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On Geometric-Arithmetic Indices of (Molecular) Trees, Unicyclic Graphs and Bicyclic Graphs

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Abstract

The geometric-arithmetic (GA) index is a newly proposed graph invariant in mathematical chemistry. We determine the *n*-vertex (molecular) trees with the second and the third for $n \geq 7$, the fourth and the fifth for $n \geq 10$, and the sixth for $n \geq 11$ maximum GA indices, unicyclic (molecular) graphs with the first for $n \geq 3$, the second and the third for $n \geq 5$, the fourth for $n \geq 7$, and the fifth and the sixth for $n \geq 9$ maximum GA indices, and bicyclic (moleclar) graphs with the first for $n \geq 4$, the second and the third for $n \geq 6$, and the fourth, the fifth and the sixth for $n \geq 8$ maximum GA indices.

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1. Introduction

A topological index is a numerical descriptor of the molecular structure derived from the corresponding molecular graph. Randić proposed a topological index called the branching index [1] that later became the famous Randić connectivity index, which is the most used molecular descriptor in QSPR and QSAR [2-5]. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, d_u denotes the degree of the vertex u in G. The Randić connectivity index of G is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

It is based on the end-vertex degrees of edges in a graph. Recently, Vukičević and Furtula [6] proposed a topological index named the geometric-arithmetic index (GA index for short) based also on the end-vertex degrees of edges in a graph. The GA index of the graph G is defined as [6]

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

It is noted in [6] that the predictive power of GA index is somewhat better than the predictive power of the Randić connectivity index for physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor. In [6], Vukičević and Furtula gave lower and upper bounds for the GA index, identified the trees with the minimum and the maximum GA indices, which are the star and the path, respectively, and thus the path is the unique molecular tree (tree with maximum degree at most four used to model carbon skeletons of acyclic hydrocarbons) with the maximum GA index. In [7], Yuan *et al.* established further bounds for the GA index using other graph invariants, lower and upper bounds for GA index of molecular graphs using the numbers of vertices and edges, and determined the molecular trees with the first, the second and the third minimum, as well as the second and the third maximum GA indices. We mention that two types of variants of the GA index were investigated in [8,9].

In this paper, we determine the n-vertex trees with the second and the third for $n \geq 7$, the fourth and the fifth for $n \geq 10$, and the sixth for $n \geq 11$ maximum GA indices, unicyclic graphs with the first for $n \geq 3$, the second and the third for $n \geq 5$, the fourth for $n \geq 7$, and the fifth and the sixth for $n \geq 9$ maximum GA indices, and bicyclic graphs with the first for $n \geq 4$, the second and the third for $n \geq 6$, and the fourth, the fifth and the sixth for $n \geq 8$ maximum GA indices.

2. Preliminaries

Note that for an edge uv of a graph G, $\frac{2\sqrt{d_u d_v}}{d_u + d_v} \leq 1$ with equality if and only if $d_u = d_v$. This fact will be used frequently in our proof.

A path $u_1 u_2 \ldots u_r$ in a graph G is said to be a pendent path at u_1 if $d_{u_1} \geq 3$, $d_{u_i} = 2$ for $i = 2, \ldots, r-1$, and $d_{u_r} = 1$. A pendent edge is an edge with one end vertex of degree one.

Lemma 1. If there are k pendent paths in a graph G, then

$$GA(G) \leq \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + |E(G)| - 2k.$$

Proof. Let uv be an edge of a graph G on n vertices. If d_u is fixed, then as a function on d_v, $\frac{2\sqrt{d_u d_v}}{d_u + d_v}$ is decreasing for $d_u \leq d_v \leq n-1$. Thus the edge of a pendent path with length 1 in G contributes to $GA(G)$ at most $\frac{2\sqrt{1 \cdot 3}}{1+3} < 1 - 2 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$, and the edges of a pendent path with length $m \geq 2$ in G contribute to $GA(G)$ at most $\frac{2\sqrt{1 \cdot 2}}{1+2} + \frac{2\sqrt{2 \cdot 2}}{2+2}(m-2) + \frac{2\sqrt{2 \cdot 3}}{2+3} = m - 2 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$. It follows that the edges of a pendent path with length $m \geq 1$ in G contribute to $GA(G)$ at most $m - 2 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$. Since there are k pendent paths in G, we have $GA(G) \leq \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + |E(G)| - 2k$. □

Recall that an n-vertex connected graph is known as a tree, a unicyclic graph and a bicyclic graph, respectively if it possesses respectively $n-1$, n and $n+1$ edges.

3. GA Indices of Trees

Among the n-vertex trees with $n \geq 4$, the path P_n is the unique tree with the maximum GA index, which is equal $n-3+\frac{4\sqrt{2}}{3}$, see [6]. In this section we determine the n-vertex trees with the second and the third for $n \geq 7$, the fourth and the fifth for $n \geq 10$, and the sixth for $n \geq 11$ maximum GA indices.

Theorem 1. Among the set of n-vertex trees,

(i) for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique trees with the second maximum GA index, which is equal to $n-7+\frac{6\sqrt{6}}{5}+2\sqrt{2}$,

(ii) for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two are the unique trees with the third maximum GA index, which is equal to $n-6+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+\frac{4\sqrt{2}}{3}$,

(iii) for $n \geq 10$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique trees with the fourth maximum GA index, which is equal to $n-9+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$,

(iv) for $n \geq 10$, the tree with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two is the unique tree with the fifth maximum GA index, which is equal to $n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}$,

(v) for $n \geq 11$, the trees with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two are the unique trees with the sixth maximum GA index, which is equal to $n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$.

Proof. Let G be an n-vertex tree different from P_n, where $n \geq 7$. Obviously, there are at least three pendent paths in G.

Suppose that there are exactly three pendent paths in G. Then there is exactly one vertex with maximum degree three in G, which is adjacent to exactly one, two or three vertices of degree two. Thus G is the tree with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two and $GA(G)=n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}$, or G is a tree with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two and $GA(G)=n-6+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+\frac{4\sqrt{2}}{3}$, or G is a tree with a single vertex of maximum degree three, adjacent to three vertices of degree two and $GA(G)=n-7+\frac{6\sqrt{6}}{5}+2\sqrt{2}.$

Suppose that there are exactly four pendent paths in G. Then there are two possibilities: (a) there is exactly one vertex of maximum degree four and other vertices are of degree one or two, and (b) there are exactly two vertices of maximum degree three in G. If (a) holds, then since $\frac{2\sqrt{1\cdot 4}}{1+4}<\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 4}}{2+4}$, we have

$$GA(G)\le 4\cdot\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 4}}{2+4}\right)+(n-1)-8<n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}.$$

Suppose that (b) holds. If there is at least one pendent path of length one in G, then

$$GA(G)\le \frac{2\sqrt{1\cdot 3}}{1+3}+3\cdot\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)+(n-1)-7<n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}.$$

Otherwise, all the four pendent paths of G are of length at least two. Denote by u and v the two vertices of degree three in G. If u and v are adjacent, then $n\ge 10$ and $GA(G)=n-9+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$, and if u and v are non-adjacent, then $n\ge 11$ and $GA(G)=n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$.

If there are $k\ge 5$ pendent paths in G, then by Lemma 1,

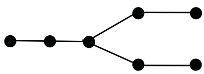
$$GA(G)\le\left(\frac{2\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}\right)k+n-1-2k\le\left(\frac{2\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}\right)\cdot 5+n-1-2\cdot 5<n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}.$$

It is easily checked that

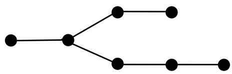
$$n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}<n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}<n-9+\frac{8\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$$
$$<n-6+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+\frac{4\sqrt{2}}{3}<n-7+\frac{6\sqrt{6}}{5}+2\sqrt{2}.$$

From the above arguments, if $GA(G)$ is not equal to one of these five values, then $GA(G)<n-11+\frac{12\sqrt{6}}{5}+\frac{8\sqrt{2}}{3}$. Now the result follows easily. □

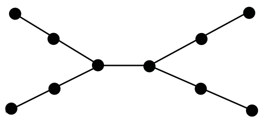
In Fig. 1, the trees in Theorem 1 (i)-(v) with the smallest numbers of vertices ($n=7$ for (i) and (ii), $n=10$ for (iii) and (iv), $n=11$ for (v)) are listed.



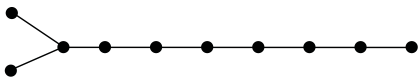
The tree in Theorem 1 (i) with $n=7$



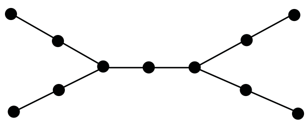
The tree in Theorem 1 (ii) with $n=7$



The tree in Theorem 1 (iii) with $n=10$



The tree in Theorem 1 (iv) with $n=10$



The tree in Theorem 1 (v) with $n=11$

Fig. 1. The trees in Theorem 1 (i)-(v) with the smallest numbers of vertices.

4. GA Indices of Unicyclic Graphs

Now we determine the n-vertex unicyclic graphs with the first for $n \geq 3$, the second and the third for $n \geq 5$, the fourth for $n \geq 7$, and the fifth and the sixth for $n \geq 9$ maximum GA indices.

Theorem 2. Among the set of n-vertex unicyclic graphs,

(i) for $n \geq 3$, the cycle C_n is the unique graph with the maximum GA index, which is equal to n,

(ii) for $n \geq 5$, the graphs with a single vertex of maximum degree three, adjacent to three vertices of degree two are the unique graphs with the second maximum GA index, which is equal to $n-4+\frac{6\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}$,

(iii) for $n \geq 5$, the graph with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two is the unique graph with the third maximum GA index, which is equal to $n-3+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}$,

(iv) for $n \geq 7$, the graphs with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two are the unique graphs with the fourth maximum GA index, which is equal to $n-6+\frac{8\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}$.

(v) for $n \geq 9$, the graphs obtained by attaching a path on at least two vertices to every vertex of a triangle are the unique graphs with the fifth maximum GA index, which is equal to $n-6+\frac{6\sqrt{6}}{5}+2\sqrt{2}$,

(vi) for $n \geq 9$, the graphs with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two are the unique graphs with the sixth maximum GA index, which is equal to $n-8+\frac{12\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}$.

Proof. Let G be an n-vertex unicyclic graph, where $n \geq 3$.

If there is no pendent path in G, then $G = C_n$ and $GA(G) = n$.

If there is exactly one pendent path in G, then either G is a graph with a single vertex of maximum degree three, adjacent to three vertices of degree two, $n \geq 5$ and $GA(G) = n - 4 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$, or G is the graph with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, $n \geq 4$ and $GA(G) = n - 3 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$.

Suppose that there are exactly two pendent paths in G. Then there are two possibilities: (a) there is exactly one vertex on the cycle of G with maximum degree four and all other vertices of G are of degree one or two, and (b) there are exactly two vertices with maximum degree three in G. If (a) holds, then since $\frac{2\sqrt{1\cdot 4}}{1+4} < \frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 4}}{2+4}$, we have

$$GA(G) \leq 2\cdot\left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 4}}{2+4}\right) + 2\cdot\frac{2\sqrt{2\cdot 4}}{2+4} + n - 6 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

Suppose that (b) holds. If both the two pendent paths are of length one in G, then

$$GA(G) \leq 2\cdot\frac{2\sqrt{1\cdot 3}}{1+3} + n - 2 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

If there is exactly one pendent path of length one in G, then there are at least three edges in G connecting vertices of degree two and three, together with the two pendent edges in G,

$$GA(G) \leq 3\cdot\frac{2\sqrt{2\cdot 3}}{2+3} + \frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{1\cdot 3}}{1+3} + n - 5 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

Suppose that both the two pendent paths are of length at least two in G. Denote by u and v the two vertices of degree three. If u and v are adjacent, then $n \geq 7$ and $GA(G) = n - 6 + \frac{8\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}$, and if u and v are non-adjacent, then $n \geq 8$ and $GA(G) = n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}$.

Suppose that there are exactly three pendent paths in G. If there is at least one pendent path of length one in G, then

$$GA(G) \le \frac{2\sqrt{1\cdot 3}}{1+3} + 2\cdot\left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 3}}{2+3}\right) + n - 5 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

Suppose that the three pendent paths in G are all of length at least two. If there is a pendent path at the vertex of degree at least four, then

$$GA(G) \le \left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 4}}{2+4}\right) + 2\cdot\left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 3}}{2+3}\right) + n - 6 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

Suppose that the three pendent paths in G are all at the vertices, say $x, y, z,$ of degree three. Note that the maximum degree of G is three. If at most two pairs of vertices x, y, z are adjacent, then there are at least five edges connecting vertices of degree two and three, together with the three pendent edges in G,

$$GA(G) \le 5\cdot\frac{2\sqrt{2\cdot 3}}{2+3} + 3\cdot\frac{2\sqrt{1\cdot 2}}{1+2} + n - 8 < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}.$$

If x, y, z are pairwise adjacent, then G is a graph obtained by attaching a path on at least two vertices to every vertex of a triangle, $n \ge 9$, and $GA(G) = n - 6 + \frac{6\sqrt{6}}{5} + 2\sqrt{2}.$

If there are $k \ge 4$ pendent paths in G, then by Lemma 1,

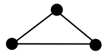
$$\begin{aligned} GA(G) &\le \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}\right)k + n - 2k \le \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}\right)\cdot 4 + n - 2\cdot 4 \\ &< n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}. \end{aligned}$$

It is easily checked that

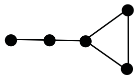
$$\begin{aligned} n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3} &< n - 6 + \frac{6\sqrt{6}}{5} + 2\sqrt{2} < n - 6 + \frac{8\sqrt{6}}{5} + \frac{4\sqrt{2}}{3} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2} < n - 4 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} < n. \end{aligned}$$

From the above arguments, if $GA(G)$ is not equal to one of these six values, then $GA(G) < n - 8 + \frac{12\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}$. Now the result follows easily. □

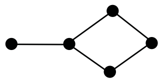
In Fig. 2, the unicyclic graphs in Theorem 2 (i)-(vi) with the smallest numbers of vertices ($n=3$ for (i), $n=5$ for (ii) and (iii), $n=7$ for (iv), $n=9$ for (v) and (vi)) are listed.



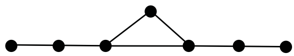
The graph in Theorem 2 (i) with $n=3$



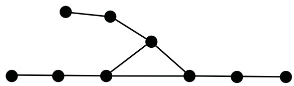
The graph in Theorem 2 (ii) with $n=5$



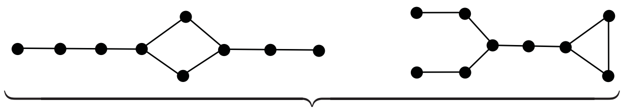
The graph in Theorem 2 (iii) with $n=5$



The graph in Theorem 2 (iv) with $n=7$



The graph in Theorem 2 (v) with $n=9$



The graphs in Theorem 2 (vi) with $n=9$

Fig. 2. The unicyclic graphs in Theorem 2 (i)-(vi) with the smallest numbers of vertices.

5. GA Indices of Bicyclic Graphs

Finally we consider the bicyclic graphs. Let $\mathbf{B}_1^1(n)$ be the set of bicyclic graphs obtained from C_n by adding an edge, where $n \geq 4$. Let $\mathbf{B}_1^2(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles C_a and C_b with $a+b=n$ by an edge, where $n \geq 6$. Let $\mathbf{B}_2(n)$ be the set of bicyclic graphs obtained from $C_a = v_0v_1\ldots v_{a-1}$ with $4 \leq a \leq n-2$ by joining v_0 and v_2 by an edge, and attaching a path on $n-a$ vertices to v_1. Let $\mathbf{B}_3^1(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_a with $4 \leq a \leq n-1$ by a path of length $n-a+1$, where $n \geq 5$. Let $\mathbf{B}_3^2(n)$ be the set of bicyclic graphs obtained by joining two vertex-disjoint cycles C_a and C_b with $a+b<n$ by a path of length $n-a-b+1$, where $n \geq 7$. Let $\mathbf{B}_4(n)$ be the set of n-vertex bicyclic graphs obtained by attaching a path on at least two vertices to the two vertices of degree two of the unique 4-vertex bicyclic graph, where $n \geq 8$. Let $\mathbf{B}_5^1(n)$ be the set of bicyclic graphs obtained from a graph in $\mathbf{B}_1^1(k)$ with $k \geq 5$ or $\mathbf{B}_1^2(k)$ with $k \geq 6$ by attaching a path on $n-k \geq 2$ vertices to a vertex of degree two, whose two neighbors are of degree two and three, where $n \geq 7$. Let $\mathbf{B}_5^2(n)$ be the set of bicyclic graphs obtained from a graph in $\mathbf{B}_3^1(k)$ with $k \geq 5$ or $\mathbf{B}_3^2(k)$ with $k \geq 7$ by attaching a path on $n-k \geq 2$ vertices to a vertex of degree two, whose two neighbors are both of degree three, where $n \geq 7$. Let $B_6(n)$ be the bicyclic graph obtained from $C_{n-1} = v_0v_1\ldots v_{n-2}$ by joining v_0 and v_2 by an edge, and attaching a vertex of degree one to v_1, where $n \geq 5$.

In the following we determine the n-vertex bicyclic graphs with the first for $n \geq 4$, the second and the third for $n \geq 6$, and the fourth, the fifth and the sixth for $n \geq 8$ maximum GA indices.

Theorem 3. Among the set of n-vertex bicyclic graphs,

(i) the graphs in $\mathbf{B}_1^1(n)$ for $n \geq 4$ and the grpahs in $\mathbf{B}_1^2(n)$ for $n \geq 6$ are the unique graphs with the maximum GA index, which is equal to $n-3+\frac{8\sqrt{6}}{5}$,

(ii) for $n \geq 6$, the graphs in $\mathbf{B}_2(n)$ are the unique graphs with the second maximum GA index, which is equal to $n-3+\frac{6\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}$,

(iii) the graphs in $\mathbf{B}_3^1(n)$ for $n \geq 6$ and the graphs in $\mathbf{B}_3^2(n)$ for $n \geq 7$ are the unique graphs with the third maximum GA index, which is equal to $n-5+\frac{12\sqrt{6}}{5}$,

(iv) for $n \geq 8$, the graphs in $\mathbf{B}_4(n)$ are the unique graphs with the fourth maximum GA index, which is equal to $n-3+\frac{4\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}$,

(v) for $n \geq 8$, the graphs in $\mathbf{B}_5^1(n)$ or $\mathbf{B}_5^2(n)$ are the unique graphs with the fifth maximum GA index, which is equal to $n-5+2\sqrt{6}+\frac{2\sqrt{2}}{3}$,

(vi) for $n \geq 8$, $B_6(n)$ is the unique graph with the sixth maximum GA index, which is equal to $n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}$.

Proof. Let G be an n-vertex bicyclic graph, where $n \geq 4$.

If there is no pendent path in G, then $G \in \mathbf{B}_1^1(n)$ or $G \in \mathbf{B}_1^2(n)$ with $n \geq 6$ and $GA(G)=n-3+\frac{8\sqrt{6}}{5}$, or $G \in \mathbf{B}_3^1(n)$ with $n \geq 5$ or $G \in \mathbf{B}_3^2(n)$ with $n \geq 7$ and $GA(G)=n-5+\frac{12\sqrt{6}}{5}$, or G is a graph obtained by identifying one vertex of two cycles and $GA(G)=n-3+\frac{8\sqrt{2}}{3}<n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}$.

Suppose that there is exactly one pendent path in G. Denote by Δ the maximum degree of G. Obviously, $3 \leq \Delta \leq 5$. First suppose that this pendent path is of length one. If $\Delta = 4, 5$, then note that there are at least two edges in G connecting vertices of degree two and Δ, together with the unique pendent edge in G, we have

$$\begin{aligned} GA(G) &\leq 2\cdot\frac{2\sqrt{2\cdot\Delta}}{2+\Delta}+\frac{2\sqrt{1\cdot 3}}{1+3}+(n+1)-3 \\ &\leq 2\cdot\frac{2\sqrt{2\cdot 4}}{2+4}+\frac{2\sqrt{1\cdot 3}}{1+3}+n-2 \\ &< n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}. \end{aligned}$$

Suppose that $\Delta = 3$. Then there are exactly three vertices, say x, y, z, of degree three in G. If at most two pairs of vertices x, y, z are adjacent, then there are at least four edges in G connecting vertices of degree two and three, together with the unique pendent edge in G, we have $GA(G) \le 4 \cdot \frac{2\sqrt{2\cdot 3}}{2+3} + \frac{2\sqrt{1\cdot 3}}{1+3} + (n+1) - 5 < n - 2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$. If x, y, z are pairwise adjacent, then $G = B_6(n)$ with $n \ge 5$, and $GA(G) = n - 2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$. Now suppose that the pendent path is of length at least two. If $\Delta = 4, 5$, then note that there are at least three edges in G connecting vertices of degree two and Δ, together with the unique pendent edge in G, we have

$$\begin{aligned} GA(G) &\le 3 \cdot \frac{2\sqrt{2\cdot \Delta}}{2+\Delta} + \frac{2\sqrt{1\cdot 2}}{1+2} + (n+1) - 4 \\ &\le 3 \cdot \frac{2\sqrt{2\cdot 4}}{2+4} + \frac{2\sqrt{1\cdot 2}}{1+2} + n - 3 \\ &< n - 2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}. \end{aligned}$$

Suppose that $\Delta = 3$. Then there are exactly three vertices, say u_1, u_2, u_3, of degree three in G. If at most one pair of vertices u_1, u_2, u_3 is adjacent, then there are at least seven edges connecting vertices of degree two and three, together with the unique pendent edge in G, we have

$$GA(G) \le 7 \cdot \frac{2\sqrt{2\cdot 3}}{2+3} + \frac{2\sqrt{1\cdot 2}}{1+2} + (n+1) - 8 < n - 2 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}.$$

If there are exactly two pairs of vertices u_1, u_2, u_3 are adjacent, then $G \in \mathbf{B}_5^1(n)$ or $\mathbf{B}_5^2(n)$ with $n \ge 7$, and $GA(G) = n - 5 + 2\sqrt{6} + \frac{2\sqrt{2}}{3}$. If u_1, u_2, u_3 are pairwise adjacent, then $G \in \mathbf{B}_2(n)$ with $n \ge 6$, and $GA(G) = n - 3 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$.

Suppose that there are exactly two pendent paths in G. Obviously, $3 \le \Delta \le 6$. If $4 \le \Delta \le 6$, then note that there are at least two edges in G connecting vertices of degree two and Δ, together with the two pendent paths in G, we have

$$GA(G) \leq 2\cdot\frac{2\sqrt{2\cdot\Delta}}{2+\Delta}+2\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)+(n+1)-6$$
$$\leq 2\cdot\frac{2\sqrt{2\cdot 4}}{2+4}+2\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)+n-5$$
$$< n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}.$$

Suppose that $\Delta = 3$. Then there are exactly four vertices, say v_1, v_2, v_3, v_4, of degree three in G. If there is at least one pendent path of length one, then

$$GA(G) \leq \frac{2\sqrt{1\cdot 3}}{1+3}+\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)+(n+1)-3 < n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}.$$

Suppose that the two pendent paths are both of length at least two. Note that at most five pairs of vertices v_1, v_2, v_3, v_4 are adjacent as G is a bicyclic graph. If at most four pairs of v_1, v_2, v_3, v_4 are adjacent, then there are at least four edges in G connecting vertices of degree two and three, together with the two pendent edges in G, we have

$$GA(G) \leq 4\cdot\frac{2\sqrt{2\cdot 3}}{2+3}+2\cdot\frac{2\sqrt{1\cdot 2}}{1+2}+(n+1)-6 < n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}.$$

If there are exactly five pairs of vertices v_1, v_2, v_3, v_4 are adjacent, then $G \in \mathbf{B}_4(n)$ with $n \geq 8$, and $GA(G) = n-3+\frac{4\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}$.

If there are $k \geq 3$ pendent paths in G, then by Lemma 1,

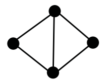
$$GA(G) \leq \left(\frac{2\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}\right)k+n+1-2k \leq \left(\frac{2\sqrt{6}}{5}+\frac{2\sqrt{2}}{3}\right)\cdot 3+n+1-2\cdot 3$$
$$< n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}.$$

It is easily checked that

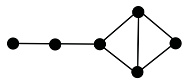
$$n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2} < n-5+2\sqrt{6}+\frac{2\sqrt{2}}{3} < n-3+\frac{4\sqrt{6}}{5}+\frac{4\sqrt{2}}{3}$$
$$< n-5+\frac{12\sqrt{6}}{5} < n-3+\frac{6\sqrt{6}}{5}+\frac{2\sqrt{2}}{3} < n-3+\frac{8\sqrt{6}}{5}.$$

From the above arguments, if $GA(G)$ is not equal to one of these six values, then $GA(G) < n-2+\frac{4\sqrt{6}}{5}+\frac{\sqrt{3}}{2}$. Now the result follows easily. □

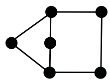
In Fig. 3, the bicyclic graphs in Theorem 3 (i)-(vi) with the smallest numbers of vertices ($n=4$ for (i), $n=6$ for (ii) and (iii), $n=8$ for (iv), (v) and (vi)) are listed.



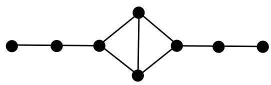
The graph in Theorem 3 (i) with $n=4$



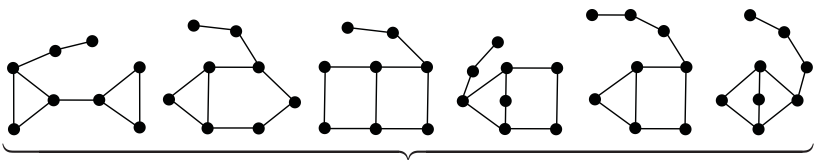
The graph in Theorem 3 (ii) with $n=6$



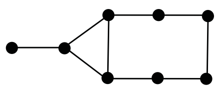
The graph in Theorem 3 (iii) with $n=6$



The graph in Theorem 3 (iv) with $n=8$



The graphs in Theorem 3 (v) with $n=8$



The graph in Theorem 3 (vi) with $n=8$

Fig. 3. The bicyclic graphs in Theorem 3 (i)-(vi) with the smallest numbers of vertices.

5. Conclusions

We have determined the *n*-vertex trees, the *n*-vertex unicyclic graphs and the *n*-vertex bicyclic graphs with the first a few largest GA indices in Theorems 1, 2 and 3, respectively. Note that these trees, unicyclic graphs and bicyclic graphs are all molecular graphs (connected graphs with maximum degree at most four) [11]. Thus, we have determined the *n*-vertex molecular trees with the second and the third for $n \geq 7$, the fourth and the fifth for $n \geq 10$, and the sixth for $n \geq 11$ maximum GA indices in Theorem 1, the *n*-vertex unicyclic molecular graphs with the first for $n \geq 3$, the second and the third for $n \geq 5$, the fourth for $n \geq 7$, and the fifth and the sixth for $n \geq 9$ maximum GA indices in Theorem 2, and the *n*-vertex bicyclic molecular graphs with the first for $n \geq 4$, the second and the third for $n \geq 6$, and the fourth, the fifth and the sixth for $n \geq 8$ maximum GA indices in Theorem 3.

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