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Note

The geometric–arithmetic index and the chromatic number of connected graphs

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ABSTRACT

In the present paper, we compare the geometric–arithmetic index GA and the chromatic number χ of a connected graph with given order. We prove, among other results, an upper bound on the ratio GA/χ. We also prove lower bounds on the chromatic number in terms of geometric–arithmetic index and number of vertices of a connected graph. The results obtained for the chromatic number χ are extended to the clique number ω.

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.

As usual, we denote by P_n the path, by C_n the cycle, by S_n the star, by $K_{a,n-a}$ the complete bipartite graph 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.*, [12,13,25]. The study of topological indices goes back to the seminal work by Wiener [28] 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 [20]. 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.*, [11,15,16,18,19] and the references therein).

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Motivated by the definition of Randić connectivity index, Vukičević and Furtula [27] 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 given in [27] 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 [27] that the predictive power of GA for physicochemical properties is somewhat better than the predictive power of the Randić connectivity index. In [27], Vukičević and Furtula gave lower and upper bounds for GA, and identified the trees with minimum and maximum GA indices, which are the star and the path, respectively. In [29], Yuan, Zhou and Trinajstić gave lower and upper bounds for GA of molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second minimum, and the third minimum, as well as the second and third maximum GA indices. The chemical applicability of the geometric–arithmetic index was highlighted in [8,10,27].

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 [21]. Also in [21], GA was compared to several 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 maximum degrees and the second Zagreb index were proved in [7].

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 number and minimum degree was discussed in [9,23].

Our main results are stated and proved in the next section. The third and last section is devoted to the statement of a few conjectures obtained after experiments using the computerized conjecture making system AutoGraphiX [2,3,5,6].

2. Main results

A *coloring* of G is an assignment of colors to the vertices of G such that two adjacent vertices have different colors. The minimum number of colors in a coloring of G is the *chromatic number* of G and is denoted by $\chi(G)$. The chromatic number χ is a very widely studied graph invariant, whose history started with the famous *four color problem*, posed by Guthrie in 1852 (see *e.g.* [4,22,24] and the work of Kempe [17] in 1879 and Heawood [14] in 1890).

A *clique* of G is a subset of mutually adjacent vertices in G. A clique is called *maximal* if it is not contained in any other clique. A clique is called *maximum* if it has maximum cardinality. The maximum size of a clique in G is called the *clique number* of G and is denoted by $\omega = \omega(G)$.

In this section, we compare the geometric–arithmetic index GA and the chromatic number χ of a connected graph with given order. Results obtained for the chromatic number χ are extended to the clique number ω.

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 [2,3,5,6].

We first prove an upper bound on the ratio GA/χ in terms of the number of vertices. We also characterize the corresponding extremal graphs.

Theorem 2.1. *For any connected graph on $n \geq 2$ vertices with chromatic number χ*

$$\frac{GA}{\chi} \leq \begin{cases} \dfrac{n^2}{8} & \text{if } n \text{ is even,} \\[2ex] \dfrac{(n^2-1)^{\frac{3}{2}}}{4n} & \text{if } n \text{ is odd,} \end{cases}$$

with equality if and only if G is the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ when n is even, and if and only if G is the complete bipartite graph $K_{\frac{n+1}{2},\frac{n-1}{2}}$ when n is odd.

Proof. We have

$$GA\left(K_{\frac{n}{2},\frac{n}{2}}\right) = \frac{n^2}{4} \qquad \text{and} \qquad GA\left(K_{\frac{n+1}{2},\frac{n-1}{2}}\right) = \frac{(n^2-1)^{\frac{3}{2}}}{4n}.$$

If $\chi = 2$ and n is even, then

$$\frac{GA}{\chi} = \frac{GA}{2} \leq \frac{m}{2} \leq \frac{n^2}{8}$$

with equality if and only if G is the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$.