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Resolving an Open Problem on the Exponential Arithmetic–Geometric Index of Unicyclic Graphs

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Abstract: Recently, the exponential arithmetic–geometric index (EAG) was introduced. The exponential arithmetic–geometric index (EAG) of a graph G is defined as $EAG(G) = \sum_{v_iv_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}$, where d_i represents the degree of the vertex v_i in G. The characterization of extreme structures in relation to graph invariants from the class of unicyclic graphs is an important problem in discrete mathematics. Cruz et al., 2022 proposed a unified method for finding extremal unicyclic graphs for exponential degree-based graph invariants. However, in the case of EAG, this method is insufficient for generating the maximal unicyclic graph. Consequently, the same article presented an open problem for the investigation of the maximal unicyclic graph with respect to this invariant. This article completely characterizes the maximal unicyclic graph in relation to EAG.

Keywords: extremal graph; exponential arithmetic–geometric index; unicyclic graph

MSC: 05C90; 05C07; 05C35

1. Introduction

In recent years, graph theory has become a crucial tool in the field of chemistry, particularly in the study of molecular structures. A topological index is a numerical quantity associated with a molecular graph that describes specific physicochemical properties. Since Wiener introduced the first such index [1], many other indices have been developed depending on various graph parameters, including degree, distance, and eccentricity [2–7]. Among these, degree-based indices have received significant attention since the 1970s due to their strong correlation with molecular properties. One important example is the arithmetic–geometric index, introduced in [8]. Let G be a simple connected graph, whose vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, with the edge set being denoted as $E(G)$. The degree of the j-th vertex v_j is denoted by d_j. The arithmetic–geometric index (AG) is defined as

$$AG(G) = \sum_{v_iv_j \in E(G)} \frac{d_i + d_j}{2\sqrt{d_id_j}}.$$

Numerous publications have extensively studied the mathematical properties of AG, specifically the extremal problems and bounds. Shegehalli et al. [9,10] computed AG for different classes of graphs. Milovanović et al. [11] established some upper bounds on AG for simple connected graphs. Hertz et al. [12] identified extremal chemical graphs for AG. Maximal chemical trees with respect to AG were characterized in [13]. Additional research

Academic Editor: Takayuki Hibi

Received: 15 March 2025
Revised: 19 April 2025
Accepted: 22 April 2025
Published: 24 April 2025

Citation: Das, K.C.; Bera, J. Resolving an Open Problem on the Exponential Arithmetic–Geometric Index of Unicyclic Graphs. *Mathematics* **2025**, *13*, 1391. https://doi.org/10.3390/math13091391

on AG can be found in [14–17]. To improve the discriminative power of topological indices, exponential versions were introduced in 2019 [18]. In [19,20], researchers provided a characterization of the extremal trees for the exponential Randić index. Das et al. [21] explored extremal graphs for the exponential atom–bond connectivity index. Jahanbani et al. [22] determined the minimum value of the exponential forgotten index for trees. Das and Mondal [23] examined sharp bounds on the exponential geometric–arithmetic index of bipartite graphs. Further studies on this concept include [24–29]. In this paper, we focus on the exponential arithmetic–geometric index (EAG), which is defined as

$$EAG(G) = \sum_{v_i v_J \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}}.$$

Previous studies have systematically characterized extremal unicyclic graphs for various degree-based indices. For example, Moon and Park [30] investigated extremal unicyclic graphs for the geometric–arithmetic index, while Cruz et al. [31] addressed the same problem with respect to AG. Liu et al. [32] presented a complete classification of extremal unicyclic graphs for the Lanzhou index. The maximal unicyclic graphs for the exponential second Zagreb and augmented Zagreb indices were described in [33,34]. For more insights into extremal unicyclic graphs, readers can refer to [35–42]. Cruz et al. [37] introduced a unified method for the identification of extremal unicyclic graphs for exponential degree-based indices, which was successfully applied to many well-known indices. However, they discovered that this method is insufficient for generating the maximal unicyclic graph in the case of EAG. Because of this, the following open problem was posed in [37]:

Problem 1 ([37])**.** *Characterize the maximal unicyclic graph with respect to EAG in terms of graph order.*

This paper aims to fully solve this problem by applying advanced combinatorial methods. Our goal is to develop new methods that will help us to identify the maximal unicyclic graph with respect to EAG.

2. Main Result

In this section, we address and resolve the open problem concerning the exponential arithmetic–geometric index of unicyclic graphs. To achieve this, we first establish the following essential results:

Lemma 1. *Let $x \geq 2$. Then, $3x^5 - 49x^4 + 310x^3 - 936x^2 + 1366x - 775 > 0$.*

Proof. Let $f(x) = 3x^5 - 49x^4 + 310x^3 - 936x^2 + 1366x - 775$. Now,

$$\begin{aligned} &3x^5 - 49x^4 + 310x^3 - 936x^2 + 1366x - 775 \\ =&x^4(3x - 49) + x^2(310x - 936) + 1366x - 775 > 0 \end{aligned}$$

for $x \geq 17$. Using Mathematica [43], we can visualize the function with a plot, which clearly shows that $f(x) > 0$ for all x in the interval $[2, 17]$. □

Lemma 2. *Let*

$$f(x) = \frac{x}{2\sqrt{x-1}} - \frac{x-1}{2\sqrt{3(x-4)}}, \; x \geq 2.$$

Then, $f(x)$ is a strictly increasing function on $x \geq 2$.

Proof. Since
$$f(x) = \frac{x}{2\sqrt{x-1}} - \frac{x-1}{2\sqrt{3(x-4)}},$$
we have
$$f'(x) = \frac{1}{4\sqrt{x-1}}\left(\frac{x-2}{x-1}\right) - \frac{1}{4\sqrt{3}\sqrt{x-4}}\left(\frac{x-7}{x-4}\right).$$
We have to prove that $f'(x) > 0$, i.e.,
$$\frac{1}{\sqrt{x-1}}\left(\frac{x-2}{x-1}\right) > \frac{1}{\sqrt{3}\sqrt{x-4}}\left(\frac{x-7}{x-4}\right),$$
that is,
$$3(x-2)^2(x-4)^3 > (x-7)(x-1)^3,$$
that is,
$$3x^5 - 49x^4 + 310x^3 - 936x^2 + 1366x - 775 > 0,$$
which is true by Lemma 1 ($x \geq 2$). This proves the result. □

Lemma 3. *Let*
$$g(x) = \frac{x}{2\sqrt{x-1}} - \frac{x+3}{2\sqrt{2(x+1)}}, \; x \geq 4.$$
Then, $g(x)$ is a strictly increasing function on $x \geq 4$.

Proof. Since $x \geq 4$, one can easily see that
$$g'(x) = \frac{1}{4\sqrt{x-1}}\left(\frac{x-2}{x-1}\right) - \frac{1}{4\sqrt{2(x+1)}}\left(\frac{x-1}{x+1}\right) > 0.$$
Therefore, $g(x)$ is a strictly increasing function on $x \geq 4$. □

Lemma 4. *Let*
$$q(x) = \frac{x+3}{2\sqrt{2(x+1)}} - \frac{x+5}{4\sqrt{x+1}}, \;\; x > 0.$$
Then, $q(x)$ is a strictly increasing function on $x > 0$.

Proof. Since $x > 0$, one can easily see that
$$q'(x) = \frac{1}{4\sqrt{2}}\frac{(x-1)}{(x+1)^{3/2}} - \frac{1}{8}\frac{(x-3)}{(x+1)^{3/2}} > 0.$$
Therefore, $q(x)$ is a strictly increasing function on $x > 0$. □

Lemma 5. *For $b \leq d_j \leq d_i \leq a$,*
$$\frac{d_i + d_j}{\sqrt{d_i d_j}} \leq \frac{a+b}{\sqrt{ab}}$$
with equality if and only if $d_i = a$, $d_j = b$.

Proof. For $b \leq d_j \leq d_i \leq a$, we obtain
$$\frac{d_i}{d_j} \leq \frac{a}{b}, \; \frac{d_j}{d_i} \geq \frac{b}{a}, \;\text{ and hence }\; \left(\frac{d_i}{d_j}\right)^{1/4} - \left(\frac{d_j}{d_i}\right)^{1/4} \leq \left(\frac{a}{b}\right)^{1/4} - \left(\frac{b}{a}\right)^{1/4}.$$

Using the above result, we obtain

$$\left(\left(\frac{d_i}{d_j}\right)^{1/4}+\left(\frac{d_j}{d_i}\right)^{1/4}\right)^2=\left(\left(\frac{d_i}{d_j}\right)^{1/4}-\left(\frac{d_j}{d_i}\right)^{1/4}\right)^2+4\le\left(\left(\frac{a}{b}\right)^{1/4}-\left(\frac{b}{a}\right)^{1/4}\right)^2+4,$$

$$\text{that is, } \sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}\le\sqrt{\frac{a}{b}}+\sqrt{\frac{b}{a}}, \text{ that is, } \frac{d_i+d_j}{\sqrt{d_i\,d_j}}\le\frac{a+b}{\sqrt{a\,b}}.$$

Moreover, the equality holds if and only if $d_i = a$, $d_j = b$. □

Let $S_{n,3}$ be a unicyclic graph of order n obtained by adding an edge to the star graph S_n (S_n is a star graph of order n).

Theorem 1. *Let G be a unicyclic graph of order n. Then,*

$$EAG(G)\le(n-3)\,e^{\frac{n}{2\sqrt{n-1}}}+2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}+e \tag{1}$$

with equality if and only if $G\cong S_{n,3}$.

Proof. Let Δ be the maximum degree in the unicyclic graph G. If $\Delta = n-1$, then $G\cong S_{n,3}$ with

$$EAG(G)=(n-3)\,e^{\frac{n}{2\sqrt{n-1}}}+2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}}+e,$$

and hence the equality holds. For $n\le 9$, in accordance to Sage [44], one can easily check that the result (1) holds with equality if and only if $G\cong S_{n,3}$. Otherwise, $\Delta\le n-2$ and $n\ge 10$. For any pendant edge $v_iv_j\in E(G)\,(1=d_j\le d_i\le n-2<n-1)$, by Lemma 5, we obtain

$$\frac{d_i+d_j}{2\sqrt{d_id_j}}<\frac{n}{2\sqrt{n-1}}. \tag{2}$$

For any non-pendant edge $v_iv_j\in E(G)\,(2\le d_j\le d_i\le n-2<n-1)$, by Lemma 5, we obtain

$$\frac{d_i+d_j}{2\sqrt{d_id_j}}<\frac{n+1}{2\sqrt{2\,(n-1)}}. \tag{3}$$

For any edge $v_iv_j\in E(G)$, from (2) and (3), we obtain

$$\frac{d_i+d_j}{2\sqrt{d_id_j}}<\frac{n}{2\sqrt{n-1}} \tag{4}$$

as

$$\frac{n+1}{2\sqrt{2\,(n-1)}}<\frac{n}{2\sqrt{n-1}}.$$

Let k be the length of the cycle in the unicyclic graph G. Then, $k\ge 3$. We consider the following two cases:

Case 1. $k=3$. Let v_1, v_2, v_3 be the three vertices on the cycle in G. We assume that $d_1\ge d_2\ge d_3\ge 2$. We consider the following cases:

Case 1.1. $d_2 = 2$. In this case, $d_2 = d_3 = 2$; hence,

$$\frac{d_2 + d_3}{2\sqrt{d_2 d_3}} = 1.$$

Let $E_1 = \{v_1v_2,\, v_2v_3,\, v_3v_1\}$. Using the above result with (3) and (4), we obtain

$$\begin{aligned} EAG(G) &= \sum_{v_iv_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &= e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} + \sum_{v_iv_j \in E(G)\setminus E_1} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &< 2\, e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e + (n-3)\, e^{\frac{n}{2\sqrt{n-1}}}. \end{aligned}$$

Inequality (1) holds strictly.

Case 1.2. $d_2 = 3$. If $d_3 = 3$, then similarly, by Case 1.1 , we obtain

$$\begin{aligned} EAG(G) &= e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} + \sum_{v_iv_j \in E(G)\setminus E_1} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\ &< 2\, e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + e + (n-3)\, e^{\frac{n}{2\sqrt{n-1}}}. \end{aligned}$$

The result (1) strictly holds. Otherwise, $d_3 = 2$. Let v_4 be the vertex adjacent to the vertex v_2 other than v_1 and v_3. Since $d_2 = 3$ and $d_3 = 2$, we have

$$\frac{d_2 + d_3}{2\sqrt{d_2 d_3}} = \sqrt{\frac{25}{24}}.$$

Again, since $d_2 = 3$ and $d_4 \le n - 4$, by Lemma 5, we obtain

$$\frac{d_2 + d_4}{2\sqrt{d_2 d_4}} \le \frac{n-1}{2\sqrt{3\,(n-4)}}.$$

Since $n \ge 10$, by Lemma 2, we obtain

$$f(n) = \frac{n}{2\sqrt{n-1}} - \frac{n-1}{2\sqrt{3(n-4)}} \ge f(10) = \frac{5}{3} - \sqrt{\frac{9}{8}} > 0.606.$$

From the above results, we obtain

$$\begin{aligned} e^{\frac{n}{2\sqrt{n-1}}} + e > e^{\frac{n-1}{2\sqrt{3(n-4)}}+0.606} + e > 1.83\, e^{\frac{n-1}{2\sqrt{3(n-4)}}} + e &> e^{\frac{n-1}{2\sqrt{3(n-4)}}} + 0.83\, e^{\frac{\sqrt{n+2}}{2\sqrt{3}}} + e \\ &\ge e^{\frac{n-1}{2\sqrt{3(n-4)}}} + 1.83\, e \\ &> e^{\frac{n-1}{2\sqrt{3(n-4)}}} + e^{\sqrt{\frac{25}{24}}} \\ &\ge e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_2+d_4}{2\sqrt{d_2d_4}}}. \end{aligned}$$

Let $E_2 = E_1 \cup \{v_2v_4\}$. By (3) and (4), we obtain

$$e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} < e^{\frac{n+1}{2\sqrt{2(n-1)}}},\ e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} < e^{\frac{n+1}{2\sqrt{2(n-1)}}},\ \text{ and } e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} < e^{\frac{n}{2\sqrt{n-1}}} \text{ for any } v_iv_j \in E(G)\backslash E_2.$$

Using the above results with $|E(G)\backslash E_2| = n-4$, we obtain

$$EAG(G) = e^{\frac{d_1+d_2}{2\sqrt{d_1d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_1}{2\sqrt{d_3d_1}}} + e^{\frac{d_2+d_4}{2\sqrt{d_2d_4}}} + \sum_{v_iv_j\in E(G)\backslash E_2} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}}$$

$$< 2\,e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e + (n-3)\,e^{\frac{n}{2\sqrt{n-1}}}.$$

The result (1) strictly holds.

Case 1.3. $d_2 \geq 4$. Let $S_1 = \{v_2v_j \in E(G) \mid \text{for all } v_j \in N_G(v_2)\}$, $S = S_1 \cup \{v_1v_3\}$ and $E_3 = E(G)\backslash S$. Since G is a unicyclic graph of order n, we have $d_1 + d_2 \leq n+1$. Thus, we have $d_1 \leq n-3$, $4 \leq d_2 \leq \frac{n+1}{2}$, and $d_3 \geq 2$. Since $d_1 \geq d_2 \geq d_3$, by Lemma 5, we obtain

$$\frac{d_1+d_2}{2\sqrt{d_1d_2}} \leq \frac{n+1}{4\sqrt{n-3}}, \frac{d_2+d_3}{2\sqrt{d_2d_3}} \leq \frac{n+5}{4\sqrt{n+1}}, \frac{d_1+d_3}{2\sqrt{d_1d_3}} \leq \frac{n-1}{2\sqrt{2(n-3)}} < \frac{n+1}{2\sqrt{2(n-1)}}. \tag{5}$$

Since $|E_3| = |E(G)\backslash S| = n - d_2 - 1$, by (4), we obtain

$$\sum_{v_iv_j\in E_3} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} < (n-d_2-1)\,e^{\frac{n}{2\sqrt{n-1}}}. \tag{6}$$

Claim 1.

$$2\,e^{\frac{n+3}{2\sqrt{2(n+1)}}} + e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} < 2\,e^{\frac{n}{2\sqrt{n-1}}} + e^{\frac{n+1}{2\sqrt{2(n-1)}}}.$$

Proof of Claim 1. For $10 \leq n \leq 11$, in accordance to Mathematica [43], one can easily check that the result holds. Otherwise, $n \geq 12$. By Lemma 3, the function $g(x) = \frac{x}{2\sqrt{x-1}} - \frac{x+3}{2\sqrt{2(x+1)}}$ is increasing on $x \geq 12$; hence,

$$g(x) \geq g(12) = \frac{6}{\sqrt{11}} - \frac{15}{2\sqrt{26}} > 0.338.$$

Since $n \geq 12$, from the above, we have

$$\frac{n}{2\sqrt{n-1}} - \frac{n+3}{2\sqrt{2(n+1)}} > 0.338 > \ln 1.4,$$

$$\text{that is, } e^{\frac{n}{2\sqrt{n-1}} - \frac{n+3}{2\sqrt{2(n+1)}}} > 1.4, \text{ that is, } e^{\frac{n}{2\sqrt{n-1}}} > 1.4\,e^{\frac{n+3}{2\sqrt{2(n+1)}}}. \tag{7}$$

By Lemma 4, the function $q(x) = \frac{x+3}{2\sqrt{2(x+1)}} - \frac{x+5}{4\sqrt{x+1}}$ is increasing on $x \geq 12$; hence,

$$q(x) \geq q(12) = \frac{15}{2\sqrt{26}} - \frac{17}{4\sqrt{13}} > 0.29.$$

Since $n \geq 12$, from the above, we have

$$\frac{n+3}{2\sqrt{2(n+1)}} - \frac{n+5}{4\sqrt{n+1}} > 0.29 > \ln\left(\frac{5}{4}\right),$$

$$\text{that is, } e^{\frac{n+3}{2\sqrt{2(n+1)}}-\frac{n+5}{4\sqrt{n+1}}} > \frac{5}{4}, \text{ that is, } 0.8\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} > e^{\frac{n+5}{4\sqrt{n+1}}}. \tag{8}$$

Since $n > 5$, one can easily see that

$$\frac{n+1}{4\sqrt{n-3}} < \frac{n+1}{2\sqrt{2(n-1)}}, \text{ that is, } e^{\frac{n+1}{4\sqrt{n-3}}} < e^{\frac{n+1}{2\sqrt{2(n-1)}}}.$$

Using the above result with (7) and (8), we obtain

$$\begin{aligned} 2\, e^{\frac{n}{2\sqrt{n-1}}} + e^{\frac{n+1}{2\sqrt{2(n-1)}}} &> 2.8\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + e^{\frac{n+1}{2\sqrt{2(n-1)}}} \\ &> 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + e^{\frac{n+1}{2\sqrt{2(n-1)}}} \\ &> 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + e^{\frac{n+1}{4\sqrt{n-3}}}. \end{aligned}$$

This completes the proof of Claim 1. □

For $v_j \in N_G(v_2) \backslash \{v_1, v_3\}$, we have $4 \le d_2 \le \frac{n+1}{2}$, $1 \le d_j \le \frac{n-3}{2}$, and by Lemma 5, we obtain

$$\frac{d_2 + d_j}{2\sqrt{d_2 d_j}} \le \frac{n+3}{2\sqrt{2(n+1)}}.$$

Using the above result with (5), we obtain

$$\begin{aligned} \sum_{v_j : v_j \in N_G(v_2)} e^{\frac{d_2+d_j}{2\sqrt{d_2 d_j}}} &= e^{\frac{d_1+d_2}{2\sqrt{d_1 d_2}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2 d_3}}} + \sum_{v_j : v_j \in N_G(v_2)\backslash\{v_1, v_3\}} e^{\frac{d_2+d_j}{2\sqrt{d_2 d_j}}} \\ &\le e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + (d_2 - 2)\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} \\ &\le e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + (d_2 - 4)\, e^{\frac{n}{2\sqrt{n-1}}} \end{aligned} \tag{9}$$

as

$$\frac{n+3}{2\sqrt{2(n+1)}} < \frac{n}{2\sqrt{n-1}}.$$

Using (5), (6), (9) and Claim 1, we obtain

$$\begin{aligned} EAG(G) &= \sum_{v_i v_j \in E(G)} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}} \\ &= e^{\frac{d_1+d_3}{2\sqrt{d_1 d_3}}} + \sum_{v_j : v_j \in N_G(v_2)} e^{\frac{d_2+d_j}{2\sqrt{d_2 d_j}}} + \sum_{v_i v_j \in E_3} e^{\frac{d_i+d_j}{2\sqrt{d_i d_j}}} \\ &< e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e^{\frac{n+1}{4\sqrt{n-3}}} + e^{\frac{n+5}{4\sqrt{n+1}}} + 2\, e^{\frac{n+3}{2\sqrt{2(n+1)}}} + (d_2 - 4)\, e^{\frac{n}{2\sqrt{n-1}}} + (n - d_2 - 1)\, e^{\frac{n}{2\sqrt{n-1}}} \\ &< (n-3)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-2)}}} < (n-3)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e. \end{aligned}$$

The result (1) strictly holds.

Case 2. $k \geq 4$. Let $v_1, v_2, \ldots, v_k$ be the vertices on the cycle C_k $(k \geq 4)$. We can assume that $d_1 = \max\{d_i : v_i \in V(C_k)\}$. Then, $d_1 \leq n-k+2 \leq n-2$ and $d_i \geq 2\,(2 \leq i \leq k)$. Then, by Lemma 5, for $v_1v_2 \in E(C_k)$ and $v_1v_k \in E(C_k)$, we obtain

$$\frac{d_1+d_2}{2\sqrt{d_1\,d_2}} \leq \frac{n}{2\sqrt{2\,(n-2)}} \quad \text{and} \quad \frac{d_1+d_k}{2\sqrt{d_1\,d_k}} \leq \frac{n}{2\sqrt{2\,(n-2)}}.$$

Since $v_2v_3 \in E(C_k)$ and $v_3v_4 \in E(C_k)$ with $2 \leq d_2, d_3, d_4 \leq \frac{n-k+4}{2} \leq \frac{n}{2}$, by Lemma 5, we obtain

$$\frac{d_2+d_3}{2\sqrt{d_2\,d_3}} \leq \frac{n+4}{4\sqrt{n}} \quad \text{and} \quad \frac{d_3+d_4}{2\sqrt{d_3\,d_4}} \leq \frac{n+4}{4\sqrt{n}}. \tag{10}$$

Claim 2.

$$2\,e^{\frac{n+4}{4\sqrt{n}}} < e^{\frac{n}{2\sqrt{n-1}}} + e.$$

Proof of Claim 2. For $10 \leq n \leq 12$, in accordance to Mathematica [43], one can easily check that the result holds. Otherwise, $n \geq 13$. Let us consider a function

$$h(x) = \frac{x}{\sqrt{x-1}} - \frac{x+4}{2\sqrt{x}}, \quad x \geq 13.$$

Then, we have

$$h'(x) = \frac{1}{4x^{3/2}\,(x-1)^{3/2}}\left[2\,x^{3/2}\,(x-2) - (x-4)\,(x-1)^{3/2}\right] > 0.$$

Thus, $h(x)$ is an increasing function on $x \geq 13$ and, hence,

$$h(x) \geq h(13) = \frac{13}{\sqrt{12}} - \frac{17}{2\sqrt{13}} > 1.395 > 2\ \ln 2.$$

From the above, we obtain

$$\frac{n}{\sqrt{n-1}} - \frac{n+4}{2\sqrt{n}} > 2\ \ln 2,$$

that is,

$$e^{\frac{n}{2\sqrt{n-1}} - \frac{n+4}{4\sqrt{n}}} > 2,$$

that is,

$$2\,e^{\frac{n+4}{4\sqrt{n}}} < e^{\frac{n}{2\sqrt{n-1}}} < e^{\frac{n}{2\sqrt{n-1}}} + e.$$

This completes the proof of Claim 2. $\square$

Let p be the number of pendant vertices in G. Since G has a cycle length of at least 4, we have $p \leq n-4$. Since $\frac{n+1}{\sqrt{2\,(n-1)}} < \frac{n}{\sqrt{n-1}}$, using (3), we obtain

$$\sum_{\substack{v_iv_j \in E(G)\setminus\{v_2v_3, v_3v_4\},\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} < (n-p-2)\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} \leq 2\,e^{\frac{n+1}{2\sqrt{2\,(n-1)}}} + (n-p-4)\,e^{\frac{n}{2\sqrt{n-1}}}.$$

Using the above result with (2), (10) and Claim 2, we obtain

$$
\begin{aligned}
EAG(G) &= \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j = 1}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} + \sum_{\substack{v_iv_j \in E(G),\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\
&< p\, e^{\frac{n}{2\sqrt{n-1}}} + e^{\frac{d_2+d_3}{2\sqrt{d_2d_3}}} + e^{\frac{d_3+d_4}{2\sqrt{d_3d_4}}} + \sum_{\substack{v_iv_j \in E(G) \setminus \{v_2v_3, v_3v_4\},\\ d_i \geq d_j \geq 2}} e^{\frac{d_i+d_j}{2\sqrt{d_id_j}}} \\
&< p\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+4}{4\sqrt{n}}} + (n-p-4)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-1)}}} \\
&< (n-3)\, e^{\frac{n}{2\sqrt{n-1}}} + 2\, e^{\frac{n+1}{2\sqrt{2(n-1)}}} + e.
\end{aligned}
$$

The result (1) strictly holds. This completes the proof of the theorem. □

3. Concluding Remarks

The exponential arithmetic–geometric index (denoted as EAG) is a recently introduced topological index in the field of mathematical chemistry. This index was first brought into the literature by Rada [18]. In [37], the authors proposed an open problem: to characterize the unicyclic graph that attains the maximum EAG value among all unicyclic graphs of a given order n. In this paper, we address and resolve this open problem by providing a complete characterization of an extremal graph. Our findings show that, among all unicyclic graphs with n vertices, the graph $S_{n,3}$ uniquely maximizes the EAG index. This result not only settles the open problem posed by Cruz, Rada, and Sánchez but also contributes to a deeper understanding of the behavior of the EAG index in relation to graph structures.

Author Contributions: Conceptualization, K.C.D. and J.B.; investigation, K.C.D. and J.B.; writing—original draft preparation, K.C.D. and J.B.; writing—review and editing, K.C.D. and J.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The data presented in this study are openly available in https://figshare.com/articles/dataset/GRAZPEDWRI-DX/14825193 (accessed on 21 April 2025).

Conflicts of Interest: The authors declare no conflicts of interest.

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