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Upper bound for the geometric-arithmetic index of trees with given domination number ☆

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ABSTRACT

Given a graph G with vertex set $V(G)$ and edge set $E(G)$, the geometric-arithmetic index is the value

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

where d_u and d_v denote the degrees of the vertices $u, v \in V(G)$, respectively. In this work we present an upper bound for the geometric-arithmetic index of trees in terms of the order and the domination number, and we characterize the extremal trees for this upper bound. Finally, using a known relation between the geometric-arithmetic and arithmetic-geometric indices, we deduce a lower bound for the arithmetic-geometric index using the same parameters.

1. Introduction

A topological index is a numerical parameter of a graph which characterizes its topology, and it is usually a graph invariant. Topological indices have been used for correlation of chemical structure with chemical reactivity, biological activity or physical properties [6,17,18]. One of the most used topological indices in applications to chemistry and pharmacology is the Randić index, that has been used in the development of QSPR/QSAR studies [10,11,13]. The geometric-arithmetic index was introduced in [20] with the aim of improving the predictive ability of the Randić index. It has been also applied in QSPR and related fields. Given a graph G with vertex set $V(G)$ and edge set $E(G)$, the *geometric-arithmetic index* is a topological index based on end-vertex degrees of edges, which is defined as

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

where uv denotes the edge connecting the vertices $u, v \in V(G)$ and d_u and d_v denote the degrees of the vertices u and v, respectively. There are many works devoted to this topological index and it is a topic of interest in recent years ([1–3,7,14]). We will focus here only on its value over trees (see [8,9]).

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Recently, many papers relating topological indices and domination number of trees have appeared in the literature [4,5,12,16,21]. A vertex set $D \subseteq V(G)$ is a *dominating set* in G if every vertex in $V(G)\backslash D$ is adjacent to some vertex of D. The *domination number* of G is the minimum cardinality among all dominating sets of G, and it is denoted by $\gamma(G)$. Following the research line in [4] and [5], in this work we give an upper bound for the geometric-arithmetic index of trees in terms of the order and the domination number, and we characterize the extremal trees for that bound. As a consequence, using a known relation between the geometric-arithmetic and arithmetic-geometric indices, we deduce a lower bound for the arithmetic-geometric index using the same parameters.

Let us start with some notation and terminology. Let G be a graph and $u \in V(G)$, we denote by $N(u) = \{v \in V(G) : uv \in E(G)\}$ the set of neighbors of u, and by d_u the *degree* of u, it means, the cardinality of $N(u)$. A *leaf* is a vertex with degree 1 and a *support vertex* is a vertex adjacent to a leaf. We use $G - \{u_1, \ldots, u_k\}$ or $G - \{e_1, \ldots, e_k\}$ to denote the graph obtained from G by deleting the vertices $u_1, \ldots, u_k$ of G or the edges $e_1, \ldots, e_k$ of G, respectively. In this paper we will work only with trees (i.e. connected acyclic graphs). As usual, by P_n and S_n we denote the path and the star with n vertices, respectively. A *rooted tree* is a tree in which there is one vertex that is distinguished from the others and is called the *root*. The *level* of a vertex is the number of edges along the unique path between it and the root. The *height* of a rooted tree is the maximum level of any vertex of the tree. Given the root or any internal vertex v of a rooted tree, the *children* of v are all those vertices that are adjacent to v and are one level farther away from the root than v. If w is a child of v, then v is called the *parent* of w, and two distinct vertices that are both children of the same parent are called *siblings*. Given two distinct vertices v and w, if v lies on the unique path between w and the root, then v is an *ancestor* of w and w is a *descendant* of v.

2. Upper bound for the geometric-arithmetic index of trees with a given domination number

In [20] the authors showed the extremal values of the geometric-arithmetic index over trees. Among trees with n vertices, the star S_n has the minimum geometric-arithmetic index and the path P_n attains the maximum geometric-arithmetic index.

Theorem 2.1. [20] *For any tree T with n vertices and different from a star S_n and a path P_n, we have*

$$\frac{2(n-1)^{\frac{3}{2}}}{n} = GA(S_n) < GA(T) < GA(P_n) = n - 3 + \frac{4\sqrt{2}}{3}.$$

Since the upper bound shown above is attained for any path, the only way to improve that bound for trees is to give some conditions about the tree or to include another parameter in the bound. The domination number is one of the most studied parameters in graphs, in this section we show a new upper bound for the geometric-arithmetic index of trees using, not only the order, but the order and the domination number.

The following lemma, which can be easily proved, will be used in the proof of the main theorem. Many times throughout this work we say that an inequality can be checked, in our case, we have checked those inequalities using the program Mathematica.

Lemma 2.2. *Let $f(x) = \frac{\sqrt{x}}{a+x} - \frac{\sqrt{x-1}}{a+x-1}$ with $a > 0$ and $x \geq 1$. Then, $f(x)$ is a negative function for every $x \geq a+1$.*

Theorem 2.3. *For any tree T with order n and domination number γ, we have*

$$GA(T) \leq 3\gamma + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n - 3\gamma) - 3 + \frac{4\sqrt{2}}{3}.$$

Proof. To simplify the computation, we define

$$f(n,\gamma) = 3\gamma + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n - 3\gamma) - 3 + \frac{4\sqrt{2}}{3},$$

which is an increasing function in both variables. Let us prove the result by induction on n. When $n = 2$ or $n = 3$ we have $GA(P_2) = 1 < 3 - \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right) - 3 + \frac{4\sqrt{2}}{3} = 3 - \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$ and $GA(P_3) = \frac{4\sqrt{2}}{3} = f(3,1)$. If $n = 4$, then T is a path or a star. If T is a star, then $GA(T) = \frac{3\sqrt{3}}{2} < f(4,1) = -3 + \frac{6\sqrt{6}}{5} + 2\sqrt{2}$. If T is a path, then $GA(T) = 1 + \frac{4\sqrt{2}}{3} < f(4,2) = 9 - \frac{12\sqrt{6}}{5}$. We suppose that the upper bound is true for any tree with $n-1$ vertices and we take a tree T with n vertices and domination number γ.

Claim 1. *Let v be a support vertex of T such that $N(v) = \{u_1, u_2, \ldots, u_j\}$ and $d_{u_i} = 1$ for every $1 \leq i \leq j-1$. If $j \geq 4$ or $j = 3$ and $d_{u_3} \leq 8$, then $GA(T) < f(n,\gamma)$.*

Proof of Claim 1. We consider $T_1 = T - \{u_1\}$. Then, we know that $\gamma(T_1) = \gamma$ and, by induction, we have

$$\begin{aligned} GA(T) &= GA(T_1) + \frac{2\sqrt{j}}{j+1} + 2(j-2)\left(\frac{\sqrt{j}}{j+1} - \frac{\sqrt{j-1}}{j}\right) \\ &\quad +2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) \\ &\le 3\gamma + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n-1-3\gamma) - 3 + \frac{4\sqrt{2}}{3} + \frac{2\sqrt{j}}{j+1} \\ &\quad +2(j-2)\left(\frac{\sqrt{j}}{j+1} - \frac{\sqrt{j-1}}{j}\right) + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right), \end{aligned}$$

thus,

$$\begin{aligned} GA(T) &\le f(n,\gamma) - \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3} + 3 + \frac{2\sqrt{j}}{j+1} + 2(j-2)\left(\frac{\sqrt{j}}{j+1} - \frac{\sqrt{j-1}}{j}\right) \\ &\quad +2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right). \end{aligned}$$

It can be checked that

$$\begin{aligned} &-\frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3} + 3 + \frac{2\sqrt{j}}{j+1} + 2(j-2)\left(\frac{\sqrt{j}}{j+1} - \frac{\sqrt{j-1}}{j}\right) \\ &\quad +2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) < 0, \end{aligned}$$

if $j \ge 4$, or $j = 3$ and $d_{u_3} \le 8$.

Claim 2. *Let v be a vertex in T such that $N(v) = \{u_1, u_2, \dots, u_j\}$, $d_{u_1} = 3$ and u_1 is adjacent to two leaves w_1, w_2. If $d_{u_i} \le j-1$ for every $i \in \{2, \dots, j-1\}$ and $\gamma(T - \{u_1, w_1, w_2\}) = \gamma - 1$, then $GA(T) < f(n,\gamma)$.*

Proof of Claim 2. If we denote $T_3 = T - \{u_1, w_1, w_2\}$, we have

$$\begin{aligned} GA(T) &= GA(T_3) + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) \\ &\quad +2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1}\right) + \frac{2\sqrt{3j}}{j+3} + \sqrt{3}. \end{aligned}$$

Due to $\gamma(T_3) = \gamma - 1$, by induction, we know that $GA(T_3) \le f(n,\gamma) - 3$, then

$$\begin{aligned} GA(T) &\le f(n,\gamma) - 3 + \frac{2\sqrt{3j}}{j+3} + \sqrt{3} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) \\ &\quad +2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1}\right). \end{aligned}$$

Since $j \ge d_{u_i} + 1$ for any $i \in \{2, \dots, j-1\}$, by Lemma 2.2 we have that $\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1} < 0$, consequently,

$$GA(T) \le f(n,\gamma) - 3 + \frac{2\sqrt{3j}}{j+3} + \sqrt{3} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right).$$

But, it can be checked that $-3 + \frac{2\sqrt{3j}}{j+3} + \sqrt{3} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right)$ is negative for any $j \ge 2$ and $d_{u_j} \ge 1$.

Claim 3. *Let v be a vertex in T such that $N(v) = \{u_1, u_2, \dots, u_j\}$, $d_{u_1} = 2$ and u_1 is adjacent to a leaf w_1. If $d_{u_i} \le j-1$ for every $i \in \{2, \dots, j-1\}$ and $\gamma(T - \{u_1, w_1\}) = \gamma - 1$, then $GA(T) < f(n,\gamma)$.*

Proof of Claim 3. If we denote $T_2 = T - \{u_1, w_1\}$, we have

$$GA(T) = GA(T_2) + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) + 2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_1}+j-1}\right) + \frac{2\sqrt{2j}}{j+2} + \frac{2\sqrt{2}}{3}.$$

By induction, we know that $GA(T_2) \le f(n,\gamma) - 6 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$, thus,

$$GA(T) \le f(n,\gamma) - 6 + \frac{4\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) + 2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1}\right) + \frac{2\sqrt{2j}}{j+2}.$$

Since $j \ge d_{u_i} + 1$ for every $i \in \{2, \dots, j-1\}$, by Lemma 2.2 we know that $\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1} < 0$, therefore,

$$GA(T) \le f(n,\gamma) - 6 + \frac{4\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2j}}{j+2} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right).$$

But, it can be checked that

$$-6 + \frac{4\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2j}}{j+2} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) < 0,$$

for any $j \ge 2$ and $d_{u_j} \ge 1$.

Claim 4. *Let v be a vertex in T such that $d_v = j \ge 4$, $N(v) = \{u_1, u_2, \dots, u_j\}$, $N(u_1) = \{v, w_1\}$, $N(w_1) = \{u_1, w_2\}$ and $d_{w_2} = 1$. If $d_{u_i} \le j-1$ for every $i \in \{2, \dots, j-1\}$, then $GA(T) < f(n,\gamma)$.*

Proof of Claim 4. If we denote $T_3 = T - \{u_1, w_1, w_2\}$, we have

$$GA(T) = GA(T_3) + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) + 2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_1}+j-1}\right) + \frac{2\sqrt{2j}}{j+2} + 1 + \frac{2\sqrt{2}}{3}.$$

By induction, we know that $GA(T_3) \le f(n,\gamma) - 3$, then

$$GA(T) \le f(n,\gamma) - 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{2j}}{j+2} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) + 2\sum_{i=2}^{j-1}\sqrt{d_{u_i}}\left(\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1}\right).$$

Since $j \ge d_{u_i} + 1$ for every $i \in \{2, \dots, j-1\}$, by Lemma 2.2 we know that $\frac{\sqrt{j}}{d_{u_i}+j} - \frac{\sqrt{j-1}}{d_{u_i}+j-1} < 0$, therefore,

$$GA(T) \le f(n,\gamma) - 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{2j}}{j+2} + 2\sqrt{d_{u_j}}\left(\frac{\sqrt{j}}{d_{u_j}+j} - \frac{\sqrt{j-1}}{d_{u_j}+j-1}\right) < f(n,\gamma),$$

for any $j \ge 4$ and $d_{u_j} \ge 1$.

Now, since the bound is trivial for a star, we consider T as a rooted tree with root v_{k+1} and height $k \ge 3$, and let $v_1, v_2, \dots, v_{k+1}$ be a path from the root to a leaf v_1 in T. By Claims 1, 2, 3 and 4, it remains to prove the result when $d_{v_2} = 2 = d_{v_3}$ and $d_{v_4} \le 3$.

Case 1. We suppose that $d_{v_4}=3$. If we denote $N(v_4)=\{v_3,v_5,w_1\}$, again by the above claims, we can assume that $d_{w_1}\le 2$. If we take $T_3=T-\{v_1,v_2,v_3\}$, then we have

$$GA(T)=GA(T_3)+2\sqrt{d_{w_1}}\left(\frac{\sqrt{3}}{d_{w_1}+3}-\frac{\sqrt{2}}{d_{w_1}+2}\right)+2\sqrt{d_{v_5}}\left(\frac{\sqrt{3}}{d_{v_5}+3}-\frac{\sqrt{2}}{d_{v_5}+2}\right)+\frac{2\sqrt{6}}{5}+1+\frac{2\sqrt{2}}{3}.$$

Since $\gamma(T_3)=\gamma-1$, by induction, we know that $GA(T_3)\le f(n,\gamma)-3$, so

$$GA(T)\le f(n,\gamma)-2+\frac{2\sqrt{2}}{3}+\frac{2\sqrt{6}}{5}+2\sqrt{d_{w_1}}\left(\frac{\sqrt{3}}{d_{w_1}+3}-\frac{\sqrt{2}}{d_{w_1}+2}\right)+2\sqrt{d_{v_5}}\left(\frac{\sqrt{3}}{d_{v_5}+3}-\frac{\sqrt{2}}{d_{v_5}+2}\right).$$

Case 1.1. We suppose that $d_{w_1}=1$. Then,

$$GA(T)\le f(n,\gamma)-2+\frac{2\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+2\sqrt{d_{v_5}}\left(\frac{\sqrt{3}}{d_{v_5}+3}-\frac{\sqrt{2}}{d_{v_5}+2}\right)<f(n,\gamma),$$

for any $d_{v_5}\ge 1$.

Case 1.2. We suppose that $d_{w_1}=2$. Then,

$$GA(T)\le f(n,\gamma)-3+\frac{2\sqrt{2}}{3}+\frac{4\sqrt{6}}{5}+2\sqrt{d_{v_5}}\left(\frac{\sqrt{3}}{d_{v_5}+3}-\frac{\sqrt{2}}{d_{v_5}+2}\right)<f(n,\gamma),$$

for every $d_{v_5}\le 10$. Therefore, we suppose $d_{v_5}=s\ge 11$. If $N(v_5)=\{v_4,v_6,z_1,\dots,z_{s-2}\}$ and $d_{z_1}\ge 4$, by the cases above, we can assume that any path starting in v_5 and containing the edge v_5z_1 does not have more than four vertices. But, in such a case, using Claims 1, 2 and 3, we are done. Consequently, we consider $d_{z_i}\le 3$ for every $i\in\{1,2,\dots,s-2\}$.

Case 1.2.1. We suppose that $N(w_1)=\{v_4,w_2\}$ and $d_{w_2}=1$. In such a case, we denote $T_6=T-\{v_1,v_2,v_3,v_4,w_1,w_2\}$, so we have that

$$GA(T)=GA(T_6)+2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s}-\frac{\sqrt{s-1}}{d_{z_i}+s-1}\right)+2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s}-\frac{\sqrt{s-1}}{d_{v_6}+s-1}\right)+\frac{2\sqrt{3s}}{3+s}+\frac{4\sqrt{6}}{5}+1+\frac{4\sqrt{2}}{3}.$$

By induction, we know that $GA(T_6)\le f(n,\gamma)-6$ and, using Lemma 2.2, we obtain

$$GA(T)<f(n,\gamma)-5+\frac{2\sqrt{3s}}{3+s}+\frac{4\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}+2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s}-\frac{\sqrt{s-1}}{d_{v_6}+s-1}\right)<f(n,\gamma),$$

for any $s\ge 11$ and $d_{v_6}\ge 1$.

Case 1.2.2. We suppose that $N(w_1)=\{v_4,w_2\}$ and $N(w_2)=\{w_1,w_3\}$. In such a case, we denote $T_7=T-\{v_1,v_2,v_3,v_4,w_1,w_2,w_3\}$ and we have

$$GA(T)=GA(T_7)+2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s}-\frac{\sqrt{s-1}}{d_{z_i}+s-1}\right)+2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s}-\frac{\sqrt{s-1}}{d_{v_6}+s-1}\right)+\frac{2\sqrt{3s}}{3+s}+\frac{4\sqrt{6}}{5}+2+\frac{4\sqrt{2}}{3}.$$

Since $\gamma(T_7)\le\gamma-2$, by induction, we know that $GA(T_7)\le f(n,\gamma)-3-\frac{6\sqrt{6}}{5}-\frac{2\sqrt{2}}{3}$, then, using also that $\frac{\sqrt{s}}{d_{z_i}+s}-\frac{\sqrt{s-1}}{d_{z_i}+s-1}<0$ for every $i\in\{1,2,\dots,s-2\}$,

$$GA(T) < f(n,\gamma) - 1 + \frac{2\sqrt{3s}}{3+s} - \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) < f(n,\gamma),$$

for any $s \geq 11$ and $d_{v_6} \geq 1$.

Case 2. If $d_{v_4} = 2$ and we take $T_3 = T - \{v_1, v_2, v_3\}$, then we have $\gamma(T_3) = \gamma - 1$ and $GA(T_3) \leq f(n,\gamma) - 3$, consequently,

$$\begin{aligned} GA(T) &= GA(T_3) + 2\sqrt{d_{v_5}}\left(\frac{\sqrt{2}}{d_{v_5}+2} - \frac{1}{d_{v_5}+1}\right) + 2 + \frac{2\sqrt{2}}{3} \\ &\leq f(n,\gamma) - 1 + \frac{2\sqrt{2}}{3} + 2\sqrt{d_{v_5}}\left(\frac{\sqrt{2}}{d_{v_5}+2} - \frac{1}{d_{v_5}+1}\right) \leq f(n,\gamma), \end{aligned}$$

for every $d_{v_5} \leq 2$. Therefore, we suppose that $d_{v_5} = s \geq 3$. If $N(v_5) = \{v_4, v_6, z_1, \ldots, z_{s-2}\}$, since any path starting in v_5 and containing the edge $v_5 z_i$ does not have more than five vertices, by the claims and the cases above, we can assume that $d_{z_i} \leq 2$ for every $i \in \{1, 2, \ldots, s-2\}$. If we take $T_4 = T - \{v_1, v_2, v_3, v_4\}$, then

$$\begin{aligned} GA(T) = GA(T_4) &+ 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \\ &+ 2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s} - \frac{\sqrt{s-1}}{d_{z_i}+s-1}\right) + \frac{2\sqrt{2s}}{2+s} + 2 + \frac{2\sqrt{2}}{3}. \end{aligned}$$

By induction, since $\gamma(T_4) \leq \gamma - 1$, we know that $GA(T_4) \leq f(n,\gamma) - \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3}$, then

$$\begin{aligned} GA(T) \leq f(n,\gamma) + 2 - \frac{6\sqrt{6}}{5} &+ 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \\ &+ 2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s} - \frac{\sqrt{s-1}}{d_{z_i}+s-1}\right) + \frac{2\sqrt{2s}}{2+s}. \end{aligned}$$

Case 2.1. We suppose $s \geq 9$. Due to $d_{z_i} \leq 2$ and $\sqrt{2}\left(\frac{\sqrt{s}}{2+s} - \frac{\sqrt{s-1}}{1+s}\right) < \frac{\sqrt{s}}{1+s} - \frac{\sqrt{s-1}}{s}$, we have that

$$\begin{aligned} & 2 - \frac{6\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \\ & \qquad + 2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s} - \frac{\sqrt{s-1}}{d_{z_i}+s-1}\right) + \frac{2\sqrt{2s}}{2+s} \\ & \leq 2 - \frac{6\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \\ & \qquad + 2(s-2)\left(\frac{\sqrt{s}}{1+s} - \frac{\sqrt{s-1}}{s}\right) + \frac{2\sqrt{2s}}{2+s} < 0, \end{aligned}$$

for every $s \geq 9$ and $d_{v_6} \geq 1$.

Case 2.2. We suppose $5 \leq s \leq 8$. Due to $d_{z_i} \leq 2$ and $\frac{\sqrt{s}}{1+s} - \frac{\sqrt{s-1}}{s} < \sqrt{2}\left(\frac{\sqrt{s}}{2+s} - \frac{\sqrt{s-1}}{1+s}\right)$, we have

$$\begin{aligned} & 2 - \frac{6\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \\ & \qquad + 2\sum_{i=1}^{s-2}\sqrt{d_{z_i}}\left(\frac{\sqrt{s}}{d_{z_i}+s} - \frac{\sqrt{s-1}}{d_{z_i}+s-1}\right) + \frac{2\sqrt{2s}}{2+s} \\ & \leq 2 - \frac{6\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{s}}{d_{v_6}+s} - \frac{\sqrt{s-1}}{d_{v_6}+s-1}\right) \end{aligned}$$

$$+2(s-2)\sqrt{2}\left(\frac{\sqrt{s}}{2+s}-\frac{\sqrt{s-1}}{1+s}\right)+\frac{2\sqrt{2s}}{2+s}<0,$$

if $5 \le s \le 8$ and $d_{v_6} \ge 1$.

Case 2.3. We suppose $s=4$. In such a case,

$$\begin{aligned}2-\frac{6\sqrt{6}}{5}+2\sqrt{d_{v_6}}\left(\frac{2}{d_{v_6}+4}-\frac{\sqrt{3}}{d_{v_6}+3}\right)\\ +2\sum_{i=1}^{2}\sqrt{d_{z_i}}\left(\frac{2}{d_{z_i}+4}-\frac{\sqrt{3}}{d_{z_i}+3}\right)+\frac{\sqrt{8}}{3}\\ \le 2-\frac{6\sqrt{6}}{5}+2\sqrt{d_{v_6}}\left(\frac{2}{d_{v_6}+4}-\frac{\sqrt{3}}{d_{v_6}+3}\right)+4\sqrt{2}\left(\frac{1}{3}-\frac{\sqrt{3}}{5}\right)+\frac{\sqrt{8}}{3}<0,\end{aligned}$$

for every $d_{v_6} \le 15$. Therefore, we suppose that $d_{v_6} \ge 16$.

Case 2.3.1. We suppose that there exists a minimum dominating set D in T such that $v_6 \in N[D \setminus \{v_5\}]$. Let T_1 and T_2 be two subtrees of $T-\{v_5v_6\}$, containing v_5 and v_6, respectively. Then, if $N(v_6)=\{v_5, w_1, \dots, w_{r-1}\}$, we have

$$\begin{aligned}GA(T)=GA(T_1)+GA(T_2)+2\sum_{i=1}^{r-1}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r}-\frac{\sqrt{r-1}}{d_{w_i}+r-1}\right)\\ +2\sum_{i=1}^{2}\sqrt{d_{z_i}}\left(\frac{2}{d_{z_i}+4}-\frac{\sqrt{3}}{d_{z_i}+3}\right)+2\sqrt{2}\left(\frac{1}{3}-\frac{\sqrt{3}}{5}\right)+\frac{2\sqrt{4r}}{4+r}.\end{aligned}$$

Since $2\sum_{i=1}^{2}\sqrt{d_{z_i}}\left(\frac{2}{d_{z_i}+4}-\frac{\sqrt{3}}{d_{z_i}+3}\right) \le 4\sqrt{2}\left(\frac{1}{3}-\frac{\sqrt{3}}{5}\right)$, by induction we have

$$\begin{aligned}GA(T) \le f(n,\gamma)-3+\frac{4\sqrt{2}}{3}+2\sum_{i=1}^{r-1}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r}-\frac{\sqrt{r-1}}{d_{w_i}+r-1}\right)\\ +6\sqrt{2}\left(\frac{1}{3}-\frac{\sqrt{3}}{5}\right)+\frac{2\sqrt{4r}}{4+r}.\end{aligned}$$

But, it can be checked that

$$-3+\frac{10\sqrt{2}}{3}-\frac{6\sqrt{6}}{5}+\frac{2\sqrt{4r}}{4+r}+2(r-1)\sqrt{x}\left(\frac{\sqrt{r}}{x+r}-\frac{\sqrt{r-1}}{x+r-1}\right)$$

is negative for any $r \ge 16$ and $x \ge 1$.

Case 2.3.2. We suppose that, for any minimum dominating set D in T, we have $D \cap N[v_6]=\{v_5\}$. If $w_1 \ne v_7$ and $d_{w_1} \ge 3$, then there exist a minimum dominating set D and $a_1 \in N(w_1) \cap D$ such that, by the above cases, any path starting in v_6 and containing v_6, w_1 and a_1 has not more than five vertices, consequently, a_1 must be adjacent to a leaf. Therefore, applying Claims 1, 2 and 3, we are done. Hence, we can suppose that $d_{w_i}=2$ for every $i \in \{1,2\dots,r-2\}$. But, if $d_{w_1}=2$, by the above cases, we can assume that $N(w_1)=\{v_6, a_1\}$, $N(a_1)=\{w_1, a_2\}$ and $d_{a_2}=1$, consequently, since $r \ge 4$, by Claim 4, we are done.

Case 2.4. We suppose $s=3$, and we distinguish two new cases.

Case 2.4.1. We suppose that $d_{z_1}=1$. Then, we have

$$\begin{aligned}2-\frac{6\sqrt{6}}{5}+2\sqrt{d_{v_6}}\left(\frac{\sqrt{3}}{d_{v_6}+3}-\frac{\sqrt{2}}{d_{v_6}+2}\right)+2\sqrt{d_{z_1}}\left(\frac{\sqrt{3}}{d_{z_1}+3}-\frac{\sqrt{2}}{d_{z_1}+2}\right)+\frac{2\sqrt{6}}{5}\\ =2-\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}+2\sqrt{d_{v_6}}\left(\frac{\sqrt{3}}{d_{v_6}+3}-\frac{\sqrt{2}}{d_{v_6}+2}\right),\end{aligned}$$

which is negative for $d_{v_6} \le 3$. Therefore, we assume that $d_{v_6}=r \ge 4$ and $N(v_6)=\{v_5, w_1, \dots, w_{r-1}\}$.

Case 2.4.1.1. We suppose that there exists a minimum dominating set D in T such that $v_6 \in N[D \setminus \{v_5\}]$. In such a case, if we denote $T_6=T-\{v_1, v_2, v_3, v_4, v_5, z_1\}$, we have

$$GA(T) = GA(T_6) + 2\sum_{i=1}^{r-1}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r} - \frac{\sqrt{r-1}}{d_{w_i}+r-1}\right)$$
$$+\frac{2\sqrt{3r}}{3+r} + \frac{2\sqrt{3}}{4} + \frac{2\sqrt{6}}{5} + 2 + \frac{2\sqrt{2}}{3}.$$

By induction, we know that $GA(T_6) \le f(n,\gamma) - 6$, then

$$GA(T) \le f(n,\gamma) - 4 + 2\sum_{i=1}^{r-1}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r} - \frac{\sqrt{r-1}}{d_{w_i}+r-1}\right)$$
$$+\frac{2\sqrt{3r}}{3+r} + \frac{2\sqrt{3}}{4} + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}.$$

But, it can be checked that

$$-4 + 2\sum_{i=1}^{r-1}\sqrt{x}\left(\frac{\sqrt{r}}{x+r} - \frac{\sqrt{r-1}}{x+r-1}\right) + \frac{2\sqrt{3r}}{3+r} + \frac{2\sqrt{3}}{4} + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} < 0,$$

for every $r \ge 4$ and $x \ge 1$.

Case 2.4.1.2. We suppose that, for any minimum dominating set D in T, we have $D \cap N[v_6] = \{v_5\}$. In such a case, since $r \ge 4$, we can do the same we did in Case 2.3.2.

Case 2.4.2. We suppose that $d_{z_1} = 2$. Then, we have

$$2 - \frac{6\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{3}}{d_{v_6}+3} - \frac{\sqrt{2}}{d_{v_6}+2}\right) + 2\sqrt{d_{z_1}}\left(\frac{\sqrt{3}}{d_{z_1}+3} - \frac{\sqrt{2}}{d_{z_1}+2}\right) + \frac{2\sqrt{6}}{5}$$
$$= 1 - \frac{2\sqrt{6}}{5} + 2\sqrt{d_{v_6}}\left(\frac{\sqrt{3}}{d_{v_6}+3} - \frac{\sqrt{2}}{d_{v_6}+2}\right),$$

which is equal to zero if $d_{v_6} = 2$. Therefore, we suppose that $d_{v_6} \ge 3$. Moreover, by the above cases, we can assume that $N(z_1) = \{v_5, a_1\}$, $N(a_1) = \{z_1, a_2\}$, $N(a_2) = \{a_1, a_3\}$ and $d_{a_3} = 1$, and, if $N(v_6) = \{v_5, v_7, w_1, \ldots, w_{r-2}\}$, by the above cases and Claims 1, 2, 3 and 4, we can also assume that $d_{w_i} \le 3$ for every $i \in \{1, 2 \ldots, r-2\}$.

Case 2.4.2.1. We suppose that there exists a minimum dominating set D in T such that $v_6 \in N[D \setminus \{v_5\}]$. In such a case, if we denote $T_9 = T - \{v_1, v_2, v_3, v_4, v_5, z_1, a_1, a_2, a_3\}$, we have

$$GA(T) = GA(T_9) + 2\sum_{i=1}^{r-2}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r} - \frac{\sqrt{r-1}}{d_{w_i}+r-1}\right)$$
$$+2\sqrt{d_{v_7}}\left(\frac{\sqrt{r}}{d_{v_7}+r} - \frac{\sqrt{r-1}}{d_{v_7}+r-1}\right) + \frac{2\sqrt{3r}}{3+r} + \frac{4\sqrt{6}}{5} + 4 + \frac{4\sqrt{2}}{3}.$$

By induction, we know that $GA(T_9) \le f(n,\gamma) - 9$, then

$$GA(T) \le f(n,\gamma) - 5 + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{2}}{3} + \frac{2\sqrt{3r}}{3+r} + 2\sqrt{d_{v_7}}\left(\frac{\sqrt{r}}{d_{v_7}+r} - \frac{\sqrt{r-1}}{d_{v_7}+r-1}\right)$$
$$+2\sum_{i=1}^{r-2}\sqrt{d_{w_i}}\left(\frac{\sqrt{r}}{d_{w_i}+r} - \frac{\sqrt{r-1}}{d_{w_i}+r-1}\right).$$

Now, using that $\max\left\{\frac{\sqrt{r}}{1+r} - \frac{\sqrt{r-1}}{r}, \sqrt{2}\left(\frac{\sqrt{r}}{2+r} - \frac{\sqrt{r-1}}{1+r}\right)\right\} \le \sqrt{3}\left(\frac{\sqrt{r}}{3+r} - \frac{\sqrt{r-1}}{2+r}\right)$ for $3 \le r \le 11$ and $\max\left\{\sqrt{2}\left(\frac{\sqrt{r}}{2+r} - \frac{\sqrt{r-1}}{1+r}\right), \sqrt{3}\left(\frac{\sqrt{r}}{3+r} - \frac{\sqrt{r-1}}{2+r}\right)\right\} \le \frac{\sqrt{r}}{1+r} - \frac{\sqrt{r-1}}{r}$ for $r \ge 12$, it can be checked that

$$-5 + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{2}}{3} + \frac{2\sqrt{3r}}{3+r} + 2\sqrt{d_{v_7}}\left(\frac{\sqrt{r}}{d_{v_7}+r} - \frac{\sqrt{r-1}}{d_{v_7}+r-1}\right)$$
$$+2(r-2)\sqrt{3}\left(\frac{\sqrt{r}}{3+r} - \frac{\sqrt{r-1}}{2+r}\right) < 0,$$

for $3 \le r \le 11$ and $d_{v_7} \ge 1$, and

$$-5+\frac{4\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}+\frac{2\sqrt{3r}}{3+r}+2\sqrt{d_{v_7}}\left(\frac{\sqrt{r}}{d_{v_7}+r}-\frac{\sqrt{r-1}}{d_{v_7}+r-1}\right)$$
$$+2(r-2)\left(\frac{\sqrt{r}}{1+r}-\frac{\sqrt{r-1}}{r}\right)<0,$$

for $r\geq 12$ and $d_{v_7}\geq 1$.

Case 2.4.2.2. We suppose that, for any minimum dominating set D in T, we have $D\cap N[v_6]=\{v_5\}$. Looking at the proof of the Case 2.3.2, we can assume that $r=3$, $N(w_1)=\{v_6,a_1\}$, $N(a_1)=\{w_1,a_2\}$ and $d_{a_2}=1$. We denote $d_{v_7}=t$ and $T_3=T-\{w,a_1,a_2\}$. Then

$$GA(T)=GA(T_3)+2\sqrt{t}\left(\frac{\sqrt{3}}{t+3}-\frac{\sqrt{2}}{t+2}\right)+2\sqrt{3}\left(\frac{\sqrt{3}}{3+3}-\frac{\sqrt{2}}{3+2}\right)$$
$$+\frac{2\sqrt{6}}{5}+1+\frac{2\sqrt{2}}{3}.$$

By induction, we know that $GA(T_3)\leq f(n,\gamma)-3$, so

$$GA(T)\leq f(n,\gamma)-1+\frac{2\sqrt{2}}{3}+2\sqrt{t}\left(\frac{\sqrt{3}}{t+3}-\frac{\sqrt{2}}{t+2}\right)<f(n,\gamma),$$

for every $t\leq 4$.

Finally, we suppose that $N(v_7)=\{v_6,v_8,b_1,b_2,\ldots,b_{t-2}\}$ with $t\geq 5$. If $d_{b_i}\geq 2$ and we consider the rooted subtree $T_{v_7b_i}$ with root v_7 and containing b_i and all its descendants, since the height is not bigger than 6, we can do in a path of this subtree from the root to a leaf with length equal to the height, the same we did with the path $v_1-v_2-v_3-v_4-v_5-v_6-v_7$ to get that $d_{b_i}\leq 3$. Therefore, if we consider the subtrees T' and T'' of $T-\{v_6v_7\}$ containing v_6 and v_7, respectively, we have that

$$GA(T)=GA(T')+GA(T'')+2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t}-\frac{\sqrt{t-1}}{d_{v_8}+t-1}\right)$$
$$+2\sum_{i=1}^{t-2}\sqrt{d_{b_i}}\left(\frac{\sqrt{t}}{d_{b_i}+t}-\frac{\sqrt{t-1}}{d_{b_i}+t-1}\right)$$
$$+2\sqrt{2}\left(\frac{\sqrt{3}}{2+3}-\frac{\sqrt{2}}{2+2}\right)+2\sqrt{3}\left(\frac{\sqrt{3}}{3+3}-\frac{\sqrt{2}}{3+2}\right)+\frac{2\sqrt{3t}}{3+t}.$$

By induction, we know that $GA(T')+GA(T'')\leq f(n,\gamma)-3+\frac{4\sqrt{2}}{3}$, then

$$GA(T)\leq f(n,\gamma)-3+\frac{4\sqrt{2}}{3}+2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t}-\frac{\sqrt{t-1}}{d_{v_8}+t-1}\right)$$
$$+2\sum_{i=1}^{t-2}\sqrt{d_{b_i}}\left(\frac{\sqrt{t}}{d_{b_i}+t}-\frac{\sqrt{t-1}}{d_{b_i}+t-1}\right)+\frac{2\sqrt{3t}}{3+t}.$$

If $5\leq t\leq 11$, then

$$-3+\frac{4\sqrt{2}}{3}+2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t}-\frac{\sqrt{t-1}}{d_{v_8}+t-1}\right)$$
$$+2\sum_{i=1}^{t-2}\sqrt{d_{b_i}}\left(\frac{\sqrt{t}}{d_{b_i}+t}-\frac{\sqrt{t-1}}{d_{b_i}+t-1}\right)+\frac{2\sqrt{3t}}{3+t}$$
$$\leq -3+\frac{4\sqrt{2}}{3}+2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t}-\frac{\sqrt{t-1}}{d_{v_8}+t-1}\right)$$
$$+2(t-2)\sqrt{3}\left(\frac{\sqrt{t}}{3+t}-\frac{\sqrt{t-1}}{3+t-1}\right)+\frac{2\sqrt{3t}}{3+t}<0,$$

for every $d_{v_8} \geq 1$.

If $t \geq 12$, then

$$\begin{aligned}
&-3 + \frac{4\sqrt{2}}{3} + 2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t} - \frac{\sqrt{t-1}}{d_{v_8}+t-1}\right) \\
&\qquad + 2\sum_{i=1}^{t-2}\sqrt{d_{b_i}}\left(\frac{\sqrt{t}}{d_{b_i}+t} - \frac{\sqrt{t-1}}{d_{b_i}+t-1}\right) + \frac{2\sqrt{3t}}{3+t} \\
&\leq -3 + \frac{4\sqrt{2}}{3} + 2\sqrt{d_{v_8}}\left(\frac{\sqrt{t}}{d_{v_8}+t} - \frac{\sqrt{t-1}}{d_{v_8}+t-1}\right) \\
&\qquad + 2(t-2)\left(\frac{\sqrt{t}}{1+t} - \frac{\sqrt{t-1}}{t}\right) + \frac{2\sqrt{3t}}{3+t} < 0,
\end{aligned}$$

for every $d_{v_8} \geq 1$. □

Let us observe that, since the function $f(n,\gamma)$, in the above proof, is an increasing function on γ and $f\left(n, \frac{n}{3}\right) = n - 3 + \frac{4\sqrt{2}}{3}$, the upper bound given in Theorem 2.3 is better that $n - 3 + \frac{4\sqrt{2}}{3}$ when the domination number of the tree satisfies $\gamma < \frac{n}{3}$.

3. Extremal trees for the geometric-arithmetic index

In this section we characterize all the trees attaining the upper bound given in Theorem 2.3. To do that, we consider the following family $\mathcal{F}$ of graphs, which we define recursively. We consider any path with $3k$ vertices in $\mathcal{F}$ and we construct new graphs in the family in two ways.

(i) If $T \in \mathcal{F}$ satisfies that there exists $v \in V(T)$ such that v belongs to a minimum dominating set in T, $N(v) = \{v_1, v_2\}$, and $d_{v_1} = 2 = d_{v_2}$, and we take any path P, whose consecutive vertices are $u_1, u_2, \ldots, u_{3t+1}$, then the graph T' such that $V(T') = V(T) \cup V(P)$ and $E(T') = E(T) \cup E(P) \cup \{vu_1\}$, belongs to $\mathcal{F}$.

(ii) If $T \in \mathcal{F}$, v is a leaf in T and we take any path P, whose consecutive vertices are $u_1, u_2, \ldots, u_{3t}$, then the graph T' such that $V(T') = V(T) \cup V(P)$ and $E(T') = E(T) \cup E(P) \cup \{vu_1\}$, belongs to $\mathcal{F}$.

Using again the function

$$f(n,\gamma) = 3\gamma + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n - 3\gamma) - 3 + \frac{4\sqrt{2}}{3},$$

we present the following results.

Lemma 3.1. *If $T \in \mathcal{F}$, then $GA(T) = f(n(T), \gamma(T))$.*

Proof. If T is a path with $3k$ vertices we can easily check that the result is true. (i) We suppose that there exists $T \in \mathcal{F}$ that satisfies that $GA(T) = f(n(T), \gamma(T))$ and there exists $v \in V(T)$ such that $N(v) = \{v_1, v_2\}$, $d_{v_1} = 2 = d_{v_2}$, and v belongs to a minimum dominating set in T. If we consider $T' \in \mathcal{F}$, attaching to v a path P, whose consecutive vertices are $u_1, u_2, \ldots, u_{3t+1}$, by the edge vu_1, we have

$$\begin{aligned}
GA(T') &= GA(T) + GA(P) - 2 + \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3} + 1 \\
&= 3\gamma(T) + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n(T) - 3\gamma(T)) - 3 + \frac{4\sqrt{2}}{3} \\
&\qquad + 3t - 2 + \frac{4\sqrt{2}}{3} - 1 + \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3} \\
&= 3(\gamma(T) + t) + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)((n(T) + 3t + 1) - 3(\gamma(T) + t)) \\
&\qquad - 3 + \frac{4\sqrt{2}}{3}
\end{aligned}$$

$$= 3\gamma(T') + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n(T') - 3\gamma(T')) - 3 + \frac{4\sqrt{2}}{3}.$$

(ii) If $T \in \mathcal{F}$ satisfies that $GA(T) = f(n(T), \gamma(T))$, T has a leaf v, P is a path whose consecutive vertices are $u_1, u_2, \ldots, u_{3t}$, and we consider the graph T' such that $V(T') = V(T) \cup V(P)$ and $E(T') = E(T) \cup E(P) \cup \{vu_1\}$, since the only neighbor of v has degree 2, we have

$$\begin{aligned} GA(T') &= GA(T) + GA(P) - \frac{2\sqrt{2}}{3} + 1 + 1 - \frac{2\sqrt{2}}{3} + 1 \\ &= 3\gamma(T) + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n(T) - 3\gamma(T)) - 3 + \frac{4\sqrt{2}}{3} \\ &\qquad + 3t - 3 + \frac{4\sqrt{2}}{3} + 3 - \frac{4\sqrt{2}}{3} \\ &= 3\gamma(T') + \left(\frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} - 3\right)(n(T') - 3\gamma(T')) - 3 + \frac{4\sqrt{2}}{3}. \quad \square \end{aligned}$$

Theorem 3.2. *$GA(T) = f(n(T), \gamma(T))$ if and only if $T \in \mathcal{F}$.*

Proof. By Lemma 3.1, we only need to prove that any tree T satisfying $GA(T) = f(n(T), \gamma(T))$ belongs to the family $\mathcal{F}$. By absurdum, we suppose that there exists a tree T such that $GA(T) = f(n(T), \gamma(T))$ and $T \notin \mathcal{F}$. We take the tree T satisfying that with the minimum number of vertices. We consider T as a rooted tree with root v_{r+1} and height r, and take $v_1, v_2, \ldots, v_{r+1}$ a path from the root to a leaf v_1 in T. If we follow the proof of Theorem 2.3, we can assume that $d_{v_2} = d_{v_3} = d_{v_4} = 2$ and $d_{v_5} = 2$ or $d_{v_5} = 3$, $d_{z_1} = 2$ and $d_{v_6} = 2$.

If $d_{v_5} = 2$ and we take $T' = T - \{v_1, v_2, v_3\}$, we have

$$GA(T) = GA(T') - \frac{2\sqrt{2}}{3} + 3 + \frac{2\sqrt{2}}{3} \le f(n(T'), \gamma(T')) + 3 = f(n(T), \gamma(T)),$$

thus, $GA(T') = f(n(T'), \gamma(T'))$. If $T' \in \mathcal{F}$, since v_4 is a leaf in T', we would have that T belongs to $\mathcal{F}$. Therefore, $T' \notin \mathcal{F}$ and we get a contradiction with the minimality of T.

If $d_{v_5} = 3$, $d_{z_1} = 2$ and $d_{v_6} = 2$ and we consider $T' = T - \{v_1, v_2, v_3, v_4\}$, we have

$$\begin{aligned} GA(T) &= GA(T') - 2 + \frac{6\sqrt{6}}{5} + 2 + \frac{2\sqrt{2}}{3} \le f(n(T'), \gamma(T')) + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \\ &\le f(n(T), \gamma(T)), \end{aligned}$$

thus, $GA(T') = f(n(T'), \gamma(T'))$ and $\gamma(T') = \gamma - 1$, it means, v_5 belongs to a minimum dominating set in T'. If $T' \in \mathcal{F}$, then T would belong to $\mathcal{F}$. Therefore, $T' \notin \mathcal{F}$ and we get a contradiction with the minimality of T. $\square$

4. Conclusions

We have determined an upper bound for the geometric-arithmetic index of trees and we have characterized the extremal trees for this bound, but these results can be applied to obtain a lower bound for another topological index, the arithmetic-geometric index. The arithmetic-geometric index, which firstly appeared in [15], is defined as

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

For any tree T with $n \ge 3$ vertices, it was recently proved in [19] that

$$AG(T) \ge n - 3 + \frac{3}{\sqrt{2}} \qquad \text{and} \qquad AG(T) + GA(T) \ge 2n - 6 + \frac{17\sqrt{2}}{6},$$

and that these lower bounds are only attained by the paths P_n with n vertices. Then, by our Theorem 2.3, it T is a tree with order n and domination number γ, we obtain

$$AG(T) \ge n + \left(4 - \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3}\right)(n - 3\gamma) - 3 + \frac{3}{\sqrt{2}},$$

and this lower bound is only attained by the paths P_{3k}. Moreover, since $4 - \frac{6\sqrt{6}}{5} - \frac{2\sqrt{2}}{3} > 0$, this lower bound improves the general one $n - 3 + \frac{3}{\sqrt{2}}$ when $\gamma(T) < \frac{n}{3}$.

The family $\mathcal{F}$ of graphs attaining the upper bound in Theorem 2.3 was already given in [4] as extremal trees for a similar upper bound. Using the same family $T_{s,r}$ they gave there for the lower bound of the Randić index, we think that the following conjecture could be true.

Conjecture 4.1. *If T is a tree with order n and domination number γ, then*

$$GA(T) \geq \frac{2(n-2\gamma+1)\sqrt{n-\gamma}}{n-\gamma+1} + \frac{2\sqrt{2}(\gamma-1)\sqrt{n-\gamma}}{n-\gamma+2} + \frac{2\sqrt{2}(\gamma-1)}{3}.$$

Moreover, this lower bound is attained if and only if $T = T_{s,r}$.

If this conjecture were true, since the inequalities

$$AG(T) \leq \frac{n\sqrt{n-1}}{2} \qquad \text{and} \qquad AG(T) + GA(T) \leq \frac{(n^2+4n-4)\sqrt{n-1}}{2n}$$

were proved in [19], and they are only attained when T is a star, we would have

$$AG(T) \leq \frac{(n^2+4n-4)\sqrt{n-1}}{2n} - \frac{2(n-2\gamma+1)\sqrt{n-\gamma}}{n-\gamma+1} - \frac{2\sqrt{2}(\gamma-1)\sqrt{n-\gamma}}{n-\gamma+2} - \frac{2\sqrt{2}(\gamma-1)}{3}.$$

This upper bound is smaller than $\frac{n\sqrt{n-1}}{2}$ when $\gamma \geq 2$.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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