Bicyclic Graphs With Maximum Geometric-Arithmetic Index^{*}

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Abstract

Let G be a simple graph with vertex set V(G) and edge set E(G). The geometric-arithmetic index (GA index for short) of graph G is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$, where the summation extends over all edges uv of G, and d_u denotes the degree of vertex u in G. Recently, Du *et al.* [On geometric arithmetic indices of (molecular) trees, unicyclic graphs and bicyclic graphs, MATCH Commun. Math. Comput. Chem. 66 (2011), 681–697] determined the first six maximum values for the GA indices of bicyclic graphs. In this paper, we determine the *n*-vertex bicyclic graphs with the seventh and eighth for $n \geq 9$, the ninth, tenth, eleventh for $n \geq 10$, the twelfth, thirteenth, fourteenth, fifteenth, sixteenth for $n \geq 11$, the seventeenth, eighteenth, nineteenth, twentieth, twenty-first, twenty-second, twenty-third, twenty-forth and twenty-fifth for $n \geq 12$ maximum GA indices.

1 Introduction

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 vertex u in G. An n-vertex connected graph G is said to be a bicyclic graph if it possesses n + 1 edges. For the notations and terminologies not mentioned here, please refer to [18].

Graph theory has provided the chemist with a variety of useful tools, one of which is the topological indices [8]. Molecules and molecular compounds are often modeled by molecular graphs. Topological indices of molecular graphs are one of the oldest and the most widely used descriptors in QSPR/QSAR research [16].

The Randić index [15] is one of the most important topological indices having a lot of applications in chemistry. For the results on Randić index, please refer [2, 6, 10].

Motivated by Randić index, Vukičević and Furtula [17] proposed a new topological index named the *geometric-arithmetic index* (GA index for short) based on the end-vertex degrees of edges in a graph. The GA index of graph G, denoted by GA(G), is defined as [17]

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

where the summation extends over all edges uv of G.

It is noted in [17] that the predictive power of GA index for several physico-chemical properties (boiling point, entropy, enthalpy and standard enthalpy of vaporization, enthalpy of formation, acentric factor) is somewhat better than the predictive power of the Randić connectivity index.

In [17], Vukičević and Furtula gave the lower and upper bounds for the GA index of graphs, and identified the trees with the minimum and maximum GA indices, which are the star and the path, respectively. In [19], Yuan *et al.* gave the lower and upper bounds for the GA index of molecular graphs in terms of the number of vertices and edges. They also determined the *n*-vertex molecular trees with the minimum, the second

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minimum and the third minimum, as well as the second maximum and the third maximum GA indices. Du et al. [9] and Husin et al. [12] presented a further ordering for the GA indices of trees and determined the first fourteen maximum values. For more results on the mathematical properties of GA indices, please refer to a recent survey [14] and papers [1, 4, 5, 7, 11, 13].

In [3], the authors collected all hitherto obtained results on the GA index of graphs. In particular, Du et al. [9] determined the *n*-vertex bicyclic (molecular) graphs with the first for $n \ge 4$, the second and the third for $n \ge 6$, and the fourth, the fifth and the sixth for $n \ge 8$ maximum GA indices. In this paper, we determine the *n*-vertex bicyclic graphs with the seventh and eighth for $n \ge 9$, the ninth, tenth, eleventh for $n \ge 10$, the twelfth, thirteenth, fourteenth, fifteenth, sixteenth for $n \ge 11$, the seventeenth, eighteenth, nineteenth, twentieth, twenty-first, twenty-second, twenty-third, twenty-forth and twenty-fifth for $n \ge 12$ maximum GA indices, and characterize the corresponding extremal graphs. This result was obtained by combining the approach used by Du et al. [9] and Deng et al. [7].

2 Preliminary Results

Note that for an edge uv of a graph G, it holds that

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \le 1$$

with equality if and only if $d_u = d_v$. This fact will be used frequently in the proofs of our main results.

A pendant vertex is a vertex of degree one. A pendant edge is an edge incident with a pendant vertex. A path $u_1u_2...u_r$ in a graph G is said to be a pendant path at u_1 if $d_{u_1} \ge 3$, $d_{u_i} = 2$ for i = 2, ..., r - 1and $d_{u_r} = 1$. An *n*-vertex connected graph is known as bicyclic if it has n + 1 edges.

Lemma 1 ([9]) If there are k pendant paths in an n-vertex bicyclic graph G, then

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

Let $\mathbf{B}_1^1(n)$ be the set of bicyclic graphs obtained from C_n by adding an edge, where $n \ge 4$. 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 ad edge, where $n \ge 6$. Let $\mathbf{B}_2(n)$ be the set of bicyclic graphs obtained from $C_a = v_0v_1 \dots v_{n-1}$ with $4 \le a \le n-2$ by joining v_0 and v_2 by an edge, and attaching a path on n-a vertices to v_1 . Let $\mathbf{B}_1^3(n)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_a with $4 \le a \le n-1$ by a path of length n-a+1, where $n \ge 5$. Let $\mathbf{B}_2^3(n)$ 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 $n \ge 7$. 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 $n \ge 8$. Let $\mathbf{B}_5^1(n)$ be the set of bicyclic graphs obtained from a graph in $\mathbf{B}_1^1(k)$ with $k \ge 5$ or $\mathbf{B}_1^2(k)$ with $k \ge 6$ by attaching a path on $n-k \ge 2$ vertices to a vertex of degree two, whose two neighbors are of degree two and three, where $n \ge 7$. Let $\mathbf{B}_5^2(n)$ be the set of bicyclic graphs obtained from a graph in $\mathbf{B}_3^1(k)$ with $k \ge 5$ or $\mathbf{B}_3^2(k)$ with $k \ge 7$ by attaching a path on $n-k \ge 2$ vertices to a vertex of degree two, whose two neighbors are both of degree three, where $n \ge 7$. Let $\mathbf{B}_6(n)$ be the bicyclic graphs obtained from $C_{n-1} = v_0v_1 \dots v_{n-2}$ by joining v_0 and v_2 by an edge, and attaching a vertex of degree one to v_1 , where $n \ge 5$.

The following result was obtained in [9].

Theorem 1 ([9]) Among the set of n-vertex bicyclic graphs,

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

- (ii) for $n \ge 6$, 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 $n \ge 6$ and the graphs in $\mathbf{B}_3^2(n)$ for $n \ge 7$ are the unique graphs with the third maximum GA index, which is equal to $n 5 + \frac{12\sqrt{6}}{5}$;
- (iv) for $n \ge 8$, 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 $n \ge 8$, 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 $n 5 + 2\sqrt{6} + \frac{2\sqrt{2}}{2}$;
- (vi) for $n \ge 8$, the graphs in $\mathbf{B}_6(n)$ are the unique graphs with the sixth maximum GA index, which is equal to $n-2+\frac{4\sqrt{6}}{2}+\frac{\sqrt{3}}{2}$.

3 Main Results

In this section, we present our main result. Let B_n be the set of bicyclic graphs with n vertices and n + 1 edges. Assume d_{ij} denotes the number of edges connecting vertex of degree i with vertex of degree j.

The following four propositions will be used to prove our main result.

Proposition 1 Among the set of n-vertex bicyclic graph G with no pendant path, different from the types of graphs described in Theorem 1(i) and (ii), and let $\tilde{B}_n^1 = \{G \in \tilde{B}_n : d_{23} = 4, d_{22} = n-3\}$. If $G \in \tilde{B}_n^1$, then $GA(G) = n-3 + \frac{8\sqrt{2}}{3}$.



Figure 1: The unique bicyclic graph in Proposition 1 with n = 10 and $GA(G) = 7 + \frac{8\sqrt{2}}{3}$.

Proposition 2 Among the set of n-vertex bicyclic graph G with exactly one pendant path, different from the types of graphs described in Theorem 1(ii), (v) and (vi),

- (i) the graphs in $\tilde{B}_n^2 = \{G \in \tilde{B}_n : d_{12} = 1, d_{23} = 7, d_{33} = 1, d_{22} = n 8\}$ are the unique graphs with the maximum GA index, which is equal to $n 7 + \frac{2\sqrt{2}}{3} + \frac{14\sqrt{6}}{5};$
- (ii) the graphs in $\tilde{B}_n^3 = \{G \in \tilde{B}_n : d_{13} = 1, d_{24} = 4, d_{33} = 2, d_{22} = n 6\}$ are the unique graphs with the second maximum GA index, which is equal to $n 4 + \frac{\sqrt{3}}{2} + \frac{8\sqrt{6}}{5};$
- (iii) the graphs in $\tilde{B}_n^4 = \{G \in \tilde{B}_n : d_{12} = 1, d_{23} = 9, d_{22} = n 9\}$ are the unique graphs with the third maximum GA index, which is equal to $n 9 + \frac{2\sqrt{2}}{3} + \frac{18\sqrt{6}}{5};$
- (iv) the graphs in $\tilde{B}_n^5 = \{G \in \tilde{B}_n : d_{13} = 1, d_{23} = 6, d_{33} = 1, d_{22} = n 7\}$ are the unique graphs with the fourth maximum GA index, which is equal to $n 6 + \frac{\sqrt{3}}{2} + \frac{12\sqrt{6}}{5}$;
- (v) the graphs in $\tilde{B}_n^6 = \{G \in \tilde{B}_n : d_{12} = 1, d_{23} = 2, d_{24} = 3, d_{34} = 1, d_{22} = n 6\}$ are the unique graphs with the fifth maximum GA index, which is equal to $n 6 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{3}}{7} + \frac{4\sqrt{6}}{5};$

- (vi) the graphs in $\tilde{B}_n^7 = \{G \in \tilde{B}_n : d_{13} = 1, d_{23} = 8, d_{22} = n 8\}$ are the unique graphs with the sixth maximum GA index, which is equal to $n 8 + \frac{\sqrt{3}}{2} + \frac{16\sqrt{6}}{5}$.
- (vii) for all other graphs G, it holds that

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

Proof. Denote by k the number of pendant paths of length one in G. There are three possible cases.

Case 1. There is exactly one vertex in G of degree five, and all other vertices of G are of degree one or two.

Case 2. There is exactly one vertex of degree four and one vertex of degree three in G, and all other vertices of G are of degree one or two.

Case 3. There are exactly three vertices in G of degree three, and all other vertices of G are of degree one or two.

Suppose that Case 1 holds. Clearly, $0 \le k \le 1$. Then

$$\begin{aligned} GA(G) &\leq \left(\frac{\sqrt{5}}{3} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{10}}{7} + 1\right)k + n + 5 - \frac{2\sqrt{2}}{3} - \frac{10\sqrt{10}}{7} \\ &\leq n + 5 - \frac{2\sqrt{2}}{3} - \frac{10\sqrt{10}}{7} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}. \end{aligned}$$

Suppose that Case 2 holds. Denote by v_1 and v_2 the two vertices of degree three and four, respectively. Let G_1^k be the graphs that the unique pendant path is attached to v_1 and G_2^k be the graphs that the unique pendant path is attached to v_2 . Then we have the next two subcases.

• Case 2-1. Suppose that v_1 and v_2 are adjacent. Table 1 gives us the result.

Graphs	k	d_{12}	d_{13}	d_{14}	d_{23}	d_{24}	d_{34}	d_{22}	GA values
G_1^k	0	1	0	0	2	3	1	n-6	n + 0.72057
G_1^k	1	0	1	0	1	3	1	n-5	n + 0.66399
G_2^k	0	1	0	0	2	3	1	n-6	n + 0.7206
G_2^k	1	0	0	1	2	2	1	n-6	n + 0.63495

Table 1: The connected bicyclic graphs and their GA values.

From Table 1, we can see that $G_1^0 \cup G_2^0 \in \tilde{B_n^6}$ with $GA(G) = n - 6 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{3}}{7} + \frac{4\sqrt{6}}{5} \approx n + 0.72057$. For both G_1^1 and G_2^1 , $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 2-2. Suppose that v_1 and v_2 are non-adjacent. Table 2 gives us the result.

Graphs	k	d_{12}	d_{13}	d_{14}	d_{23}	d_{24}	d_{22}	GA values
G_1^k	0	1	0	0	3	4	n-7	n + 0.6534
G_1^k	1	0	1	0	2	4	n-6	n + 0.5969
G_2^k	0	1	0	0	3	4	n-7	n + 0.6534
G_2^k	1	0	0	1	3	3	n-6	n + 0.5678

Table 2: The connected bicyclic graphs and their GA values.

From Table 2, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

Suppose that Case 3 holds. Denote by v_1, v_2, v_3 the three vertices of degree three in G of degree three. Clearly, $0 \le k \le 1$. Then we have the next four subcases.

- Case 3-1. Suppose that there are exactly three pairs of v_1, v_2, v_3 are adjacent in G. If k = 0, graph G is described in Theorem 1(ii), and if k = 1, graph G is described in Theorem 1(vi). So, there is no need to consider such cases.
- Case 3-2. Suppose that there are exactly two pairs of v_1, v_2, v_3 are adjacent in G. If k = 0, graph G is described in Theorem 1(v) and such case is no need to be considered. If k = 1, $G \in \tilde{B}_n^3$ and $GA(G) = n 4 + \frac{\sqrt{3}}{2} + \frac{8\sqrt{6}}{5} \approx n + 0.7852$.
- Case 3-3. Suppose that there are exactly one pair of v_1, v_2, v_3 are adjacent in G. If $k = 0, G \in \tilde{B_n^2}$ with $GA(G) = n 7 + \frac{2\sqrt{2}}{3} + \frac{14\sqrt{6}}{5} \approx n + 0.8014$. If $k = 1, G \in \tilde{B_n^5}$ and $GA(G) = n 6 + \frac{\sqrt{3}}{2} + \frac{12\sqrt{6}}{5} \approx n + 0.7448$.
- Case 3-4. Suppose that v_1, v_2, v_3 are pairwise non-adjacent in G. If $k = 0, G \in \tilde{B}_n^4$ with $GA(G) = n 9 + \frac{2\sqrt{2}}{3} + \frac{18\sqrt{6}}{5} \approx n + 0.76097$. If $k = 1, G \in \tilde{B}_n^7$ and $GA(G) = n 8 + \frac{\sqrt{3}}{2} + \frac{16\sqrt{6}}{5} \approx n + 0.7044$.

Finally, it is easy to check that

$$\begin{array}{rcl} n-8+\frac{\sqrt{3}}{2}+\frac{16\sqrt{6}}{5} &< n-6+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{3}}{7}+\frac{4\sqrt{6}}{5} < n-6+\frac{\sqrt{3}}{2}+\frac{12\sqrt{6}}{5} \\ &< n-9+\frac{2\sqrt{2}}{3}+\frac{18\sqrt{6}}{5} < n-4+\frac{\sqrt{3}}{2}+\frac{8\sqrt{6}}{5} \\ &< n-7+\frac{2\sqrt{2}}{3}+\frac{14\sqrt{6}}{5}. \end{array}$$

Moreover, from the above arguments, if GA(G) is not equal to one of these six values, then

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

This completes the proof. \blacksquare

Proposition 3 Among the set of n-vertex bicyclic graph G with exactly two pendant paths, different from the types of graphs described in Theorem 1(iv),

- (i) the graphs in $\tilde{B}_{n}^{8} = \{G \in \tilde{B}_{n} : d_{12} = 2, d_{23} = 4, d_{33} = 4, d_{22} = n 9\}$ are the unique graphs with the maximum GA index, which is equal to $n 5 + \frac{4\sqrt{2}}{3} + \frac{8\sqrt{6}}{5};$
- (ii) the graphs in $\tilde{B}_n^9 = \{G \in \tilde{B}_n : d_{12} = 1, d_{13} = 1, d_{23} = 1, d_{33} = 5, d_{22} = n 7\}$ are the unique graphs with the second maximum GA index, which is equal to $n 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3}}{2};$
- (iii) the graphs in $\tilde{B}_n^{10} = \{G \in \tilde{B}_n : d_{12} = 2, d_{23} = 6, d_{33} = 3, d_{22} = n 10\}$ are the unique graphs with the third maximum GA index, which is equal to $n 7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5};$
- (iv) the graphs in $\tilde{B}_n^{11} = \{G \in \tilde{B}_n : d_{12} = 1, d_{13} = 1, d_{23} = 3, d_{33} = 4, d_{22} = n 8\}$ are the unique graphs with the fourth maximum GA index, which is equal to $n 4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2};$
- (v) the graphs in $\tilde{B}_n^{12} = \{G \in \tilde{B}_n : d_{12} = 2, d_{23} = 8, d_{33} = 2, d_{22} = n 11\}$ are the unique graphs with the fifth maximum GA index, which is equal to $n 9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5}$;
- (vi) the graphs in $\tilde{B}_n^{13} = \{G \in \tilde{B}_n : d_{12} = 2, d_{23} = 2, d_{24} = 2, d_{34} = 2, d_{33} = 1, d_{22} = n 8\}$ are the unique graphs with the sixth maximum GA index, which is equal to $n 7 + \frac{8\sqrt{2}}{5} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7};$

- (vii) the graphs in $\tilde{B}_n^{14} = \{G \in \tilde{B}_n : d_{12} = 1, d_{13} = 1, d_{23} = 5, d_{33} = 3, d_{22} = n 9\}$ are the unique graphs with the seventh maximum GA index, which is equal to $n 6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6};$
- (viii) the graphs in $\tilde{B}_n^{15} = \{G \in \tilde{B}_n : d_{13} = 2, d_{23} = 2, d_{33} = 4, d_{22} = n 7\}$ are the unique graphs with the eighth maximum GA index, which is equal to $n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Proof. There are five possible subcases.

Case 1. There is exactly one vertex in G of degree six, and all other vertices of G are of degree one or two.

Case 2. There is exactly one vertex of degree five and one vertex of degree three in G, and all other vertices of G are of degree one or two.

Case 3. There are exactly two vertices in G of degree four, and all other vertices of G are of degree one or two.

Case 4. There is exactly one vertex of degree four and two vertices of degree three in G, and all other vertices of G are of degree one or two.

Case 5. There are exactly four vertices of degree three in G, and all other vertices of G are of degree one or two.

Suppose that Case 1 holds. Denote by k the number of pendant path of length one in G. Clearly, $0 \le k \le 2$. Then

$$GA(G) = \left(\frac{2\sqrt{6}}{7} - \frac{2\sqrt{2}}{3} - \frac{\sqrt{3}}{2} + 1\right) \cdot k + n - 7 + \frac{4\sqrt{2}}{3} + 3\sqrt{3}$$

$$\leq n - 7 + \frac{4\sqrt{2}}{3} + 3\sqrt{3}$$

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

Suppose that Case 2 holds. Denote by v_1 and v_2 be the two vertices of degree three and five, respectively. Without loss of generality, denote by k_1 the number of pendant paths attached to v_1 in G, and k_2 the number of pendant paths attached to v_2 in G. Clearly, $k_1 + k_2 = 2$. Then we have the next two subcases.

• Case 2-1. Suppose that v_1 and v_2 are adjacent. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k_1 + \left(\frac{\sqrt{5}}{3} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{10}}{7} + 1\right) \cdot k_2$$
$$+ n - 8 + \frac{\sqrt{15}}{4} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{10}}{7}$$
$$\leq n - 8 + \frac{\sqrt{15}}{4} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{10}}{7}$$
$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

• Case 2-2. Suppose that v_1 and v_2 are non-adjacent. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k_1 + \left(\frac{\sqrt{5}}{3} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{10}}{7} + 1\right) \cdot k_2 + n - 9 + \frac{4\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{10\sqrt{10}}{7} \\ \leq n - 9 + \frac{4\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{10\sqrt{10}}{7} \\ < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

Suppose that Case 3 holds. Assume there are two vertices v_1 and v_2 of degree four in G. Denote by k the number of pendant path of length one in G. Clearly, $0 \le k \le 2$. Then we have the next two subcases.

• Case 3-1. Suppose that v_1 and v_2 are adjacent in G. Then

$$\begin{split} GA(G) &= k \cdot \frac{2\sqrt{1 \cdot 4}}{1 + 4} + (2 - k) \left(\frac{2\sqrt{1 \cdot 2}}{1 + 2}\right) + (6 - k) \left(\frac{2\sqrt{2 \cdot 4}}{2 + 4}\right) + n + 1 - (8 - k) \\ &= \left(\frac{4}{5} - \frac{4\sqrt{2}}{3} + 1\right) \cdot k + n - 7 + \frac{16\sqrt{2}}{3} \\ &\leq n - 7 + \frac{16\sqrt{2}}{3} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}. \end{split}$$

• Case 3-2. Suppose that v_1 and v_2 are non-adjacent in G. Then

$$\begin{split} GA(G) &= k \cdot \frac{2\sqrt{1 \cdot 4}}{1 + 4} + (2 - k) \left(\frac{2\sqrt{1 \cdot 2}}{1 + 2}\right) + (8 - k) \left(\frac{2\sqrt{2 \cdot 4}}{2 + 4}\right) + n + 1 - (10 - k) \\ &= \left(\frac{4}{5} - \frac{4\sqrt{2}}{3} + 1\right) \cdot k + n - 9 + \frac{20\sqrt{2}}{3} \\ &\leq n - 9 + \frac{20\sqrt{2}}{3} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}. \end{split}$$

Suppose that Case 4 holds. There are exactly one vertex v_1 of degree four and two vertices v_2, v_3 of degree three in G. Then we have the next four cases.

• Case 4-1. Suppose that there are exactly three pairs of v_1, v_2, v_3 which are adjacent in G. Table 3 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	2	0	0	2	0	2	1	n-6	n + 0.5391
D_2	0	0	2	2	2	2	1	n-8	n + 0.7103
D_3	1	0	1	2	1	2	1	n-7	n + 0.6247
D_4	1	1	0	1	1	2	1	n-6	n + 0.5681
D_5	0	1	1	1	2	2	1	n-7	n + 0.6537
D_6	0	2	0	0	2	2	1	n-6	n + 0.5972

Table 3: The connected bicyclic graphs and their GA values.

From Table 3, let $G = D_2 \in \tilde{B}_n^{13}$ and $GA(G) = n - 7 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7} \approx n + 0.7103$. For other bicyclic graph $G, GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 4-2. Suppose that there are exactly two pairs of v_1, v_2, v_3 which are adjacent in G. Table 4 gives

us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	2	0	0	4	0	2	0	n-7	n + 0.4987
D_2	0	0	2	4	2	2	0	n-9	n + 0.6699
D_3	1	0	1	4	1	2	0	n-8	n + 0.5843
D_4	1	1	0	3	1	2	0	n-7	n + 0.5277
D_5	0	1	1	3	2	2	0	n-8	n + 0.6133
D_6	0	2	0	2	2	2	0	n-7	n + 0.5567

Table 4: The connected bicyclic graphs and their GA values.

From Table 4, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 4-3. Suppose that there are exactly one pair of v_1, v_2, v_3 which are adjacent in G. Table 5 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	2	0	0	4	2	0	1	n-8	n + 0.4048
D_2	0	0	2	4	4	0	1	n - 10	n + 0.5760
D_3	1	0	1	4	3	0	1	n-9	n + 0.4904
D_4	1	1	0	3	3	0	1	n-8	n + 0.4338
D_5	0	1	1	3	4	0	1	n-9	n + 0.5195
D_6	0	2	0	2	4	0	1	n-8	n + 0.4629

Table 5: The connected bicyclic graphs and their GA values.

From Table 5, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 4-4. Suppose that v_1, v_2, v_3 are pairwise non-adjacent in G. Table 6 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	2	0	0	4	2	0	1	n-8	n + 0.4315
D_2	0	0	2	4	4	0	1	n - 10	n + 0.6028
D_3	1	0	1	4	3	0	1	n-9	n + 0.5172
D_4	1	1	0	3	3	0	1	n-8	n + 0.4606
D_5	0	1	1	3	4	0	1	n-9	n + 0.5462
D_6	0	2	0	2	4	0	1	n-8	n + 0.4896

Table 6: The connected bicyclic graphs and their GA values.

From Table 6, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

Suppose that Case 5 holds. There are exactly four vertices v_1, v_2, v_3, v_4 of degree three in G. Denote by k the number of pendant path of length one in G. Clearly, $0 \le k \le 2$. Then we have the next six subcases.

• Case 5-1. Suppose that v_1, v_2, v_3, v_4 are adjacent in G. Then

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

If k = 0, the graph G is described in Theorem 1(iv), so there is no need to consider such case. If k = 1, then $G \in \tilde{B}_n^9$ and $GA(G) = n - 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3}}{2} \approx n + 0.7866$. If k = 2, n = 6, then $GA(G) = n - 1 + \sqrt{3} \approx 6.7321 < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 5-2. Suppose that there are exactly four pairs of v_1, v_2, v_3, v_4 are adjacent in G. Then

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

If k = 0, then $G \in \tilde{B}_n^8$ and $GA(G) = n - 5 + \frac{4\sqrt{2}}{3} + \frac{8\sqrt{6}}{5} \approx n + 0.8048$. If k = 1, then $G \in \tilde{B}_n^{11}$ and $GA(G) = n - 4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2} \approx n + 0.7482$. If k = 2, then $G \in \tilde{B}_n^{15}$ and $GA(G) = n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 5-3. Suppose that there are exactly three pairs of v_1, v_2, v_3, v_4 are adjacent in G. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k + n - 7 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$$

If k = 0, then $G \in \tilde{B}_n^{10}$ and $GA(G) = n - 7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5} \approx n + 0.7644$. If k = 1, then $G \in \tilde{B}_n^{14}$ and $GA(G) = n - 6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6} \approx n + 0.7078$. If k = 2, then $GA(G) = n - 5 + \frac{8\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6512 < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 5-4. Suppose that there are exactly two pairs of v_1, v_2, v_3, v_4 are adjacent in G. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k + n - 9 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$$

If k = 0, then $G \in B_n^{\tilde{1}2}$ and $GA(G) = n - 9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5} \approx n + 0.72399$. If k = 1, 2, then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k + n - 9 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$$
$$\leq \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot 1 + n - 9 + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$$
$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

• Case 5-5. Suppose that there are exactly one pair of v_1, v_2, v_3, v_4 are adjacent in G. Then

$$\begin{aligned} GA(G) &= \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k + n - 11 + \frac{4\sqrt{2}}{3} + 4\sqrt{6} \\ &\leq n - 11 + \frac{4\sqrt{2}}{3} + 4\sqrt{6} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}. \end{aligned}$$

• Case 5-6. Suppose that all vertices v_1, v_2, v_3, v_4 are not adjacent in G. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k + n - 13 + \frac{4\sqrt{2}}{3} + \frac{24\sqrt{6}}{5}$$
$$\leq n - 13 + \frac{4\sqrt{2}}{3} + \frac{24\sqrt{6}}{5}$$
$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

Finally, it is easy to check that

$$\begin{split} n-3 + \frac{4\sqrt{6}}{5} + \sqrt{3} < n-6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6} < n-7 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7} < \\ n-9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5} < n-4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2} < n-7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5} < \\ n-2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3}}{2} < n-5 + \frac{4\sqrt{2}}{3} + \frac{8\sqrt{6}}{5}. \end{split}$$

This completes the proof. \blacksquare

Proposition 4 Among the set of n-vertex bicyclic graph G with exactly three pendant paths,

- (i) the graphs in $\tilde{B}_n^{16} = \{G \in \tilde{B}_n : d_{12} = 3, d_{23} = 3, d_{33} = 6, d_{22} = n 11\}$ are the unique graphs with the maximum GA index, which is equal to $n 5 + 2\sqrt{2} + \frac{6\sqrt{6}}{5}$;
- (ii) the graphs in $\tilde{B}_n^{17} = \{G \in \tilde{B}_n : d_{12} = 3, d_{23} = 5, d_{33} = 5, d_{22} = n 12\}$ are the unique graphs with the second maximum GA index, which is equal to $n 7 + 2\sqrt{2} + 2\sqrt{6}$;
- (iii) the graphs in $\tilde{B}_n^{18} = \{G \in \tilde{B}_n : d_{12} = 2, d_{13} = 1, d_{23} = 2, d_{33} = 6, d_{22} = n 10\}$ are the unique graphs with the third maximum GA index, which is equal to $n 4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{2}}{5};$
- (iv) the graphs in $\tilde{B}_n^{19} = \{G \in \tilde{B}_n : d_{12} = 3, d_{23} = 2, d_{24} = 1, d_{34} = 3, d_{33} = 2, d_{22} = n 10\}$ are the unique graphs with the fourth maximum GA index, which is equal to $n 8 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{3}}{7};$
- (\mathbf{v}) for all other graphs G, it holds that

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

Proof. There are seven possible cases.

Case 1. There is exactly one vertex on the cycle of G of maximum degree seven, and all other vertices of G are of degree one or two.

Case 2. There is exactly one vertex of degree six and one vertex of degree three in G, and all other vertices of G are of degree one or two.

Case 3. There is exactly one vertex of degree five and one vertex of degree four in G, and all other vertices of G are of degree one or two.

Case 4. There is exactly one vertex of degree five and two vertices of degree three in G, and all other vertices of G are of degree one or two.

Case 5. There is exactly one vertex of degree four and three vertices of degree three in G, and all other vertices of G are of degree one or two.

Case 6. There are exactly two vertices of degree four and one vertex of degree three in G, and all other vertices of G are of degree one or two.

Case 7. There are exactly five vertices in G of degree three, and all other vertices of G are of degree one or two.

Suppose that Case 1 holds. Denote by k the number of pendant path of length one in G. Clearly, $0 \le k \le 3$. Then

$$\begin{aligned} GA(G) &= \left(\frac{\sqrt{7}}{4} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{14}}{9} + 1\right) \cdot k + n - 9 + 2\sqrt{2} + \frac{14\sqrt{14}}{9} \\ &\leq n - 9 + 2\sqrt{2} + \frac{14\sqrt{14}}{9} \\ &< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}. \end{aligned}$$

Suppose that Case 2 holds. Denote by v_1 and v_2 the two vertices of degree three and six, respectively. Denote by k_1 the number of pendant paths of length one attached to v_1 in G and k_2 the number of pendant paths of length one attached to v_2 in G. Clearly, $k_1 + k_2 = 3$. Then we have the next two subcases.

• Case 2-1. Suppose that v_1 and v_2 are adjacent in G. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k_1 + \left(\frac{2\sqrt{6}}{7} - \frac{2\sqrt{2}}{3} - \frac{\sqrt{3}}{2} + 1\right) \cdot k_2 + n - 10 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{5\sqrt{3}}{2} \\ \leq n - 10 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{5\sqrt{3}}{2} \\ < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

• Case 2-2. Suppose that v_1 and v_2 are not adjacent in G. Then

$$GA(G) = \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) \cdot k_1 + \left(\frac{2\sqrt{6}}{7} - \frac{2\sqrt{2}}{3} - \frac{\sqrt{3}}{2} + 1\right) \cdot k_2$$
$$+ n - 11 + 2\sqrt{2} + 3\sqrt{3} + \frac{6\sqrt{6}}{5}$$
$$\leq n - 11 + 2\sqrt{2} + 3\sqrt{3} + \frac{6\sqrt{6}}{5}$$
$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

Suppose that Case 3 holds. Denote by v_1 and v_2 the two vertices of degree four and five, respectively. Denote by k_1 the number of pendant paths of length one attached to v_1 in G and k_2 the number of pendant paths of length one attached to v_2 in G. Clearly, $k_1 + k_2 = 3$. Then we have the next two subcases.

• Case 3-1. Suppose that v_1 and v_2 are adjacent in G. Then

$$GA(G) = \left(\frac{4}{5} - \frac{4\sqrt{2}}{3} + 1\right) \cdot k_1 + \left(\frac{\sqrt{5}}{3} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{10}}{2} + 1\right) \cdot k_2$$
$$+ n - 10 + 4\sqrt{2} + \frac{4\sqrt{5}}{9} + \frac{8\sqrt{10}}{7}$$
$$\leq n - 10 + 4\sqrt{2} + \frac{4\sqrt{5}}{9} + \frac{8\sqrt{10}}{7}$$
$$< n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

• Case 3-2. Suppose that v_1 and v_2 are not adjacent in G. Then

$$GA(G) = \left(\frac{4}{5} - \frac{4\sqrt{2}}{3} + 1\right) \cdot k_1 + \left(\frac{\sqrt{5}}{3} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{10}}{7} + 1\right) \cdot k_2 + n - 11 + \frac{14\sqrt{2}}{3} + \frac{10\sqrt{10}}{7} \\ \leq n - 11 + \frac{14\sqrt{2}}{3} + \frac{10\sqrt{10}}{7} \\ < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

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Suppose that Case 4 holds. There are exactly one vertex of degree five v_1 and two vertices of degree three v_2 and v_3 in G. Then we have the next four subcases.

Graphs	d_{15}	d_{13}	d_{12}	d_{23}	d_{25}	d_{35}	d_{33}	d_{22}	GA values
D_1	0	0	3	2	3	2	1	n - 10	n + 0.4350
D_2	3	0	0	2	0	2	1	n-7	n + 0.1322
D_3	1	0	2	2	2	2	1	n-9	n + 0.3341
D_4	2	0	1	2	1	2	1	n-8	n + 0.2331
D_5	1	2	0	0	2	2	1	n-7	n + 0.2209
D_6	0	2	1	0	3	2	1	n-8	n + 0.3219
D_7	0	1	2	1	3	2	1	n-9	n + 0.37855
D_8	1	1	1	1	2	2	1	n-8	n + 0.2775
D_9	2	1	0	1	1	2	1	n-7	n + 0.1765

• Case 4-1. Suppose that v_1, v_2, v_3 are pairwise adjacent in G. Table 7 gives us the result.

Table 7: The connected bicyclic graphs and their GA values.

From Table 7, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 4-2. Suppose that there are exactly two pairs of v_1, v_2, v_3 are adjacent in G. Table 8 gives us the result.

Graphs	d_{15}	d_{13}	d_{12}	d_{23}	d_{25}	d_{35}	d_{33}	d_{22}	GA values
D_1	0	0	3	4	3	2	0	n - 11	n + 0.3946
D_2	3	0	0	4	0	2	0	n-8	n + 0.0917
D_3	1	0	2	4	2	2	0	n - 10	n + 0.2937
D_4	2	0	1	4	1	2	0	n-9	n + 0.1927
D_5	1	2	0	2	2	2	0	n-8	n + 0.1805
D_6	0	2	1	2	3	2	0	n-9	n + 0.2815
D_7	0	1	2	3	3	2	0	n - 10	n + 0.3381
D_8	1	1	1	3	2	2	0	n-9	n + 0.2371
D_9	2	1	0	3	1	2	0	n-8	n + 0.1361

Table 8: The connected bicyclic graphs and their GA values.

From Table 8, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

- Case 4-3. Suppose that there are exactly one pair of v_1, v_2, v_3 are adjacent in G. It is easy to handle cases 4-3 in the same fashion as cases 4-1 and 4-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 4-4. Suppose that v_1, v_2, v_3 are pairwise non-adjacent in G. It is easy to handle cases 4-4 in the same fashion as cases 4-1 and 4-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Suppose that Case 5 holds. There are exactly one vertex v_1 of degree four and three vertices v_2 and v_3 of degree three in G. Then we have the next six subcases.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	0	0	3	1	2	2	3	n - 10	n + 0.6733
D_2	2	1	0	0	0	2	3	n-7	n + 0.4455
D_3	0	1	2	0	2	2	3	n-9	n + 0.6167
D_4	2	0	1	1	0	2	3	n-8	n + 0.5021
D_5	1	0	2	1	1	2	3	n-9	n + 0.5877
D_6	1	1	1	0	1	2	3	n-8	n + 0.5311
D_7	0	0	3	2	1	3	2	n - 10	n + 0.7001
D_8	1	2	0	0	0	3	2	n-7	n + 0.5013
D_9	0	2	1	0	1	3	2	n-8	n + 0.5869
D_{10}	1	0	2	2	0	3	2	n-9	n + 0.6144
D_{11}	0	1	2	1	1	3	2	n-9	n + 0.6435
D_{12}	1	1	1	1	0	3	2	n-8	n + 0.5579

• Case 5-1. Suppose that v_1, v_2, v_3, v_4 are pairwise adjacent in G. Table 9 gives us the result.

Table 9: The connected bicyclic graphs and their GA values.

From Table 9, let $G = D_7 \in \tilde{B}_n^{19}$ and $GA(G) = n - 8 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{3}}{7} \approx n + 0.7001$. For other bicyclic graph $G, GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 5-2. Suppose that there are exactly four vertices v_1, v_2, v_3, v_4 are adjacent in G. Table 10 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{33}	d_{22}	GA values
D_1	0	0	3	2	3	1	3	n - 11	n + 0.6062
D_2	3	0	0	2	0	1	3	n-8	n + 0.3493
D_3	1	0	2	2	2	1	3	n - 10	n + 0.5206
D_4	2	0	1	2	1	1	3	n-9	n + 0.43495
D_5	0	0	3	4	1	3	1	n - 11	n + 0.6597
D_6	1	2	0	2	0	3	1	n-8	n + 0.4609
D_7	0	2	1	2	1	3	1	n-9	n + 0.5465
D_8	1	0	2	4	0	3	1	n - 10	n + 0.5740
D_9	0	1	2	3	1	3	1	n - 10	n + 0.6031
D_{10}	1	1	1	3	0	3	1	n-9	n + 0.5175
D_{11}	0	0	3	3	2	2	2	n - 11	n + 0.6329
D_{12}	0	3	0	0	2	2	2	n-8	n + 0.4632
D_{13}	0	1	2	2	2	2	2	n - 10	n + 0.5763
D_{14}	0	2	1	1	2	2	2	n-9	n + 0.5198

Table 10: The connected bicyclic graphs and their GA values.

From Table 10, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

- Case 5-3. Suppose that there are exactly three vertices v_1, v_2, v_3, v_4 are adjacent in G. It is easy to handle case 5-3 in the same fashion as cases 5-1 and 5-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 5-4. Suppose that there are exactly three vertices v_1, v_2, v_3, v_4 are not adjacent in G. It is easy to handle case 5-4 in the same fashion as cases 5-1 and 5-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 5-5. Suppose that there are exactly two vertices v_1, v_2, v_3, v_4 are not adjacent in G. It is easy to handle case 5-5 in the same fashion as cases 5-1 and 5-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

• Case 5-6. Suppose that v_1, v_2, v_3, v_4 are pairwise non-adjacent in G. It is easy to handle case 5-6 in the same fashion as cases 5-1 and 5-2, and we obtain $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Suppose that Case 6 holds. There are exactly one vertex v_1 of degree three and two vertices v_2 and v_3 of degree four in G. Then we have the next four cases.

• Case 6-1. Suppose that v_1, v_2, v_3 are pairwise adjacent in G. Table 11 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{22}	GA values
D_1	0	0	3	1	4	2	n-9	n + 0.55895
D_2	3	0	0	1	1	2	n-6	n + 0.3021
D_3	1	0	2	1	3	2	n-8	n + 0.4733
D_4	2	0	1	1	2	2	n-7	n + 0.3877
D_5	2	1	0	0	2	2	n-6	n + 0.3311
D_6	0	1	2	0	4	2	n-8	n + 0.5024
D_7	1	1	1	0	3	2	n-7	n + 0.4168

Table 11: The connected bicyclic graphs and their GA values.

From Table 11, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 6-2. Suppose that there are exactly two pairs of v_1, v_2, v_3, v_4 are adjacent in G. Table 12 gives us the result.

Graphs	d_{14}	d_{13}	d_{12}	d_{23}	d_{24}	d_{34}	d_{44}	d_{22}	GA values
D_1	0	0	3	1	6	2	0	n - 11	n + 0.4446
D_2	2	1	0	0	4	2	0	n-8	n + 0.2168
D_3	0	1	2	0	6	2	0	n - 10	n + 0.38798
D_4	2	0	1	1	4	2	0	n-9	n + 0.2733
D_5	1	0	2	1	5	2	0	n - 10	n + 0.3589
D_6	1	1	1	0	5	2	0	n-9	n + 0.3024
D_7	3	0	0	1	3	2	0	n-8	n + 0.1877
D_8	0	0	3	2	5	1	1	n - 11	n + 0.4918
D_9	2	1	0	1	3	1	1	n-8	n + 0.26399
D_{10}	0	1	2	1	5	1	1	n - 10	n + 0.4352
D_{11}	2	0	1	2	3	1	1	n-9	n + 0.3206
D_{12}	1	0	2	2	4	1	1	n - 10	n + 0.4062
D_{13}	1	1	1	1	4	1	1	n - 10	n + 0.3496
D_{14}	3	0	0	2	2	1	1	n-8	n + 0.23495

Table 12: The connected bicyclic graphs and their GA values.

From Table 12, we can see that $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

- Case 6-3. Suppose that there are exactly one pair of v_1, v_2, v_3 are adjacent in G. It is easy to handle case 6-3 in the same fashion as cases 6-1 and 6-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 6-4. Suppose that v_1, v_2, v_3 are pairwise non-adjacent in G. It is easy to handle case 6-4 in the same fashion as cases 6-1 and 6-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Suppose that **Case 7** holds. There are exactly five vertices v_1, v_2, v_3, v_4, v_5 of degree three in G. Then we have the next seven subcases.

• Case 7-1. Suppose that there are exactly six pairs of v_1, v_2, v_3, v_4, v_5 are adjacent in G. Table 13 gives us the result.

Graphs	d_{13}	d_{12}	d_{23}	d_{33}	d_{22}	GA values	
D_1	0	3	3	6	n - 11	n + 0.7678	
D_2	3	0	0	6	n-8	n + 0.5981	
D_3	1	2	2	6	n - 10	n + 0.7112	
D_4	2	1	1	6	n-9	n + 0.6547	

Table 13: The connected bicyclic graphs and their GA values.

From Table 13, let $G = D_1 \in \tilde{B_n^{16}}$ and $GA(G) = n - 5 + 2\sqrt{2} + \frac{6\sqrt{6}}{5} \approx n + 0.7678$. Let $G = D_3 \in \tilde{B_n^{18}}$ and $GA(G) = n - 4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} \approx n + 0.7112$. For other bicyclic graph $G, GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

• Case 7-2. Suppose that there are exactly five pairs of v_1, v_2, v_3, v_4, v_5 are adjacent in G. Table 14 gives us the result.

Graphs	d_{13}	d_{12}	d_{23}	d_{33}	d_{22}	GA values
D_1	0	3	5	5	n - 12	n + 0.7274
D_2	3	0	2	5	n-9	n + 0.5577
D_3	1	2	4	5	n - 11	n + 0.6708
D_4	2	1	3	5	n - 10	n + 0.6143

Table 14: The connected bicyclic graphs and their GA values.

From Table 14, let $G = D_1 \in \tilde{B_n^{17}}$ and $GA(G) = n - 7 + 2\sqrt{2} + 2\sqrt{6} \approx n + 0.7274$. For other bicyclic graph $G, GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3} \approx n + 0.6916$.

- Case 7-3. Suppose that there are exactly four pairs of v_1, v_2, v_3, v_4, v_5 are adjacent in G. It is easy to handle case 7-3 in the same fashion as cases 7-1 and 7-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 7-4. Suppose that there are exactly three pairs of v_1, v_2, v_3, v_4, v_5 are adjacent in G. It is easy to handle case 7-4 in the same fashion as cases 7-1 and 7-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 7-5. Suppose that there are exactly two pairs of v_1, v_2, v_3, v_4, v_5 are adjacent in G. It is easy to handle case 7-5 in the same fashion as cases 7-1 and 7-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 7-6. Suppose that there are exactly one pair of v_1, v_2, v_3, v_4, v_5 are adjacent in G. It is easy to handle case 7-6 in the same fashion as cases 7-1 and 7-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.
- Case 7-7. Suppose that v_1, v_2, v_3, v_4, v_5 are not adjacent in G. It is easy to handle case 7-7 in the same fashion as cases 7-1 and 7-2, and we obtain $GA(G) < n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Finally, it is easy to check that

$$\begin{split} n-8 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{3}}{7} &< n-4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} \\ &< n-7 + 2\sqrt{2} + 2\sqrt{6} < n-5 + 2\sqrt{2} + \frac{6\sqrt{6}}{5}. \end{split}$$

Moreover, from the above arguments, if GA(G) is not equal to one of these four values, then

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

This completes the proof. \blacksquare

Some bicyclic graphs in Propositions 2, 3 and 4 with the smallest number of vertices are listed in Appendix. Now, we present our main result. **Theorem 2** Among the set of n-vertex bicyclic graphs,

- (i) for $n \ge 9$, the graphs in \tilde{B}_n^8 are the unique graphs with the seventh maximum GA index, which is equal to $n-5+\frac{4\sqrt{2}}{5}+\frac{8\sqrt{6}}{5}$;
- (ii) for $n \ge 9$, the graphs in \tilde{B}_n^2 are the unique graphs with the eighth maximum GA index, which is equal to $n 7 + \frac{2\sqrt{2}}{3} + \frac{14\sqrt{6}}{5}$;
- (iii) for $n \ge 10$, the graphs in \tilde{B}_n^9 are the unique graphs with the ninth maximum GA index, which is equal to $n-2+\frac{2\sqrt{2}}{3}+\frac{2\sqrt{6}}{5}+\frac{\sqrt{3}}{2};$
- (iv) for $n \ge 10$, the graphs in \tilde{B}_n^3 are the unique graphs with the tenth maximum GA index, which is equal to $n-4+\frac{\sqrt{3}}{2}+\frac{8\sqrt{6}}{5}$;
- (v) for $n \ge 10$, the graphs in \tilde{B}_n^1 are the unique graphs with the eleventh maximum GA index, which is equal to $n-3+\frac{8\sqrt{2}}{3}$;
- (vi) for $n \ge 11$, the graphs in \tilde{B}_n^{16} are the unique graph with the twelfth maximum GA index, which is equal to $n-5+2\sqrt{2}+\frac{6\sqrt{6}}{5}$;
- (vii) for $n \ge 11$, the graphs in \tilde{B}_n^{10} are the unique graph with the thirteenth maximum GA index, which is equal to $n 7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5}$;
- (viii) for $n \ge 11$, the graphs in \tilde{B}_n^4 are the unique graph with the fourteenth maximum GA index, which is equal to $n 9 + \frac{2\sqrt{2}}{3} + \frac{18\sqrt{6}}{5}$;
- (ix) for $n \ge 11$, the graphs in \tilde{B}_n^{11} are the unique graph with the fifteenth maximum GA index, which is equal to $n 4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$;
- (x) for $n \ge 11$, the graphs in \tilde{B}_n^5 are the unique graph with the sixteenth maximum GA index, which is equal to $n 6 + \frac{\sqrt{3}}{2} + \frac{12\sqrt{6}}{5}$;
- (xi) for $n \ge 12$, the graphs in \tilde{B}_n^{17} are the unique graph with the seventeenth maximum GA index, which is equal to $n 7 + 2\sqrt{2} + 2\sqrt{6}$;
- (xii) for $n \ge 12$, the graphs in \tilde{B}_n^{12} are the unique graphs with the eighteenth maximum GA index which is equal to $n 9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5}$;
- (xiii) for $n \ge 12$, the graphs in \tilde{B}_n^6 are the unique graphs with the nineteenth maximum GA index which is equal to $n 6 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{3}}{7} + \frac{4\sqrt{5}}{5};$
- (xiv) for $n \ge 12$, the graphs in \tilde{B}_n^{18} are the unique graphs with the twentieth maximum GA index which is equal to $n 4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}$;
- (xv) for $n \ge 12$, the graphs in $\tilde{B}_n^{\tilde{1}3}$ are the unique graphs with the twenty-first maximum GA index which is equal to $n 7 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7};$
- (xvi) for $n \ge 12$, the graphs in \tilde{B}_n^{14} are the unique graphs with the twenty-second maximum GA index which is equal to $n 6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6}$;
- (xvii) for $n \ge 12$, the graphs in \tilde{B}_n^7 are the unique graphs with the twenty-third maximum GA index which is equal to $n 8 + \frac{\sqrt{3}}{2} + \frac{16\sqrt{6}}{5}$;

- (xviii) for $n \ge 12$, the graphs in \tilde{B}_n^{19} are the unique graphs with the twenty-forth maximum GA index which is equal to $n 8 + \frac{5\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{3}}{7}$;
- (xix) for $n \ge 12$, the graphs in \tilde{B}_n^{15} are the unique graphs with the twenty-fifth maximum GA index which is equal to $n 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$.

Proof. Let G be an n-vertex bicyclic graph different from the graphs mentioned in Theorem 1 with the first six maximum GA indices, where $n \ge 8$. If there are $k \ge 4$ pendant paths in G, then by Lemma 1, we have

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

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

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

If G has exactly no pendant path, then from Proposition 1, the unique GA index is

$$n-3+\frac{8\sqrt{2}}{3}.$$

and $GA(G) < n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$. If G has exactly one pendant paths, then from Proposition 2, the first sixth maximum GA indices are, respectively,

$$n - 7 + \frac{2\sqrt{2}}{3} + \frac{14\sqrt{6}}{5}, \quad n - 4 + \frac{\sqrt{3}}{2} + \frac{8\sqrt{6}}{5}, \quad n - 9 + \frac{2\sqrt{2}}{3} + \frac{18\sqrt{6}}{5},$$
$$n - 6 + \frac{\sqrt{3}}{2} + \frac{12\sqrt{6}}{5}, \quad n - 6 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{3}}{7} + \frac{4\sqrt{6}}{5}, \quad n - 8 + \frac{\sqrt{3}}{2} + \frac{16\sqrt{6}}{5},$$

and for all other graphs G,

$$GA(G) < n-3 + \frac{4\sqrt{6}}{5} + \sqrt{3}$$

If G has exactly two pendant paths, then from Proposition 3, the first eighth maximum GA indices are, respectively

$$n - 5 + \frac{4\sqrt{2}}{3} + \frac{8\sqrt{6}}{5}, \quad n - 2 + \frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} + \frac{\sqrt{3}}{2}, \quad n - 7 + \frac{4\sqrt{2}}{3} + \frac{12\sqrt{6}}{5}$$
$$n - 4 + \frac{2\sqrt{2}}{3} + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2}, \quad n - 9 + \frac{4\sqrt{2}}{3} + \frac{16\sqrt{6}}{5}, \quad n - 7 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{8\sqrt{3}}{7}$$
$$n - 6 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2} + 2\sqrt{6}, \quad n - 3 + \frac{4\sqrt{6}}{5} + \sqrt{3}.$$

If G has exactly three pendant paths, then from Proposition 4, the first fourth maximum GA indices are, respectively

$$n - 5 + 2\sqrt{2} + \frac{6\sqrt{6}}{5}, \quad n - 7 + 2\sqrt{2} + 2\sqrt{6},$$
$$n - 4 + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3} + \frac{4\sqrt{6}}{5}, \quad n - 8 + \frac{8\sqrt{2}}{3} + \frac{4\sqrt{6}}{5} + \frac{12\sqrt{3}}{7}$$

,

and for all other graphs G,

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

At the end, we can be check that

$$\begin{split} n-3+\frac{4\sqrt{6}}{5}+\sqrt{3} &< n-8+\frac{5\sqrt{2}}{3}+\frac{4\sqrt{6}}{5}+\frac{12\sqrt{3}}{7} \\ &< n-8+\frac{\sqrt{3}}{2}+\frac{16\sqrt{6}}{5} < n-6+\frac{2\sqrt{2}}{3}+\frac{\sqrt{3}}{2}+2\sqrt{6} \\ &< n-7+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{6}}{5}+\frac{8\sqrt{3}}{7} < n-4+\frac{\sqrt{3}}{2}+\frac{4\sqrt{2}}{3}+\frac{4\sqrt{6}}{5} \\ &< n-6+\frac{8\sqrt{2}}{3}+\frac{4\sqrt{3}}{7}+\frac{4\sqrt{6}}{5} < -9+\frac{4\sqrt{2}}{3}+\frac{16\sqrt{6}}{5} \\ &< n-7+2\sqrt{2}+2\sqrt{6} < n-6+\frac{\sqrt{3}}{2}+\frac{12\sqrt{6}}{5} \\ &< n-4+\frac{2\sqrt{2}}{3}+\frac{6\sqrt{6}}{5}+\frac{\sqrt{3}}{2} < n-9+\frac{2\sqrt{2}}{3}+\frac{18\sqrt{6}}{5} \\ &< n-7+\frac{4\sqrt{2}}{3}+\frac{12\sqrt{6}}{5} < n-5+2\sqrt{2}+\frac{6\sqrt{6}}{5} \\ &< n-3+\frac{8\sqrt{2}}{3} < n-4+\frac{\sqrt{3}}{3}+\frac{8\sqrt{6}}{5} \\ &< n-2+\frac{2\sqrt{2}}{3}+\frac{2\sqrt{6}}{5}+\frac{\sqrt{3}}{2} < n-7+\frac{2\sqrt{2}}{3}+\frac{14\sqrt{6}}{5} \\ &< n-5+\frac{4\sqrt{2}}{3}+\frac{8\sqrt{6}}{5}. \end{split}$$

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

Now the result follows easily. This completes the proof. ■

4 Conclusion

In this paper, we presented a further ordering for the GA indices of bicyclic graphs, and determined the first twenty-fifth maximum GA indices of bicyclic graphs. In particular, in our proof, we mainly investigated the GA indices of bicyclic graphs with at most three pendant paths. If we want to order more bicyclic graphs with large GA indices, we need only to consider such graphs with more pendant paths (e.g., the bicyclic graphs with exactly four or five pendant paths).

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5 Appendix

In the following figures, we list some bicyclic graphs in Propositions 2, 3 and 4 with the smallest number of vertices.



Figure 2: The bicyclic graphs in Proposition 4(i) with n = 9.



Figure 3: The bicyclic graphs in Proposition 4(ii) with n = 10.



Figure 4: The bicyclic graphs in Proposition 4(iii) with n = 11.



Figure 5: The bicyclic graphs in Proposition 4(iv) with n = 11.



Figure 7: The bicyclic graphs in Proposition 4(vi) with n = 12.



Figure 8: The bicyclic graphs in Proposition 5(i) with n = 9.



Figure 9: The bicyclic graphs in Proposition 5(ii) with n = 10.



Figure 10: The bicyclic graphs in Proposition 5(iii) with n = 11.



Figure 11: The bicyclic graphs in Proposition 5(iv) with n = 11.



Figure 12: The bicyclic graphs in Proposition 5(v) with n = 12.



Figure 13: The bicyclic graphs in Proposition 5(vi) with n = 12.



Figure 14: The bicyclic graphs in Proposition 5(vii) with n = 12.



Figure 15: The bicyclic graphs in Proposition 5(viii) with n = 12.



Figure 16: The bicyclic graphs in Proposition 6(i) with n = 11.



Figure 17: The bicyclic graphs in Proposition 6(ii) with n = 12.



Figure 18: The bicyclic graphs in Proposition 6(iii) with n = 12.



Figure 19: The bicyclic graphs in Proposition 6(iv) with n = 12.