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Research Article

Conjecture Involving Arithmetic-Geometric and Geometric-Arithmetic Indices

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The geometric-arithmetic (GA) index of a graph G is the sum of the ratios of geometric and arithmetic means of end-vertex degrees of edges of G. Similarly, the arithmetic-geometric (AG) index of G is defined. Recently, Vujošević et al. conjectured that a tree attaining the maximum value of the addition $AG + GA$ or difference $AG - GA$ of the AG and GA indices in the class of all n-vertex molecular trees must contain at most one vertex of degree 2 and at most one vertex of degree 3, but not both, for every fixed integer $n \geq 11$. In this paper, the aforementioned conjecture is p.

1. Introduction

In graph theory, a graph invariant is any property of graphs that depends only on the abstract structure not on graph representations such as particular labellings or drawings of the graph. A graph invariant may be a polynomial (e.g., the characteristic polynomial), a set of numbers (e.g., the spectrum of a graph), or a numerical value. Numerical graph invariants that quantitate topological characteristics of graphs are called topological indices [1]. Topological indices play an important role in studying QSARs (quantitative structure-activity relationships) and QSPRs (quantitative structure-property relationships). It has already been observed that some topological indices can be used very effectively in predicting different physicochemical properties of chemical compounds such as boiling point and surface tension. Over the years, many topological indices were proposed and studied based on degrees, distances, and other parameters of graphs.

This paper is concerned with the geometric-arithmetic (GA) index, a topological index introduced in [2], and its closely related variant arithmetic-geometric (AG) index (see, for example [3]). The GA and AG indices for a graph G are defined as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \tag{1}$$

and

$$AG(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}, \tag{2}$$

where $E(G)$ denotes the edge set of G and d_u is the degree of the vertex $u \in V(G)$. For the graph-theoretical notation and terminology used in this paper, without defining them here, they can be found in [4, 5]. The GA index has attracted a considerable attention recently. In [6], the effect on the AG index is studied under the deletion of an edge from a graph. Rodríguez et al. [7] derived various bounds on the AG index. Gutman [8] noticed that the GA and AG indices are linearly correlated and remarked that there is no mathematical or chemical justification to study these indices independently. The detail about the GA index can be found in the recent survey [9] and related references listed therein.

By an n-vertex tree, we mean a tree of order n. A tree of maximum degree at most 4 is known as a molecular tree. Let $\mathbb{T}_{n;1}$ be the class of all those n-vertex molecular trees that contain only vertices of degrees 1 and 4. Denoted by $\mathbb{T}_{n;2}$, the

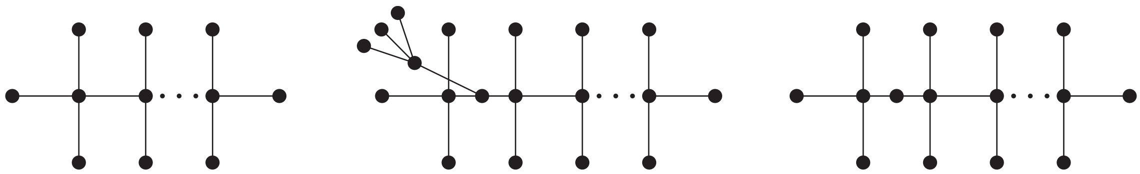

Figure 1: Some examples of the trees belonging to the class $\mathbb{T}_n^*$.

class of all those n-vertex molecular trees that do not contain any vertex of degree 3 has only one vertex of degree 2, and the unique vertex of degree 2 has only neighbors of degree 4. We take $\mathbb{T}_n^* = \mathbb{T}_{n;1} \cup \mathbb{T}_{n;2} \cup \mathbb{T}_{n;3}$. The following conjecture about the addition and difference of the AG and GA indices was described in [3].

Conjecture 1 (see [3]). *A tree T has the maximum value of the addition $AG + GA$ or difference $AG - GA$ of the AG and GA indices in the class of all n vertex molecular trees if and only if $T \in \mathbb{T}_n^*$, for every fixed integer $n \geq 11$.*

The authors of [3] wrote (Line 1, Page 13): "the cells with the stars contain the conjectures which are obtained by using computer programs"; they referred to cells of the table given at the end of Page 12 of [3]. The entry numbers 7 and 9 in the last column of the mentioned table yield Conjecture 1.

We remark here that the extremal trees mentioned in Conjecture Search#12 are the same as the trees attaining the maximum value of the difference between the atom-bond connectivity index and the Randić index among all n-vertex molecular trees, see [10]. The main purpose of the present paper is to prove Conjecture 1.

2. Proof of Conjecture 1

Note that the difference $AG - GA$ of the AG and GA indices for a graph G can be written as

$$(AG - GA)(G) = \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{2(d_u + d_v)\sqrt{d_u d_v}}. \tag{3}$$

Denoted by n_i, the number of those vertices of a molecular tree T that has the degree i. Let $x_{i,j}$ be the number of those edges of T whose end-vertices have degrees i and j. For a nontrivial n vertex molecular tree T, we obtain

$$(AG - GA)(T) = \sum_{1 \leq i \leq j \leq 4} \frac{(i - j)^2}{2(i + j)\sqrt{ij}} x_{i,j}, \tag{4}$$

$$n_1 + n_2 + n_3 + n_4 = n, \tag{5}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1), \tag{6}$$

$$x_{1,2} + x_{1,3} + x_{1,4} = n_1, \tag{7}$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} + x_{2,4} = 2n_2, \tag{8}$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4} = 3n_3, \tag{9}$$

$$x_{1,4} + x_{2,4} + x_{3,4} + 2x_{4,4} = 4n_4. \tag{10}$$

By solving equations (5)–(10) for the unknowns $n_1, n_2, n_3, n_4, x_{1,4}, x_{4,4}$ and then substituting the values of $x_{1,4}$ and $x_{4,4}$ (these two values are well known, firstly derived in 1999, see [11]) in equation (3), we have

$$\begin{aligned}(AG - GA)(T) \approx \frac{3(n+1)}{10} &- 0.482x_{1,2} - 0.211x_{1,3} \\ &- 0.3x_{2,2} - 0.159x_{2,3} \\ &- 0.032x_{2,4} - 0.1x_{3,3} - 0.029x_{3,4}.\end{aligned} \tag{11}$$

We take

$$\begin{aligned}\Gamma_{\text{AG-GA}}(T) \approx &- 0.482x_{1,2} - 0.211x_{1,3} - 0.3x_{2,2} \\ &- 0.159x_{2,3} - 0.032x_{2,4} \\ &- 0.1x_{3,3} - 0.029x_{3,4}.\end{aligned} \tag{12}$$

Then, equation (11) becomes

$$(AG - GA)(T) \approx \frac{3(n+1)}{10} + T_{AG-GA}(T). \tag{13}$$

From equation (13), it is clear that a tree T attains the maximum value of the difference $AG - GA$ in the class of all n vertex molecular trees only if T attains the maximum value of Γ_{AG-GA} in the considered class of molecular trees, for every fixed integer $n \geq 11$. Thereby, in the following lemma, we consider $\Gamma_{AG-GA}(T)$ instead of $(AG - GA)(T)$.

Lemma 1. *Let T be a molecular tree of order $n \geq 11$.*

(i) If any of the numbers $x_{2,2}$, $x_{2,3}$, $x_{3,3}$, $x_{1,2}$, and $x_{1,3}$ is nonzero

(ii) If $n_2 + n_3 \geq 2$ then

$$\Gamma_{AG-GA}(T) < \frac{1}{140}(5\sqrt{3} - 21) \approx -0.088. \tag{14}$$

Proof

(i) If any of the numbers $x_{2,2}, x_{2,3}, x_{3,3}, x_{1,2}, x_{1,3}$ is nonzero, then the desired inequality directly follows from (12).

(ii) Suppose, to the contrary, we have

$$\Gamma_{AG-GA}(T) \geq \frac{1}{140}(5\sqrt{3} - 21), \tag{15}$$

then by using part (i), we have $x_{2,2} = x_{2,3} = x_{3,3} = x_{1,2} = x_{1,3} = 0$, and hence, the identities $x_{2,4} = 2n_2$ and $x_{3,4} = 3n_3$ hold because of equations (8) and (9). Thus, by using (12), we have

$$\Gamma_{AG-GA}(T) \approx -0.064n_2 - 0.088n_3, \tag{16}$$

together with the assumption

$$\Gamma_{AG-GA}(T) \geq \frac{1}{140}(5\sqrt{3} - 21) \approx -0.088. \tag{17}$$

We imply that $n_2 + n_3 \leq 1$, which is a contradiction. □

Proof of Conjecture 2. It can be easily observed that if T is a molecular tree of order $n \geq 11$ such that $x_{2,2} = x_{2,3} = x_{3,3} = x_{1,2} = x_{1,3} = 0$ and $n_2 + n_3 \leq 1$, then exactly one of the following three possibilities holds:

(i) $\Gamma_{AG-GA}(T) = 0$,
(ii) $\Gamma_{AG-GA}(T) \approx -0.064$,
(iii) $\Gamma_{AG-GA}(T) \approx -0.088$.

Therefore, from Lemma 1 and equation (13), it is observed that a tree T has the maximum value of the difference $AG - GA$ in the class of all n vertex molecular trees only if $T \in \mathbb{T}_n^*$, for every fixed integer $n \geq 11$. Examples of the extremal trees are depicted in Figure 1.

In a similar manner, one proves that a tree T has the maximum value of the addition $AG + GA$ in the class of all $n$vertex molecular trees only if $T \in \mathbb{T}_n^*$, for every fixed integer $n \geq 11$. □

Data Availability

The data are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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