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A STUDY OF THE GEOMETRIC–ARITHMETIC INDEX AND CHROMATIC NUMBER IN CONNECTED GRAPHS

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Abstract

In this paper, we analyze and compare the geometric–arithmetic index (GAI) and the chromatic number (χ) of a connected graph with a specified order. Among our findings, we establish an upper bound for the ratio of GAI/χ. Additionally, we derive lower bounds for the chromatic number in terms of the geometric-arithmetic index and the number of vertices in a connected graph. Furthermore, the results obtained for the chromatic number (χ) are extended to the clique number(ω).

Keywords: *geometric–arithmetic index, chromatic number, connected graph, clique number.*

1. Introduction

In this paper, we focus exclusively on simple, undirected, and finite graphs, meaning undirected graphs with a finite number of vertices, without any multiple edges or loops.. A graph is denoted by $G = G(V,E)$, where V is its vertex set and E its edge set. The order of G is the number $m = |V|$ of its vertices and its size is the number $n = |E|$ of its edges.

We represent by P_m the path, by C_m the cycle, by S_m the star, by $K_{r,n-r}$ the complete bipartite graph and by K_m the complete graph, each on m vertices.

Molecular descriptors are crucial in mathematical chemistry, particularly in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) studies. Among these descriptors, topological indices are of special interest. They help simplify the understanding of physicochemical properties of chemical compounds, as they condense several properties of a molecule into a single value. Over the past few decades, numerous topological indices have been introduced and have found various applications in chemistry (see, for example, [12,13,25]). The exploration of topological indices traces back to the pioneering work of Wiener [28], who used the sum of all shortest-path distances, now known as the Wiener index, in a (molecular) graph to model the physical properties of alkanes.

Another significant molecular descriptor, introduced by Randić [20], is the Randić (connectivity) index, defined as

$$Ra = Ra(G) = \sum_{xy\in E} \frac{1}{\sqrt{d_x d_y}}$$

where d_x denotes the degree (number of neighbors) of x in G. The Randić index is probably the most studied moleculardescriptor in mathematical chemistry. Actually, there are more than two thousand papers and five books devoted to thisindex (see, e.g., [11,15,16,18,19] and the references therein).

Inspired by the definition of the Randić connectivity index, Vukičević and Furtula [27] introduced the geometric-arithmetic index. It is named as such because its definition incorporates both the geometric and arithmetic means of the degrees of the endpoints of the edges in a graph. For a simple graph G with edge set E(G), the geometric-arithmetic index GAI(G) of the graph G is defined as given in [27] by:

$$GAI(G) = \sum_{xy\in E(G)} \frac{2\sqrt{d_x d_y}}{\sqrt{d_x + d_y}}$$

Where d_x denotes the degree of x in G.

It is mentioned in [27] that the predictive ability of the geometric-arithmetic index (GAI) for physicochemical properties is somewhat superior to that of the Randić connectivity index. In [27], Vukičević and Furtula provided both lower and upper bounds for GAI and identified the trees with the minimum and maximum GAI indices, which are the star and the path, respectively. In [29], Yuan, Zhou, and Trinajstić established lower and upper bounds for GAI of molecular graphs based on the number of vertices and edges. They also identified the m-vertex molecular trees with the minimum, second minimum, and third minimum GAI indices, as well as the second and third maximum GAI indices. The chemical relevance of the geometric-arithmetic index was emphasized in [8, 10, 27].

Lower and upper bounds on the geometric-arithmetic index in terms of order m, size n, minimum degree δ and/ormaximum degree were proved in [21]. Also in [21], GAI was compared to several other well known topological indices such asthe Randić index, the first and second Zagreb indices, the harmonic index and the sum connectivity index. Other lower andupper bounds, on the geometric-arithmetic index, involving the order m, the size n, the minimum and maximum degreesand the second Zagreb index were proved in [7].

In [1], various bounds and comparisons involving the geometric-arithmetic index and other graph parameters were established. The issue of lower bounding GAI for the class of connected graphs with a fixed number of vertices and a minimum degree was addressed in [9, 23]. Our primary results are presented and proven in the following section. The third and final section is dedicated to stating several conjectures derived from experiments conducted using the computerized conjecture-making system AutoGraphiX [2, 3, 5, 6].

2. Results

A coloring of G is an assignment of colors to the vertices of G such that two adjacent vertices have different colors. Theminimum 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 otherclique. A clique is called maximum if it has maximum cardinality. The maximum size of a clique in G is called the cliquenumber of G and is denoted by $\omega = \omega(G)$.

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

We first prove an upper bound on the ratio $\frac{GAI}{\chi}$ in terms of the number of vertices. We also characterize thecorresponding extreml graphs.

Theorem 2.1.

For any connected graph on $m \geq 2$ vertices with chromatic number χ

$$\frac{GAI}{\chi} \leq \begin{cases} \frac{m^2}{8} & if\ m\ is\ even \\ \frac{(m^2-1)^{\frac{3}{2}}}{4m} & if\ m\ is\ odd \end{cases}$$

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

Proof.

We have

$$GAI\left(K_{\frac{m}{2},\frac{m}{2}}\right) = \frac{m^2}{8},$$

$$GAI\left(K_{\frac{m+1}{2},\frac{m-1}{2}}\right) = \frac{(m^2-1)^{\frac{3}{2}}}{4m}$$

If m is even, $\chi = 2$, then

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

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

If $G = K_{\frac{m+1}{2},\frac{m-1}{2}}$, then

$$\frac{GAI}{\chi} = \frac{(m^2-1)^{\frac{3}{2}}}{8m}$$

If m is odd and $G \neq K_{\frac{m+1}{2},\frac{m-1}{2}}$, $\chi = 2$, then

$$\frac{GAI}{\chi} = \frac{GAI}{2} \leq \frac{n}{2} \leq \frac{m^2-5}{8} < \frac{(m^2-1)^{\frac{3}{2}}}{8m}$$

By Turan's theorem [26], $\chi \geq 3$

$$\frac{GAI}{\chi} I \leq n \leq \frac{m}{2\chi}\left(m - \frac{m}{\chi}\right) = \frac{m^2(\chi-1)}{2\chi^2}$$

If m is odd and $G \neq K_{\frac{m+1}{2},\frac{m-1}{2}}$, $\chi = 2$, then

Which is decreasing with respect to χ, so $\chi = 3$

$$\frac{GAI}{\chi} \leq \frac{m^2}{9}$$

With a few more algebraic manipulations, we obtain the result

$$\frac{GAI}{\chi} \leq \frac{m^2}{9} < \begin{cases} \dfrac{m^2}{8} & if\ m\ is\ even \\ \dfrac{(m^2-1)^{\frac{3}{2}}}{4m} & if\ m\ is\ odd \end{cases}$$

For all $n \geq 3$.

Similarly, the following result can be proved using the clique number in place of the chromatic number.

Theorem 2.2.

For any connected graph on $m \geq 2$ vertices with chromatic number ω

$$\frac{GAI}{\omega} \leq \begin{cases} \dfrac{m^2}{8} & if\ m\ is\ even \\ \dfrac{(m^2-1)^{\frac{3}{2}}}{4m} & if\ m\ is\ odd \end{cases}$$

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

Proposition 2.1.

Let G be a connected graph with chromatic number χ, the geometric-arithmetic index GAI and maximum degree Δ, then

$$\chi \geq \frac{4GAI}{m\Delta}$$

with equality if and only if m is even and G is a regular bipartite graph.

Proof.

We have

$m\Delta \geq 2n$ with equality if and only if G is regular, $\chi \geq 2$ with equality if and only if G is bipartite,

$n \geq GAI$ with equality if and only if G is regular.

Thus $\chi m\Delta \geq 4GAI$ with equality if and only if G is regular bipartite.

By following the same steps as in the previous proof, but with $m\bar{d} = 2n$ instead of $m\Delta \geq 2n$, we get the next proposition.

Proposition 2.2.

Let G be a connected graph with chromatic number χ, the geometric-arithmetic index GAI and maximum degree $\bar{d}$, then

$$\chi \geq \frac{4GAI}{m\bar{d}}$$

with equality if and only if m is even and G is a regular bipartite graph.

By using the clique number ω in the place of the chromatic number χ in the above two propositions, we can similarly prove the following result.

Proposition 2.3.

Let G be a connected graph with clique number ω, geometric-arithmetic index GAI and average degree $\bar{d}$, then

$$\omega \geq \frac{4GAI}{m\bar{d}} \chi \geq \frac{4GAI}{m\Delta}$$

with equality if and only if is even and G is a regular bipartite graph..

4. Conclusions

In this study, we analyzed and compared the geometric–arithmetic index (GAI) and the chromatic number (χ) of connected graphs with a given order. We established an upper bound for the ratio GAI/χ, contributing to the understanding of how these two graph invariants interact. Moreover, we derived new lower bounds for the chromatic number in terms of the geometric–arithmetic index and the number of vertices. These findings not only deepen the relationship between GAI and chromatic properties but also extend to the clique number (ω), offering broader applicability to graph theory problems involving coloring and clique structures.

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