Discrete Mathematics Letters
www.dmlett.com

Discrete Math. Lett. **9** (2022) 38–43
DOI: 10.47443/dml.2021.s207

Research Article

Extremal trees for the geometric-arithmetic index with the maximum degree

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(Received: 29 December 2021. Received in revised form: 2 January 2022. Accepted: 15 January 2022. Published online: 27 January 2022.)

Abstract

For a graph G, the geometric-arithmetic index of G, denoted by $GA(G)$, is defined as the sum of the quantities $2\sqrt{d_x \times d_y}/(d_x + d_y)$ over all edges $xy \in E(G)$. Here, d_x indicates the vertex degree of x. For every tree T of order $n \geq 3$, Vukičević and Furtula [*J. Math. Chem.* **46** (2009) 1369–1376] demonstrated that $GA(T) \leq \frac{4\sqrt{2}}{3} + (n-3)$. This result is extended in the present paper. Particularly, for any tree $\mathscr{T}$ of order $n \geq 5$ and maximum degree Δ, it is proved that

$$GA(\mathscr{T}) \leq \begin{cases} 2\left(\frac{(2\Delta-n+1)\sqrt{\Delta}}{\Delta+1} + \frac{(n-\Delta-1)\sqrt{3}}{3} + \frac{(n-\Delta-1)\sqrt{2\Delta}}{\Delta+2}\right) & \text{if } \Delta > \frac{n-1}{2}, \\ 2\left(\frac{\Delta\sqrt{2}}{3} + \frac{\Delta\sqrt{2\Delta}}{\Delta+2} + \frac{2(n-2\Delta-1)}{4}\right) & \text{if } \Delta \leq \frac{n-1}{2}. \end{cases}$$

and the corresponding extremal trees are characterized.

Keywords: topological indices; geometric-arithmetic index; degree of a vertex.

2020 Mathematics Subject Classification: 05C09, 05C92.

1. Introduction

Let G be a simple connected graph with the vertex set $V(G)$ and the edges set $E(G)$. The order $n(G)$ of G is the cardinality of the vertex set $V(G)$ and the size $m(G)$ of G is the cardinality of the edge set $E(G)$. The set $N(y) = \{x \in V(G) \mid xy \in E(G)\}$ is the open neighbourhood of a vertex $y \in V(G)$. Also, for a vertex $y \in V(G)$, its degree d_y is equal to the cardinality of $N(y)$. The maximum and minimum degrees of a graph G are denoted by $\Delta(G)$ and $\delta(G)$, respectively. A vertex of degree one in a tree is known as a leaf. A vertex adjacent to a leaf is referred to as a stem. A strong stem is a vertex adjacent to two or more leaves. An end stem is a vertex whose only neighbours are leaves, except one. A rooted tree is a directed rooted tree with a distinct vertex ν (see [9]).

Many degree-based topological indices have been widely studied; for example, see [5, 6, 11]. In this paper, we study one of the degree-based topological indices, namely the geometric-arithmetic index proposed in [12]. The definition of the geometric-arithmetic (GA) index for a simple connected graph G is

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

In [2, 14], the first three minimum and maximum values of the GA index were determined, and some lower and upper bounds on the GA index for molecular graphs were obtained. Additional details about the mathematical study of the GA index can be found in [1, 3, 4, 7, 10].

In [12], Vukičević and Furtula demonstrated the upper bound, given in the next theorem, on the geometric-arithmetic index for trees.

Theorem 1.1. *If T is a tree with n vertices, then*

$$GA(T) \leq \frac{4\sqrt{2}}{3} + (n-3)$$

where the upper bound is achieved if and only if T is the path graph.

In this work, we extend Theorem 1.1 by providing an upper bound on the geometric-arithmetic index for trees T in terms of order and maximum degree of T. We also characterize all the extremal trees attaining the bound.

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2. Some lemmas

This section gives some lemmas that will be used for proving the main result of this paper. A rooted tree with root ν is denoted by $\mathscr{T}$, where ν is a vertex of maximum degree and $\mathscr{N}(\nu) = \{v_1, v_2, \ldots, v_\Delta\}$. In addition, $ga_\nu = E(\mathscr{T}) \to \mathbb{R}$ is the function defined by $ga_\nu(xy) = \frac{\sqrt{d_x \times d_y}}{d_x + d_y}$. So, $GA(\mathscr{T}) = \sum\limits_{e \in E(\mathscr{T})} ga_\nu(e)$.

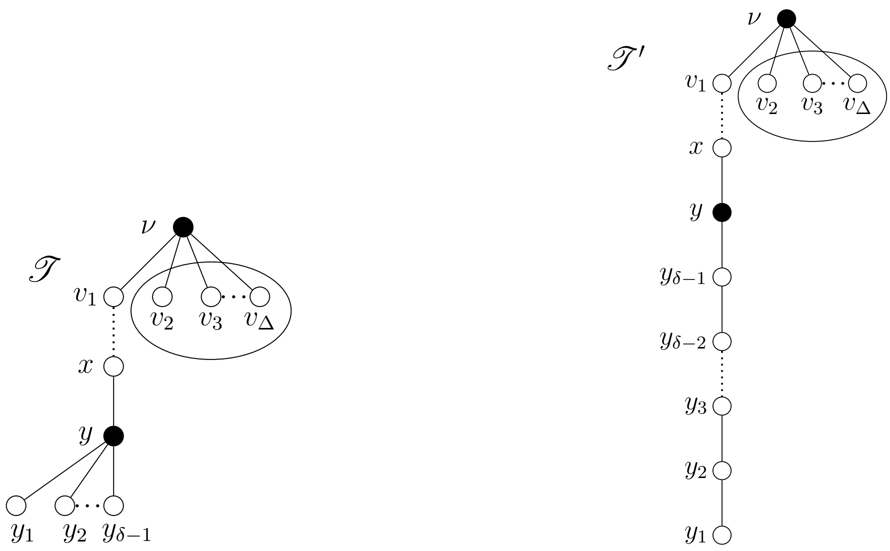


Figure 1: The trees $\mathscr{T}$ and $\mathscr{T}'$ used in the proof of Lemma 2.1.

Lemma 2.1. *Let n be the order of the tree $\mathscr{T}$ and Δ be its maximum degree. If $\mathscr{T}$ contains at least one vertex of degree three, an end-stem, and it differs from ν; then there exists a tree $\mathscr{T}'$ of order n and maximum degree Δ such that $GA(\mathscr{T}) < GA(\mathscr{T}')$.*

Proof. In $\mathscr{T}$, assume that y ($\neq \nu$) is an end-stem with $d(y) = \delta \geq 3$ and let $\mathscr{N}(y) = \{y_1, y_2, \ldots, y_{\delta-1}, x\}$, where x is the parent of y. Take $d(x) = u$ and $S = \{yy_1, yy_2, \ldots, yy_{\delta-1}, yx\}$. Let $\mathscr{T}'$ be the tree formed by adding the path $y_{\delta-1}y_{\delta-2}\ldots y_2y_1$ to $\mathscr{T} \setminus \{y_1, \ldots, y_{\delta-2}\}$ (see Figure 1). Obviously, $\mathscr{T}'$ is a tree of an order n and $\Delta(\mathscr{T}) = \Delta(\mathscr{T}')$. We have

$$\begin{aligned}\frac{1}{2}GA(\mathscr{T}) &= \sum_{xy \notin S} ga_\nu(xy) + \sum_{xy \in S} ga_\nu(xy) \\ &= \sum_{xy \notin S} ga_\nu(xy) + \frac{\sqrt{\delta u}}{\delta + u} + \frac{(\delta-2)\sqrt{\delta}}{\delta+1} + \frac{\sqrt{\delta}}{\delta+1} \qquad (1)\end{aligned}$$

and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy \notin S} ga_\nu(xy) + \frac{\sqrt{2u}}{2+u} + \frac{(\delta-2)}{2} + \frac{\sqrt{2}}{3}. \qquad (2)$$

We derive $GA(\mathscr{T}) < GA(\mathscr{T}')$ by combining (1) and (2), and by using the fact that $\delta \geq 3$. □

Lemma 2.2. *Let n be the order of the tree $\mathscr{T}$ and Δ be its maximum degree. If $\mathscr{T}$ contains at least one vertex of degree three, a stem, and it differs from ν; then there exists a tree $\mathscr{T}'$ of maximum degree Δ and order n such that $GA(\mathscr{T}) < GA(\mathscr{T}')$.*

Proof. Assume that x ($\neq \nu$) is a stem of $\mathscr{T}$ with $d(x) = \delta \geq 3$ and let $\mathscr{N}(x) = \{x_1, x_2, \ldots, x_{\delta-1}, y\}$, where x_1 is the parent of x and $d(y) = 1$. The vertex x is not an end-stem by Lemma 2.1. Let $\mathscr{T}_i$ be the component of $\mathscr{T} \setminus \nu$ that contains v_i. Let w be the parent of the leaf $q_i \in V(\mathscr{T}_i)$ and q_i be the maximum distance from v_i (see Figure 2). Then, by Lemma 2.1, $d(w) = 2$.

Let $\mathscr{T}'$ be the tree formed by adding a pendent edge q_iy to $\mathscr{T} \setminus xy$ (see Figure 2) and $S = \{q_iw, xy, xx_1, xx_2, \ldots, xx_{\delta-1}\}$. Obviously, $\mathscr{T}'$ is a tree of order n with $\Delta(\mathscr{T}) = \Delta(\mathscr{T}')$. We have

$$\begin{aligned}\frac{1}{2}GA(\mathscr{T}) &= \sum_{xy \notin S} ga_\nu(xy) + \sum_{xy \in S} ga_\nu(xy) \\ &= \sum_{xy \notin S} ga_\nu(xy) + \frac{\sqrt{\delta}}{\delta+1} + \sum_{i=1}^{\delta-1} \frac{\sqrt{\delta d_{x_i}}}{\delta + d_{x_i}} + \frac{\sqrt{2}}{3} \qquad (3)\end{aligned}$$

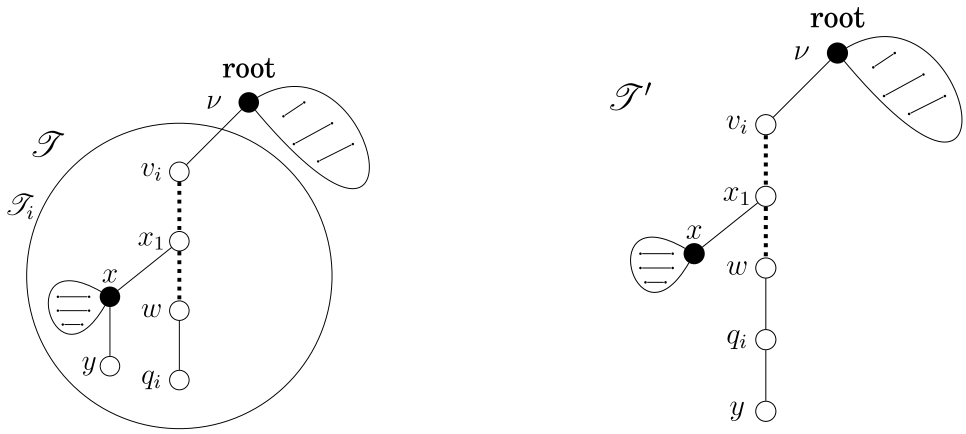


Figure 2: The trees $\mathscr{T}$ and $\mathscr{T}'$ used in the proof of Lemma 2.2.

and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy\notin S} ga_\nu(xy) + \frac{1}{2} + \sum_{i=1}^{\delta-1}\frac{\sqrt{(\delta-1)d_{x_i}}}{(\delta-1)+d_{x_i}} + \frac{\sqrt{2}}{3}. \tag{4}$$

We obtain $GA(\mathscr{T}) < GA(\mathscr{T}')$ by combining (3) and (4). This completes the proof. □

Lemma 2.3. *Let n be the order of the tree $\mathscr{T}$ and Δ be its maximum degree. If $\mathscr{T}$ contains at least one vertex of degree three and it differs from ν, then there exists a tree $\mathscr{T}'$ of maximum degree Δ and order n such that $GA(\mathscr{T}) < GA(\mathscr{T}')$.*

Proof. Let $y \neq \nu$ and $d(y) = \delta \geq 3$, i.e., $d(y,\nu)$ should probably be large. Let $\mathscr{N}(y) = \{x_1^0, x_2^0, \ldots, x_{\delta-1}^0, x_\delta\}$, where x_δ is the parent of y. Let $x_i^0 x_i^1 \ldots x_i^{u_i}$ be a longest path in $\mathscr{T}_i$ starting at x_i^0 for $i = 1, \ldots, \delta-1$. Assume that $q_i \in V(\mathscr{T}_i)$ is a leaf and w be its parent, such that it has the maximum distance from v_i (see Figure 3). Suppose that $q_i \notin \{x_1^{u_1}, \ldots, x_{\delta-2}^{u_{\delta-2}}\}$. We assume that $d(w) = 2$, by Lemma 2.1 and 2.2 and by using the option of y and that, apart from leaves, every descendant of y has degree two. We examine two cases.

Case 1. $\delta = 3$.
Let $\mathscr{T}'$ be the tree formed by adding an edge $q_i x_1^0$ to $\mathscr{T} \setminus yx_1^0$ (see Figure 3) and $S = \{yx_1^0, yx_2^0, yx_3, q_i w\}$. Obviously, $\mathscr{T}'$ is a tree of order n with $\Delta(\mathscr{T}) = \Delta(\mathscr{T}')$. We have

$$\begin{aligned}\frac{1}{2}GA(\mathscr{T}) &= \sum_{xy\notin S} ga_\nu(xy) + \sum_{xy\in S} ga_\nu(xy)\\ &= \sum_{xy\notin S} ga_\nu(xy) + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3\times d_{x_3}}}{3+d_{x_3}} + \frac{\sqrt{2}}{3}\end{aligned} \tag{5}$$

and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy\notin S} ga_\nu(xy) + \frac{1}{2} + \frac{1}{2} + \frac{\sqrt{2\times d_{x_3}}}{2+d_{x_3}} + \frac{1}{2}. \tag{6}$$

We obtain $GA(\mathscr{T}) < GA(\mathscr{T}')$ by combining (5) and (6).

Case 2. $\delta \geq 4$.
Let $q_i \neq x_{\delta-1}^{u_{\delta-1}}$. Let $\mathscr{T}'$ be the tree formed by adding edges $x_1^0 q_i, x_2^0 x_1^{u_1}, x_3^0 x_2^{u_2}, \ldots, x_{\delta-1}^0 x_{\delta-2}^{u_{\delta-2}}$ to $\mathscr{T} \setminus x_1^0 y, x_2^0 y, \ldots, x_{\delta-1}^0 y$. Clearly, $\mathscr{T}'$ is a tree of order n and $\Delta(\mathscr{T}) = \Delta(\mathscr{T}')$. Let $S = \{q_i w, yx_\delta\} \cup \{yx_i^0, x_i^{u_i} x_i^{u_i - 1} | 1 \leq i \leq \delta - 1\}$. By definition, we have

$$\begin{aligned}\frac{1}{2}GA(\mathscr{T}) &= \sum_{xy\notin S} ga_\nu(xy) + \sum_{xy\in S} ga_\nu(xy)\\ &= \sum_{xy\notin S} ga_\nu(xy) + \frac{(\delta-1)\sqrt{2}}{3} + \frac{(\delta-1)\sqrt{2\delta}}{\delta+2} + \frac{\sqrt{\delta\times d_{x_\delta}}}{\delta+d_{x_\delta}} + \frac{\sqrt{2}}{3}\end{aligned} \tag{7}$$

and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy\notin S} ga_\nu(xy) + \frac{2(\delta-1)}{4} + \frac{\sqrt{2}}{3} + \frac{2(\delta-1)}{4} + \frac{\sqrt{d_{x_\delta}}}{1+d_{x_\delta}}. \tag{8}$$

From (7) and (8), we obtain $GA(\mathscr{T}) < GA(\mathscr{T}')$.

Next, let $q_i = x_{\delta-1}^{u_{\delta-1}}$. Let $\mathscr{T}'$ be the tree formed by adding edges $x_1^0 q_i, x_i^{u_i} x_{i+1}^0$ for $1 \le i \le \delta - 3$ to $\mathscr{T} \setminus yx_i^0$ for $i = 1, \ldots, \delta-2$. Assume that $S = \{yx_\delta\} \cup \{yx_i^0, x_i^{u_i} x_i^{u_i - 1} | 1 \le i \le \delta - 1\}$. By definition, we have

$$\frac{1}{2}GA(\mathscr{T}) = \sum_{xy \notin S} ga_\nu(xy) + \sum_{xy \in S} ga_\nu(xy)$$

$$= \sum_{xy \notin S} ga_\nu(xy) + \frac{(\delta-1)\sqrt{2}}{3} + \frac{(\delta-1)\sqrt{2\delta}}{\delta+2} + \frac{\sqrt{\delta \times d_{x_\delta}}}{\delta + d_{x_\delta}} \tag{9}$$

and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy \notin S} ga_\nu(xy) + \frac{\delta-2}{2} + \frac{\sqrt{2}}{3} + \frac{\delta-1}{2} + \frac{\sqrt{2 \times d_{x_\delta}}}{2 + d_{x_\delta}}. \tag{10}$$

Note that

$$\frac{\sqrt{\delta \times d_{u_\delta}}}{\delta + d_{u_\delta}} < \frac{\sqrt{2 \times d_{u_\delta}}}{2 + d_{u_\delta}},$$

$$\frac{(\delta-2)\sqrt{2}}{3} + \frac{(\delta-1)\sqrt{2\delta}}{\delta+2} \le \frac{(\delta-3)\sqrt{2\delta} + 2\sqrt{2}}{2},$$

$$\frac{\delta-2}{2} + \frac{\sqrt{2}}{3} + \frac{\delta-1}{2} = \frac{(\delta-3)\sqrt{2\delta} + 2\sqrt{2}}{2} + \frac{1}{7}.$$

Thus, from (9) and (10) we conclude that $GA(\mathscr{T}) < GA(\mathscr{T}')$. □

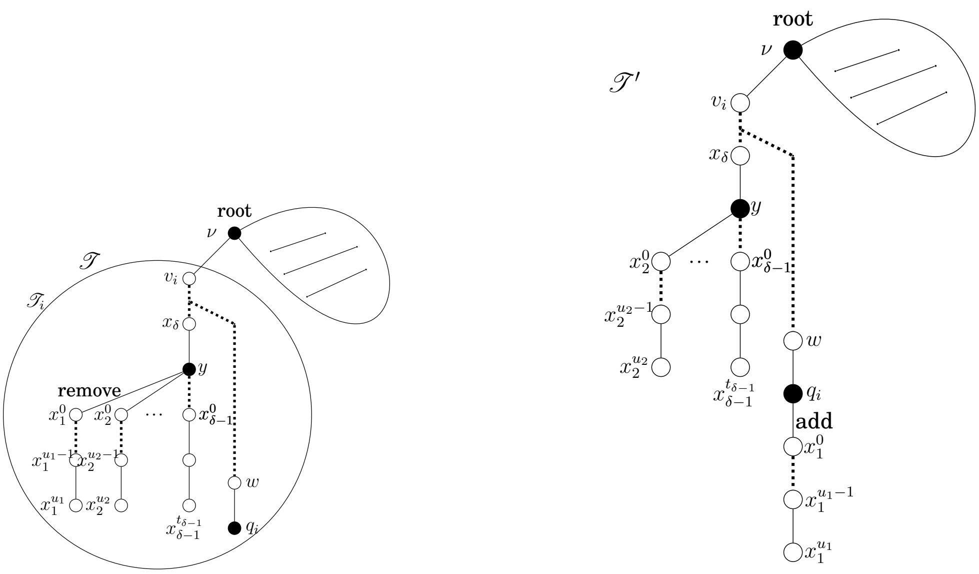


Figure 3: The trees $\mathscr{T}$ and $\mathscr{T}'$ used in the proof of Lemma 2.3.

A spider tree (also known as a star-like tree) [8,13] has at most one vertex (known as the center) of degree greater than two; see [9] for more information. A leg of a spider tree is a path that connects its center to a vertex of degree one.

Lemma 2.4. *Let n be the order of the spider tree $\mathscr{T}$ with $k \ge 3$ legs. If $\mathscr{T}$ has a leg of length one and a leg of length at least 3, then there exists a spider tree $\mathscr{T}'$ of order n with k legs such that $GA(\mathscr{T}) < GA(\mathscr{T}')$.*

Proof. Let the center of $\mathscr{T}$ be ν and $\mathscr{N}(\nu) = \{v_1, v_2, \ldots, v_k\}$. Let ν be the root of $\mathscr{T}$. Let $d(v_1) = 1$, without loss of generality, and let the leg $v_k z_1 z_2 \ldots z_u$ be a longest one in $\mathscr{T}$. Let the tree $\mathscr{T}'$ be formed by adding a pendent edge $v_1 z_u$ to $\mathscr{T} \setminus z_u z_{u-1}$. Assume that $S = \{v_1\nu, z_u z_{u-1}, z_{u-2} z_{u-1}\}$. By definition, we have

$$\frac{1}{2}GA(\mathscr{T}) = \sum_{xy \notin S} ga_\nu(xy) + \sum_{xy \in S} ga_\nu(xy)$$

$$= \sum_{xy \notin S} ga_{\nu}(xy) + \frac{2}{k+1} + \frac{\sqrt{2}}{3} + \frac{\sqrt{3}}{4} \tag{11}$$

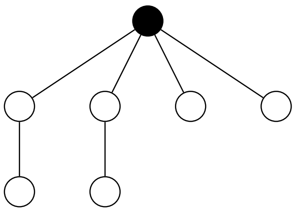
and

$$\frac{1}{2}GA(\mathscr{T}') = \sum_{xy \notin S} ga_{\nu}(xy) + \frac{\sqrt{2k}}{k+2} + \frac{\sqrt{2}}{3} + \frac{\sqrt{2}}{3}. \tag{12}$$

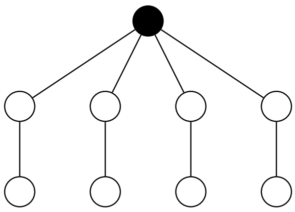
From (11) and (12), we see that $GA(\mathscr{T}) < GA(\mathscr{T}')$. $\square$

3. Main result

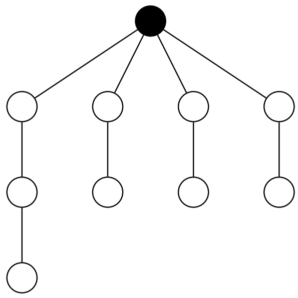
In this section, we present the main result of this paper. Figure 4 represents trees with the maximum GA index among trees of maximum degree 4 and order n for $n = 7, 9, 10$.



(a) $GA(\mathscr{T}_7) = \frac{40\sqrt{2}+24}{15}$



(b) $GA(\mathscr{T}_9) = \frac{16\sqrt{2}}{3}$



(c) $GA(\mathscr{T}_{10}) = \frac{64\sqrt{2}+12}{12}$

Figure 4: Trees attaining the maximum GA index among trees of maximum degree 4 and orders 7, 9, and 10.

Theorem 3.1. *If $\mathscr{T}$ is a tree of order $n \geq 5$ and maximum degree Δ then*

$$GA(\mathscr{T}) \leq \begin{cases} 2\Big(\frac{(2\Delta-n+1)\sqrt{\Delta}}{\Delta+1} + \frac{(n-\Delta-1)\sqrt{3}}{3} + \frac{(n-\Delta-1)\sqrt{2\Delta}}{\Delta+2}\Big) & \text{if } \Delta > \frac{n-1}{2} \\ 2\Big(\frac{\Delta\sqrt{2}}{3} + \frac{\Delta\sqrt{2\Delta}}{\Delta+2} + \frac{2(n-2\Delta-1)}{4}\Big) & \text{if } \Delta \leq \frac{n-1}{2} \end{cases}$$

with equality if and only if $\mathscr{T}$ is a spider tree and all of its legs have lengths at most two or all of its legs have lengths at least two.

Proof. Let $GA(\mathscr{T}_1) = \max\{GA(\mathscr{T}) \mid \mathscr{T}$ be a tree of order n and maximum degree $\Delta\}$. Let ν be the root of $\mathscr{T}_1$ and its degree be Δ. If $\Delta = 2$, then $\mathscr{T}$ is the path of order n, and the result follows from Theorem 1.1. Next, we assume that $\Delta \geq 3$. By using Lemmas 2.1, 2.2 and 2.3, we conclude that $\mathscr{T}_1$ is a spider tree with center ν. By Lemma 2.4, all the legs of $\mathscr{T}_1$ have lengths either at most two or at least two.

Suppose that all the legs of $\mathscr{T}_1$ have lengths at least two. Then, it is obvious that $\Delta \leq \frac{n-1}{2}$ and

$$GA(\mathscr{T}_1) = 2\Big(\frac{\Delta\sqrt{2}}{3} + \frac{\Delta\sqrt{2\Delta}}{\Delta+2} + \frac{(n-2\Delta-1)}{2}\Big).$$

Next, assume that all the legs of $\mathscr{T}_1$ have lengths at most two. Suppose $\mathscr{T}_1$ has at least one leg of length one. The result is immediate if $\mathscr{T}_1$ is a star graph. If $\mathscr{T}_1$ is not a star, then $(2\Delta+1-n)\sqrt{\Delta}$ is the number of leaves adjacent to ν and thence

$$GA(T) = 2\Big(\frac{(2\Delta+1-n)\sqrt{\Delta}}{\Delta+1} + \frac{(n-\Delta-1)\sqrt{3}}{3} + \frac{(n-\Delta-1)\sqrt{2\Delta}}{\Delta+2}\Big).$$

The proof is completed. $\square$

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