G are denoted by δ, $\overline{d}$ and Δ, respectively.

As usual, we denote by P_n the path, 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.*, [11, 12, 20]. The study of topological indices goes back to the seminal work by Wiener [22] 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 [17]. 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.*, [10, 13, 14, 15, 16] and the references therein).

Motivated by the definition of Randić connectivity index, Vukičević and Furtula [21] 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 with edge set $E(G)$, the geometric–arithmetic index $GA(G)$ of a graph G is defined as in [21] by

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

where d_u denotes the degree of u in G.

It is noted in [21] that the predictive power of GA for physico-chemical properties is somewhat better than the predictive power of the Randić connectivity index. In [21], Vukičević and Furtula gave the 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 [23] 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 [7, 9, 21].

Lower and upper bound on the geometric–arithmetic index in terms of order n, size m, minimum degree δ and/or maximum degree were proved in [18]. Also in [18], 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 [6].

In [1], several bounds and comparisons, involving the geometric–arithmetic index and several other graph parameters, were proved.

The problem of lower bounding GA over the class of connected graphs with fixed order of vertices and minimum degree was discussed in [8, 19].

2 Main results

In this section, we first prove bounds on the ratios GA/δ, $GA/\overline{d}$ and GA/Δ, in terms of the order n, over the class of connected graphs on n vertices, where GA, δ, $\overline{d}$ and Δ denote the geometric–arithmetic index and the minimum, average and maximum degrees of G, respectively. Thereafter, we prove bounds where, in addition to the geometric–arithmetic index GA, the Randić index Ra and the maximum degree Δ are involved.

Note that all results proved in the present paper were first conjectured, or at least tested, using the conjecture-making system in graph theory AutoGraphiX [2, 3, 4, 5].

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

Lemma 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 sides 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 1 *For any connected graph on $n \geq 3$ vertices 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 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. □

We next prove a lower bound on the ratio GA/δ and characterize the corresponding extremal graphs.

Theorem 2 *For any connected graph on $n \geq 3$ vertices with minimum degree δ and geometric–arithmetic index GA,*

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

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

Proof. If $\delta = 1$, it is trivial that the bound is true and reached if and only if G is the star S_n. Assume that $\delta \geq 2$. In this case, it is proved in [18] that if $\delta \geq k$ (for some integer $k \geq 2$), then

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

In our case, since both functions involved in the min operator are increasing with respect to k and $\delta \geq 2$, we have

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

for all $n \geq 3$. □

In the next theorem, we prove a lower and an upper bound on the ratio $GA/\overline{d}$. We also characterize the corresponding extremal graphs, in both cases.

Theorem 3 *For any connected graph on $n \geq 3$ vertices with average degree $\overline{d}$ and geometric–arithmetic index GA,*

$$\sqrt{n-1} \leq \frac{GA}{\overline{d}} \leq \frac{n}{2}$$

with equality if and only if G is the star S_n (resp. regular) for the lower (resp. upper) bound.

Proof. For the lower bound and assuming, without loss of generality, that $d_i \leq d_j$, we have

$$\frac{GA}{\overline{d}} = \frac{\sum_{ij\in E}\frac{2\sqrt{d_i d_j}}{d_i+d_j}}{\frac{2}{n}\sum_{ij\in E}1} = \frac{\sum_{ij\in E}\frac{2\sqrt{d_i/d_j}}{d_i/d_j+1}}{\frac{2}{n}\sum_{ij\in E}1} \geq \frac{\sum_{ij\in E}\frac{2\sqrt{1/(n-1)}}{1/(n-1)+1}}{\frac{2}{n}\sum_{ij\in E}1} = \sqrt{n-1}.$$

Equality being reached if and only if $d_i = 1$ and $d_j = n-1$ for all edges $ij \in E$, *i.e.*, if and only if G is the star S_n.

For the upper bound, we have

$$\frac{GA}{\overline{d}} = \frac{\sum_{ij\in E}\frac{2\sqrt{d_i d_j}}{d_i+d_j}}{\frac{2}{n}\sum_{ij\in E}1} \leq \frac{\sum_{ij\in E}1}{\frac{2}{n}\sum_{ij\in E}1} = \frac{n}{2}.$$

Equality being reached if and only if $d_i = d_j$ for all edges $ij \in E$, *i.e.*, if and only if G is regular. □

In the next theorem, we prove a lower and an upper bounds on the ratio GA/Δ. We also characterize the corresponding extremal graphs, in both cases.

Theorem 4 *For any connected graph on $n \geq 3$ vertices with maximum degree Δ and geometric–arithmetic index GA,*

$$\frac{2\sqrt{n-1}}{n} \leq \frac{GA}{\Delta} \leq \frac{n}{2}$$

with equality if and only if G is the star S_n (resp. regular) for the lower (resp. upper) bound.

Proof. For the lower bound, it is well-known that the minimum value of GA over all connected graphs on n vertices is reached only for the star S_n, which also maximizes Δ.

The upper bound, as well as the characterization of the extremal graphs, follows immediately from the corresponding case in Theorem 3. □

Among the the results proved in [1], we recall the following theorem.

Theorem 5 ([1]) *For any connected graph G with minimum degree $\delta \geq 2$*

$$\frac{GA}{Ra} \leq n-1$$

with equality if and only if G is the complete graph K_n.

Experiments with the hepl of AutoGraphiX led to a conjecture, improving the above theorem, proved in the next proposition.

Proposition 1 *For any connected graph G with geometric–arithmetic index GA, Randić index Ra and maximum degree Δ*

$$\frac{GA}{Ra} \leq \Delta$$

with equality if and only if G is Δ-regular.

Proof. It is well-known that $GA \leq m$ with equality if and only G is regular. In addition,

$$Ra = \sum_{ij\in E} \frac{1}{\sqrt{d_i d_j}} \geq \sum_{ij\in E} \frac{1}{\Delta} = \frac{m}{\Delta}$$

with equality if and only if G is Δ-regular. Combining the above inequalities, we get

$$\frac{GA}{Ra} \leq \frac{m\Delta}{m} = \Delta$$

with equality if and only if G is Δ-regular. □

Also, among the results proved in [1], we recall the following.

Theorem 6 ([1]) *For any connected graph with minimum degree $\delta \geq 2$*

$$GA \geq \delta Ra$$

with equality if and only if G is δ-regular.

To sum up the latter results we have a chain of inqualities which we state in the following theorem.

Theorem 7 *For any connected graph on $n \geq 2$ vertices with m edges, we have*

$$\delta \cdot Ra \leq GA \leq m \leq \Delta \cdot Ra \leq (n-1) \cdot Ra.$$

Furthermore all equalities hold simultaneously if and only if G is the complete graph K_n; and all equalities, but the last one, hold simultaneously if and only if G is a non-complete Δ-regular graph.

Note that we can not insert $\overline{d} \cdot Ra$ into the chain since there exist graphs with $GA < \overline{d} \cdot Ra$ (see Figure 1 for an example) and others with $GA > \overline{d} \cdot Ra$ (see Figure 2 for an example).

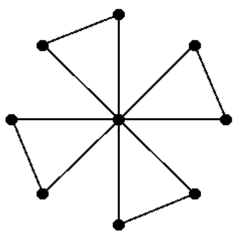

Figure 1: A graph with $GA < \overline{d} \cdot Ra$.

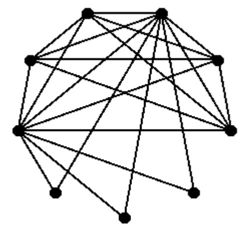

Figure 2: A graph with $GA > \overline{d} \cdot Ra$.

To conclude, we state a conjecture obtained with the help of AutoGraphiX. But first, we need the following definition. A *pineapple* $PA_{n,k}$ is the graph obtained from a clique (a set of mutual adjacent vertices) on k vertices by attaching $n-k$ pendant edges to one of its vertices. The pineapple $PA_{10,6}$ is illustrated in Figure 3.

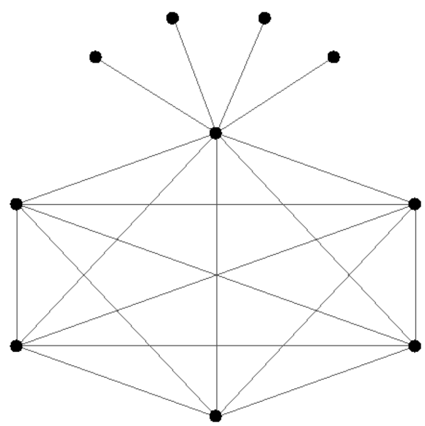

Figure 3: The pineapple $PA_{10,6}$.

Conjecture 1 *Let G be a connected graph on $n \geq 3$ vertices with geometric–arithmetic index GA, Randić index Ra and minimum degree δ. Then*

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

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

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