Computational and Applied Mathematics (2024) 43:317
https://doi.org/10.1007/s40314-024-02815-2

Open problem on the maximum exponential augmented Zagreb index of unicyclic graphs

Kinkar Chandra Das[1] · Sourav Mondal[1,2] · Da-yeon Huh[1]

Received: 2 January 2024 / Revised: 19 May 2024 / Accepted: 5 June 2024 /
Published online: 5 July 2024

Abstract

A topological index is a numerical property of a molecular graph that explains structural features of molecules. The potential of topological indices to discriminate between distinct structures is a significant topic to investigate. In this context, the exponential degree-based indices were put forward in the literature. The present work focuses on the exponential augmented Zagreb index (EAZ), which is defined for a graph G as

$$EAZ(G) = \sum_{v_i v_j \in E(G)} e^{\left(\frac{d_i\, d_j}{d_i + d_j - 2}\right)^3},$$

where d_i represents the degree of the vertex v_i and $E(G)$ denotes the edge set of G. This work characterizes the maximal unicyclic graph for EAZ in terms of graph order, which was posed as an open problem in the recent article Cruz et al. (MATCH Commun Math Comput Chem 88:481-503, 2022).

Keywords Topological index · Exponential AZ index · Extremal graph · Unicyclic graph

Mathematics Subject Classification 05C07 · 05C09 · 05C35

1 Introduction

Throughout this article, we consider G as a simple connected graph of order n and size m having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. A graph G is said to be unicyclic if $m = n$. The degree of vertex $v_i \in V(G)$ is defined as the number of vertices

✉ Sourav Mondal
souravmath94@gmail.com

Kinkar Chandra Das
kinkardas2003@gmail.com

Da-yeon Huh
dayeonhuh7@gmail.com

1 Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea

2 Department of Mathematics, College of Sciences, University of Sharjah, Sharjah 27272, UAE

adjacent to v_i. Let $N_G(v_i)$ be the neighbor set of the vertex v_i, that is, $N_G(v_i) = \{v_k \in V(G) : v_i v_k \in E(G)\}$. The double star $DS_{p,q}$ is a graph that is obtained after joining two central vertices of two stars S_p and S_q.

Topological indices are numerical descriptors used in the field of mathematical chemistry and chem-informatics to characterize the topology of molecular structures. These indices provide a quantitative measure of the structural features of a molecule, focusing on the spatial arrangement of atoms and bonds rather than their chemical nature. The origin of topological indices lies in graph theory, where a molecule is depicted as a graph featuring atoms as vertices and bonds as edges. From a mathematical perspective, it is conceptualized as a function mapping all molecular graphs to real numbers, ensuring its invariance under graph isomorphism. These indices are employed to explain different physical and chemical properties of molecules, which supports researchers working on drug design, material science, and other branches of chemistry (Basak and Vracko 2020). After Wiener's seminal work in 1947 Wiener (1947), a multitude of indices have been introduced in literature, utilizing various parameters such as degree, distance, eccentricity, and spectrum (Liu 2023; Hayat et al. 2023; Liu 2022; Maitreyi et al. 2023; Liu and Huang 2023; Du and Dimitrov 2020; Ghanbari 2022; Ali et al. 2021; Das et al. 2018; Gutman and Das 2004; Das and Vetrík 2023; Hosseini et al. 2022). While each category has its own set of applications and benefits, the domain of chemical graph theory is notably influenced by degree-based indices. The augmented Zagreb index (AZ) (Furtula et al. 2010) is one of the well-known degree based indices, which is formulated as

$$AZ(G) = \sum_{v_i v_j \in E(G)} \left(\frac{d_i\, d_j}{d_i + d_j - 2} \right)^3.$$

Widespread investigation of the AZ index is apparent in Chen et al. (2022); Sun et al. (2018); Cheng et al. (2021); Ali et al. (2021); Li et al. (2019, 2021); Ali (2021). To investigate the discrimination capability of topological indices, Rada (2019) proposed the exponential degree-based indices. A comprehensive identification of extremal trees for such invariants was reported in Cruz and Rada (2019). The path graph was established to be the maximal tree for the exponential Randić index (Cruz et al. 2020). Eliasi provided characterization of the maximal unicyclic and bicyclic graphs with respect to the exponential second Zagreb index in Eliasi (2022). For further insight on this direction, readers are referred to Xu et al. (2023); Cruz et al. (2021); Das et al. (2021); Wang and Wu (2022); Das and Mondal (2023); Carballosa et al. (2023). The present work focuses on the exponential augmented Zagreb index (Rada 2019), which is defined as

$$EAZ(G) = \sum_{v_i v_j \in E(G)} e^{\left(\frac{d_i\, d_j}{d_i + d_j - 2} \right)^3}.$$

Cruz and Rada (2019) determined that the star graph serves as the smallest tree for EAZ. They left the problem of identifying the maximal tree open, and this was resolved in Das et al. (2021). The distinct extremal graphs for EAZ within the set of graphs with n non-isolated vertices were identified in Cruz and Rada (2022). For more works on the EAZ index, readers are referred to Das and Mondal (2024); Das et al. (2024). Let C_n and S_n' be cycle and unicyclic graphs of order n, respectively, where S_n' is generated from the star graph S_n of order n by attaching two pendent vertices. Most of the degree based indices yield C_n or S_n' as maximal unicyclic graph in terms of graph order n. A unified approach reported by Cruz et al. (2022)

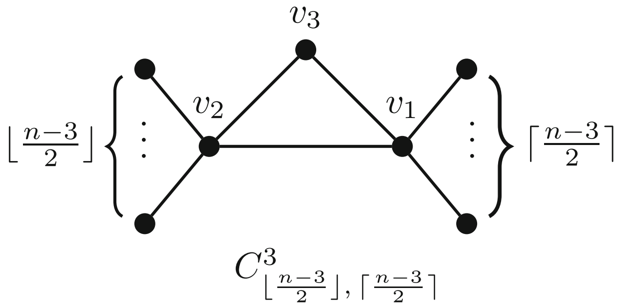

Fig. 1 Unicyclic graph $C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}$

to characterize extremal unicyclic graphs for degree-based indices also confirmed this fact. However, in case of EAZ, this approach is inadequate to generate maximal unicyclic graph. As a consequence, the problem of characterizing maximal unicyclic graph for EAZ in terms of graph order n is posed as an open problem in Cruz et al. (2022). The ultimate aim of this work is to solve this problem. We are surprised to state an amazing property of this extremal graph (see, Fig. 1) that the contribution of EAZ corresponding to one edge $v_1 v_2$ of this structure greater than the EAZ value of all other unicyclic graphs. Such scenario is rare to observe in extremal graph theory literature.

2 Main result

In this section, our aim is to explore the maximal unicyclic graph for the EAZ index.Let $C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}$ be a unicyclic graph (see, Fig. 1) of order n containing a cycle $C_3 : v_1 v_2 v_3 v_1$ such that $\lceil \frac{n-3}{2} \rceil$ pendent edges are incident on v_1 and $\lfloor \frac{n-3}{2} \rfloor$ pendent edges are incident on v_2. We first obtain the following lemma which will be employed to generate the main outcome.

Lemma 1 *Let $C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}$ be a unicyclic graph of order n as displayed in Fig. 1. Then there exists an edge $v_1 v_2 \in E\left(C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}\right)$ such that*

$$e^{\left(\frac{d_1 d_2}{d_1 + d_2 - 2}\right)^3} > \begin{cases} n\, e^{\frac{(n+3)^3}{64}} & \text{if } n \text{ is odd,} \\ n\, e^{\frac{1}{64}\left(\frac{(n+4)(n-2)}{n-1}\right)^3} & \text{if } n \text{ is even.} \end{cases}$$

Proof Using Sage (2015), one can easily verify that the assertion holds for $n \leq 9$. We now investigate the case where $n \geq 10$.

First we assume that $n = 2p + 1$. Then $d_1 = p + 1 = d_2$ and

$$\left(\frac{d_1 d_2}{d_1 + d_2 - 2}\right)^3 = \frac{(p+1)^6}{8p^3} = \frac{1}{8}\left(p + 2 + \frac{1}{p}\right)^3. \tag{1}$$

Now,

$$\frac{1}{2}\left(p+2+\frac{1}{p}\right)-\frac{1}{2}\,(p+2)=\frac{1}{2p}.$$

Then

$$\begin{aligned}\frac{1}{8}\left(p+2+\frac{1}{p}\right)^3&=\frac{(p+2)^3}{8}+\frac{3\,(p+2)^2}{8p}+\frac{3\,(p+2)}{8\,p^2}+\frac{1}{8p^3}\\&>\frac{(p+2)^3}{8}+\frac{3\,(p+2)^2}{8p}\\&>\frac{(n+3)^3}{64}+\frac{3\,(n+7)}{16}.\end{aligned}\tag{2}$$

Now,

$$e^{\frac{3\,(n+7)}{16}}>1+\frac{3\,(n+7)}{16}+\frac{9\,(n+7)^2}{512}+\frac{27\,(n+7)^3}{24,576}+\frac{81\,(n+7)^4}{1572864}.$$

For $n\geq 11$, we obtain

$$1+\frac{3\,(n+7)}{16}+\frac{9\,(n+7)^2}{512}+\frac{27\,(n+7)^3}{24,576}+\frac{81\,(n+7)^4}{1572864}>n$$

and hence

$$e^{\frac{3\,(n+7)}{16}}>n.$$

Using the above result with (2), from (1), we obtain

$$e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3}>e^{\frac{(n+3)^3}{64}}\times e^{\frac{3\,(n+7)}{16}}>n\,e^{\frac{(n+3)^3}{64}}.$$

Next we assume that $n=2p$. Then $d_1=p+1$ and $d_2=p$. Now,

$$\begin{aligned}\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3&=\left(\frac{p\,(p+1)}{2p-1}\right)^3\\&=\left(\frac{(p+2)\,(p-1)}{2p-1}+\frac{2}{2p-1}\right)^3\\&=\left(\frac{(p+2)\,(p-1)}{2p-1}\right)^3+\frac{8}{(2p-1)^3}+\frac{6\,(p+2)^2(p-1)^2}{(2p-1)^3}\\&\quad+\frac{12\,(p+2)\,(p-1)}{(2p-1)^3}\\&>\left(\frac{(p+2)\,(p-1)}{2p-1}\right)^3+\frac{6\,(p+2)^2(p-1)^2}{(2p-1)^3}\end{aligned}$$

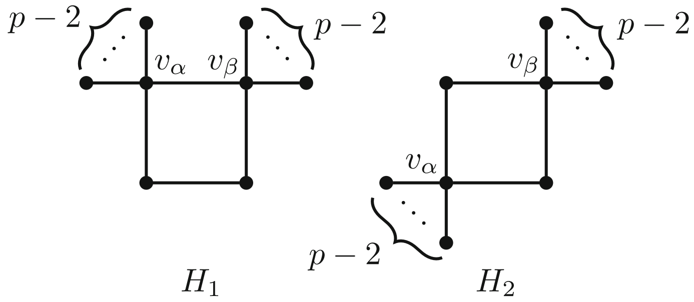

Fig. 2 Two unicyclic graphs H_1 and H_2

$$=\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3+\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}. \tag{3}$$

Now one can write

$$e^{\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}}>1+\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}+\frac{9\,(n+4)^4\,(n-2)^4}{128\,(n-1)^6}.$$

For $n\geq 10$, it is easy to check that

$$1+\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}+\frac{9\,(n+4)^4\,(n-2)^4}{128\,(n-1)^6}>n,$$

which implies

$$e^{\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}}>n.$$

In view of above result, we obtain from (3) that

$$e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3}>e^{\frac{3\,(n+4)^2\,(n-2)^2}{8\,(n-1)^3}}\times e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3}$$

$$>n\,e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3}.$$

Hence, the proof is done. □

Lemma 2 *Let G be a unicyclic graph of even order n. Then there exists $v_\alpha,\ v_\beta\in V(G)$ such that $d_\alpha=d_\beta=\frac{n}{2}$ if and only if $G\cong H_k$, $k=1,\ 2,\ 3,\ 4,\ 5$, where H_k's are reported in Figs. 2, 3, 4 and 5.*

Proof Suppose $n=2p$. First assume that there exists $v_\alpha,\ v_\beta\in V(G)$ such that $d_\alpha=d_\beta=\frac{n}{2}=p$. We have

$$d_\alpha+d_\beta=|N_G(v_\alpha)\cup N_G(v_\beta)|+|N_G(v_\alpha)\cap N_G(v_\beta)|. \tag{4}$$

Let $d_G(v_\alpha,\ v_\beta)$ be the shortest distance between v_α and v_β in G. Then $d_G(v_\alpha,\ v_\beta)\geq 1$. Now we build the proof in the three cases listed below.

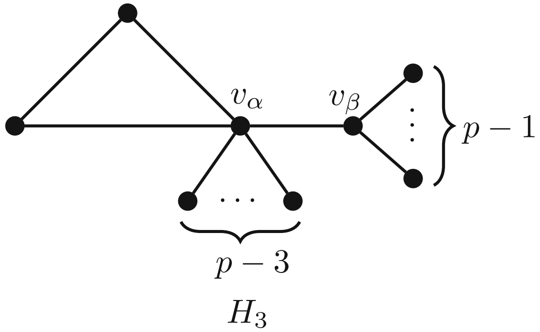

Fig. 3 Unicyclic graph H_3

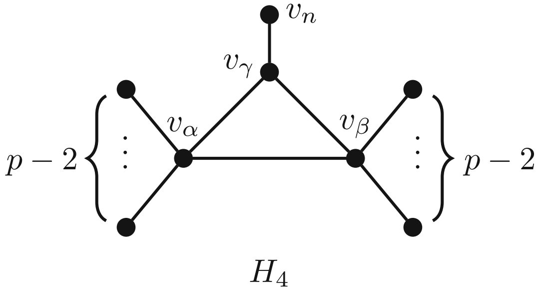

Fig. 4 Unicyclic graph H_4

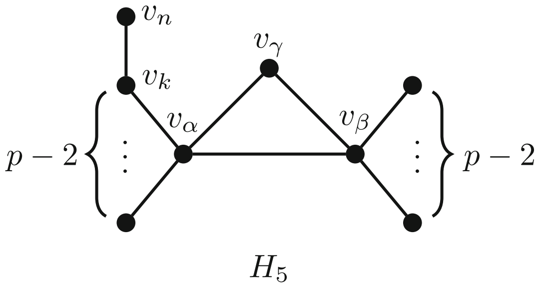

Fig. 5 Unicyclic graph H_5

Case 1. $d_G(v_\alpha,\ v_\beta) = 1$. Since G is a unicyclic graph, $0 \le |N_G(v_\alpha) \cap N_G(v_\beta)| \le 1$. First we assume that $|N_G(v_\alpha) \cap N_G(v_\beta)| = 0$. By (4), we have $|N_G(v_\alpha) \cup N_G(v_\beta)| = d_\alpha + d_\beta = n$. All the vertices in S are adjacent to either v_α or v_β, where $S = V(G)\backslash\{v_\alpha,\ v_\beta\}$. Since $d_\alpha = d_\beta = \frac{n}{2} = p$ and $v_\alpha v_\beta \in E(G)$, $DS_{p-1,p-1}$ is a subgraph of G. Since G is a unicyclic graph with $d_\alpha = d_\beta = \frac{n}{2} = p$, we have $v_i v_j \in E(G)$, where $v_i \in N_G(v_\alpha)$, $v_j \in N_G(v_\beta)$; or $v_i,\ v_j \in N_G(v_\alpha)$ (or $v_i,\ v_j \in N_G(v_\beta)$), that is, $G \cong H_1$ (see, Fig. 2) or $G \cong H_3$ (see, Fig. 3).

Next we assume that $|N_G(v_\alpha) \cap N_G(v_\beta)| = 1$. Let $v_\gamma \in N_G(v_\alpha) \cap N_G(v_\beta)$. By (4), we have $|N_G(v_\alpha) \cup N_G(v_\beta)| = d_\alpha + d_\beta - 1 = n - 1$. Using this result with $d_\alpha = d_\beta = \frac{n}{2} = p$ and $v_\alpha v_\beta \in E(G)$, we conclude that H_0 (see, Fig. 6) is a subgraph of G with $|V(H_0)| = n - 1$. Let $v_n \in V(G)\backslash V(H_0)$. Since G is unicyclic of order n, vertex v_n is adjacent to v_γ, or

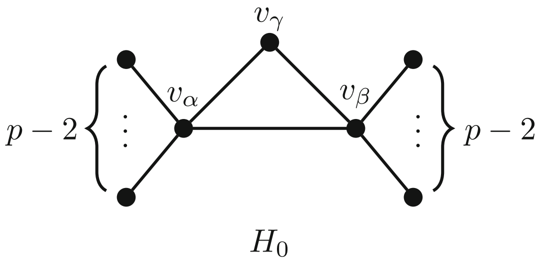

Fig. 6 Unicyclic graph H_0 of order $2p-1$

$v_n v_k \in E(G)$, where $v_k \in N_G(v_\alpha)$ or $v_k \in N_G(v_\beta)$, that is, $G \cong H_4$ (see, Fig. 4) or $G \cong H_5$ (see, Fig. 5).

Case 2. $d_G(v_\alpha, v_\beta) = 2$. In this case $|N_G(v_\alpha) \cup N_G(v_\beta)| \le n-2$. Since G is a unicyclic graph, $1 \le |N_G(v_\alpha) \cap N_G(v_\beta)| \le 2$. If $|N_G(v_\alpha) \cap N_G(v_\beta)| = 1$, then by (4), we obtain $d_\alpha + d_\beta = |N_G(v_\alpha) \cup N_G(v_\beta)| + |N_G(v_\alpha) \cap N_G(v_\beta)| \le n-1 < n = d_\alpha + d_\beta$, a contradiction. Otherwise, $|N_G(v_\alpha) \cap N_G(v_\beta)| = 2$. Again by (4), we have $|N_G(v_\alpha) \cup N_G(v_\beta)| = n-2$. Since $v_\alpha, v_\beta \notin N_G(v_\alpha) \cup N_G(v_\beta)$, all the vertices in S are adjacent to v_α or v_β or both, where $S = V(G) \backslash \{v_\alpha, v_\beta\}$. Since $d_\alpha = d_\beta = \frac{n}{2} = p$ with $|N_G(v_\alpha) \cap N_G(v_\beta)| = 2$, we must have $G \cong H_2$ (see, Fig. 2).

Case 3. $d_G(v_\alpha, v_\beta) \ge 3$. In this case $|N_G(v_\alpha) \cap N_G(v_\beta)| = 0$ and $v_\alpha, v_\beta \notin N_G(v_\alpha) \cup N_G(v_\beta)$. This with (4), we obtain $|N_G(v_\alpha) \cup N_G(v_\beta)| \le n-2 < n = d_\alpha + d_\beta = |N_G(v_\alpha) \cup N_G(v_\beta)|$, a contradiction.

Conversely, we assume that $G \cong H_k$, $k = 1, 2, 3, 4, 5$. Then from Figs. 2, 3, 4 and 5, it is evident that there exists $v_\alpha, v_\beta \in V(G)$ such that $d_\alpha = d_\beta = \frac{n}{2}$. Hence the proof is done. $\square$

Lemma 3 *Let G be a unicyclic graph of even order n. If G contains an edge $v_\alpha v_\beta$ with $d_\alpha = d_\beta = \frac{n}{2}$, then*

$$EAZ(G) < EAZ(C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}).$$

Proof Employing Lemma 2, we can write $G \cong H_k$, $k = 1, 2, 3, 4, 5$. From Figs. 2, 3, 4 and 5, it is clear that

$$EAZ(H_k) = \begin{cases} e^{\frac{n^6}{64\,(n-2)^3}} + (n-4)\, e^{\left(\frac{n}{n-2}\right)^3} + 3e^8 & \text{if } k = 1, 3, \\ (n-4)\, e^{\left(\frac{n}{n-2}\right)^3} + 4e^8 & \text{if } k = 2, \\ e^{\frac{n^6}{64\,(n-2)^3}} + (n-4)\, e^{\left(\frac{n}{n-2}\right)^3} + 2e^{\frac{27n^3}{(n+2)^3}} + e^{\frac{27}{8}} & \text{if } k = 4, \\ e^{\frac{n^6}{64\,(n-2)^3}} + (n-5)\, e^{\left(\frac{n}{n-2}\right)^3} + 4e^8 & \text{if } k = 5. \end{cases}$$

One can easily find that $EAZ(H_k) < EAZ\left(C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}\right)$ for $n = 4, 6, 8, 10$, and $k = 1, 2, 3, 4, 5$. Now we consider $n \ge 12$. Note that $d_i \le p$ for any $v_i \in V(H_k)$

($k = 1,\ 2,\ 3,\ 4,\ 5.$). For any $v_i v_j \in E(H_k)$ satisfying $d_i \ge d_j \ge 2$, we obtain

$$\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i\, d_j} = \frac{1}{d_i} + \frac{1}{d_j}\left(1 - \frac{2}{d_i}\right) \ge \frac{1}{p} + \frac{1}{d_i}\left(1 - \frac{2}{p}\right) \ge \frac{1}{p} + \frac{1}{p}\left(1 - \frac{2}{p}\right),$$

which exerts

$$\frac{d_i\, d_j}{d_i + d_j - 2} \le \frac{p^2}{2p - 2} = \frac{n^2}{4\,(n-2)} < \frac{(n+4)\,(n-2)}{4\,(n-1)}, \quad \text{as } n \ge 12.$$

For any $v_i v_j \in E(H_k)$ satisfying $d_i \ge d_j = 1$, we obtain

$$\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i\, d_j} = 1 - \frac{1}{d_i} \ge \frac{1}{2},$$

that is,

$$\frac{d_i\, d_j}{d_i + d_j - 2} \le 2 < \frac{(n+4)\,(n-2)}{4\,(n-1)} \quad \text{as } n \ge 12.$$

Thus by Lemma 1, we obtain

$$\begin{aligned} EAZ(H_k) &< n\, e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3} < e^{\left(\frac{d_1\, d_2}{d_1 + d_2 - 2}\right)^3} \\ &< EAZ\left(C^3_{\lfloor \frac{n-3}{2} \rfloor,\, \lceil \frac{n-3}{2} \rceil}\right) \end{aligned}$$

for $k = 1,\ 2,\ 3,\ 4,\ 5$. Hence the proof is completed. □

We are now ready to prove our main result of this paper.

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

$$EAZ(G) \le \begin{cases} e^{\left(\frac{n\,(n+2)}{4\,(n-1)}\right)^3} + \frac{n-2}{2}\, e^{\left(\frac{n+2}{n}\right)^3} + \frac{n-4}{2}\, e^{\left(\frac{n}{n-2}\right)^3} + 2e^8 & \textit{if } n \textit{ is even,} \\ e^{\left(\frac{(n+1)^6}{64\,(n-1)^3}\right)} + (n-3)\, e^{\left(\frac{n+1}{n-1}\right)^3} + 2e^8 & \textit{if } n \textit{ is odd,} \end{cases} \tag{5}$$

with equality if and only if $G \cong C^3_{\lfloor \frac{n-3}{2} \rfloor,\, \lceil \frac{n-3}{2} \rceil}$.

Proof Using Sage (2015), it is straightforward to examine the result to be true for $n \le 9$. Therefore, our task is to establish the result for $n \ge 10$. Suppose $v_i v_j \in E(G)$ with $d_i \ge d_j$. As G is a unicyclic graph, we must have $d_i + d_j \le n + 1$. We consider the subsequent two cases:

Case 1. $n = 2p+1$. In this case $p \ge 5$. Thus we have $d_j \le p+1$ (Otherwise, $d_i \ge d_j \ge p+2$, that is, $d_i + d_j \ge 2p+4 = n+3$, a contradiction). If $d_j = p+1$, then $d_i = p+1$ (Otherwise, $d_i \ge p+2$, that is, $d_i + d_j \ge 2p+3 = n+2$, a contradiction) and hence $G \cong C^3_{\lfloor \frac{n-3}{2} \rfloor,\, \lceil \frac{n-3}{2} \rceil}$ (see, Fig. 1). Thus we have

$$EAZ(G) = e^{\left(\frac{(n+1)^6}{64\,(n-1)^3}\right)} + (n-3)\, e^{\left(\frac{n+1}{n-1}\right)^3} + 2e^8$$

and hence equality appears in (5). Otherwise, $d_j \le p$. We take into account the following two cases:

Case 1.1. $d_i \le p+1$. Now,

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}=\frac{1}{d_i}+\frac{1}{d_j}\left(1-\frac{2}{d_i}\right)\ge\frac{1}{d_i}+\frac{1}{p}\left(1-\frac{2}{d_i}\right)=\frac{1}{p}+\frac{1}{d_i}\left(1-\frac{2}{p}\right)$$
$$\ge\frac{1}{p}+\frac{1}{p+1}\left(1-\frac{2}{p}\right),$$

that is,

$$\frac{d_i\,d_j}{d_i+d_j-2}\le\frac{p\,(p+1)}{2p-1}=\frac{1}{2}\left(p+\frac{3}{2}+\frac{3}{2\,(2p-1)}\right)<\frac{p+2}{2}=\frac{n+3}{4},$$

as $n \ge 11$. Since G is a unicyclic graph, employing the above finding with Lemma 1, it is clear that

$$EAZ(G)=\sum_{v_iv_j\in E(G)} e^{\left(\frac{d_i\,d_j}{d_i+d_j-2}\right)^3}<n\,e^{\frac{(n+3)^3}{64}}<e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3}$$
$$<EAZ\left(C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}\right).$$

Again the result (5) strictly holds.

Case 1.2. $d_i \ge p+2$. Since $d_i+d_j \le n+1$, we address the two subcases listed below:
Case 1.2.1. $d_i+d_j \le n$. First we have to prove that

$$\frac{d_i\,d_j}{d_i+d_j-2}<\frac{n+3}{4}. \tag{6}$$

For $d_i \ge d_j \ge 2$, we obtain

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}\ge\frac{1}{d_j}+\frac{1}{2p+1-d_j}\left(1-\frac{2}{d_j}\right).$$

Consider

$$f(x)=\frac{1}{x}+\frac{1}{2p+1-x}\left(1-\frac{2}{x}\right),\quad 2\le x\le p.$$

Then

$$f'(x)=-\frac{1}{x^2}+\frac{1}{(2p+1-x)^2}\left(1-\frac{2}{x}\right)+\frac{2}{(2p+1-x)\,x^2}$$
$$=-\frac{(2\,p-1)\,(2p+1-2x)}{(2p+1-x)^2\,x^2}<0\quad\text{as } x\le p.$$

Thus $f(x)$ is strictly decreasing on $2 \le x \le p$, and hence

$$f(x)\ge f(p)=\frac{1}{p}+\frac{1}{p+1}\left(1-\frac{2}{p}\right)=\frac{2p-1}{p(p+1)},$$

that is,

$$\frac{d_i\,d_j}{d_i+d_j-2}\le\frac{p(p+1)}{2p-1}=\frac{1}{2}\left(p+\frac{3}{2}+\frac{3}{2\,(2p-1)}\right)<\frac{p+2}{2}=\frac{n+3}{4}.$$

The result (6) holds. For $d_i \ge d_j = 1$, we obtain

$$\frac{d_i\,d_j}{d_i+d_j-2}=\frac{d_i}{d_i-1}<\frac{p+2}{2}=\frac{n+3}{4}$$

as $p \geq 5$. Again the result (6) holds. Similarly, as before, we obtain

$$EAZ(G) < n\,e^{\frac{(n+3)^3}{64}} < e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3} < EAZ\left(C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}\right).$$

Again the result (5) strictly holds.

Case 1.2.2. $d_i + d_j = n + 1$. In this case

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}=\frac{1}{d_j}+\frac{1}{2p+2-d_j}\left(1-\frac{2}{d_j}\right).$$

Similarly, as **Case 1.2.1**, the function $\frac{1}{x}+\frac{1}{2p+2-x}\left(1-\frac{2}{x}\right)$ is a strictly decreasing function on $x \leq p$ and hence

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}=\frac{1}{d_j}+\frac{1}{2p+2-d_j}\left(1-\frac{2}{d_j}\right)\geq\frac{2}{p+2},$$

that is,

$$\frac{d_i\,d_j}{d_i+d_j-2}\leq\frac{p+2}{2}=\frac{n+3}{4}.$$

Now,

$$EAZ(G) \leq n\,e^{\frac{(n+3)^3}{64}} < e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3} < EAZ\left(C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}\right).$$

Again the result (5) strictly holds.

Case 2. $n = 2p$. In this case $p \geq 5$. Since $d_i + d_j \leq n + 1 = 2p + 1$, we must have $d_j \leq p$. If $d_j = p$, then either $d_i = p$ or $d_i = p + 1$. For $d_i = p + 1$, we have $G \cong C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}$ (see, Fig. 1) as G is unicyclic. Thus

$$EAZ(G) = e^{\left(\frac{n\,(n+2)}{4\,(n-1)}\right)^3}+\frac{n-2}{2}\,e^{\left(\frac{n+2}{n}\right)^3}+\frac{n-4}{2}\,e^{\left(\frac{n}{n-2}\right)^3}+2e^8,$$

and hence the equality holds in (5). For $d_i = p$, by Lemma 3, the result (5) strictly holds. Otherwise, $d_j \leq p - 1$. The remaining portion of the proof can be developed by addressing the subsequent two cases:

Case 2.1. $d_i \leq p + 2$. Now, we obtain

$$\begin{aligned}\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}&=\frac{1}{d_i}+\frac{1}{d_j}\left(1-\frac{2}{d_i}\right)\\&\geq\frac{1}{d_i}+\frac{1}{p-1}\left(1-\frac{2}{d_i}\right)=\frac{1}{p-1}+\frac{1}{d_i}\left(1-\frac{2}{p-1}\right).\end{aligned}$$

Combining the above fact with $d_i \leq p + 2$ and $p \geq 5$, we have

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}\ge\frac{1}{p-1}+\frac{1}{p+2}\left(1-\frac{2}{p-1}\right),$$

which exerts

$$\frac{d_i\,d_j}{d_i+d_j-2}\le\frac{(p+2)\,(p-1)}{2p-1}=\frac{(n+4)\,(n-2)}{4\,(n-1)}.$$

It is evident from Lemma 1 that

$$EAZ(G)\le n\,e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3}<e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3}<EAZ\left(C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}\right).$$

Again the result (5) strictly holds.

Case 2.2. $d_i\ge p+3$. Since $d_i+d_j\le n+1$, we consider the following two subcases:
Case 2.2.1. $d_i+d_j\le n$. First we have to prove that

$$\frac{d_i\,d_j}{d_i+d_j-2}<\frac{(n+4)\,(n-2)}{4\,(n-1)}. \tag{7}$$

For $d_i\ge d_j\ge 2$, we obtain

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_i\,d_j}\ge\frac{1}{d_j}+\frac{1}{2p-d_j}\left(1-\frac{2}{d_j}\right).$$

Let us consider a function

$$g(x)=\frac{1}{x}+\frac{1}{2p-x}\left(1-\frac{2}{x}\right),\quad x\le p-1.$$

Similarly, as **Case 1.2.1**, the function $g(x)$ is a strictly decreasing function on $x\le p-1$, and hence

$$g(x)\ge g(p-1)=\frac{1}{p-1}+\frac{1}{p+1}\left(1-\frac{2}{p-1}\right)=\frac{2}{p+1},$$

that is,

$$\frac{d_i\,d_j}{d_i+d_j-2}\le\frac{p+1}{2}=\frac{n+2}{4}<\frac{(n+4)\,(n-2)}{4\,(n-1)},\quad as\ n\ge 10.$$

Thus (7) holds. For $d_i\ge d_j=1$, we obtain

$$\frac{d_i\,d_j}{d_i+d_j-2}=\frac{d_i}{d_i-1}<\frac{n+2}{4}<\frac{(n+4)\,(n-2)}{4\,(n-1)},\quad as\ n\ge 10.$$

Again (7) holds. Similarly, as before, we obtain

$$EAZ(G)<n\,e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3}<e^{\left(\frac{d_1\,d_2}{d_1+d_2-2}\right)^3}<EAZ\left(C^3_{\lfloor\frac{n-3}{2}\rfloor,\lceil\frac{n-3}{2}\rceil}\right).$$

Case 2.2.2. $d_i+d_j=n+1$. Let us construct a function

$$h(x)=x\,(n+1-x),\quad x\le\frac{n-2}{2}.$$

Subsequently, it becomes evident that the function $h(x)$ is increasing for $x\le\frac{n-2}{2}$, and hence

$$h(x) \leq h(n/2-1) = \frac{(n-2)\,(n+4)}{4}.$$

Employing the aforementioned result, it is apparent that

$$\frac{d_i\, d_j}{d_i + d_j - 2} = \frac{(n+1-d_j)\, d_j}{n-1} \leq \frac{(n+4)\,(n-2)}{4\,(n-1)}.$$

Similarly, as before, we obtain

$$EAZ(G) \leq n\, e^{\frac{1}{64}\left(\frac{(n+4)\,(n-2)}{n-1}\right)^3} < e^{\left(\frac{d_1\, d_2}{d_1 + d_2 - 2}\right)^3} < EAZ\left(C^3_{\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil}\right).$$

Again the result (5) strictly holds. This completes the proof of the theorem. □

3 Concluding remarks

In this work, we have solved an open problem that was posed in Cruz et al. (2022). The maximal unicyclic graph has been characterized for the EAZ index in terms of graph order n. We are delighted to report a remarkable characteristic of this extremal graph (see, Fig. 1) that the contribution of EAZ associated with a single edge $v_1 v_2$ of this structure exceeds the EAZ values of all other unicyclic graphs individually. Observing such a scenario is uncommon in the literature of extremal graph theory.

Acknowledgements The authors are grateful to the referees for their valuable comments, which have considerably improved the presentation of this paper. K. C. Das is supported by National Research Foundation funded by the Korean government (Grant No. 2021R1F1A1050646).

Data availability No data is associated with this work.

Declarations

Conflict of interest The authors declare no conflict of interest.

References

Ali A (2021) A note on minimal augmented Zagreb index of tricyclic graphs of fixed order. MATCH Commun Math Comput Chem 85:247–256

Ali A, Furtula B, Gutman I, Vukičević D (2021) Augmented Zagreb index: extremal results and bounds. MATCH Commun Math Comput Chem 85:211–244

Basak SC, Vracko MG (2020) Parsimony principle and its proper use/ application in computer-assisted Drug Design and QSAR. Curr Comput Aided Drug Des 16:1–5

Carballosa W, Quintana Y, Rodríguez JM, Sigarreta JM (2023) Exponential topological indices: optimal inequalities and applications. J Math Chem 61:933–949

Chen C, Liu M, Gu X, Das KC (2022) Extremal augmented Zagreb index of trees with given numbers of vertices and leaves. Discrete Math 345:112753

Cheng K, Liu M, Belardo F (2021) The minimal augmented Zagreb index of k-apex trees for $k \in \{1, 2, 3\}$. Appl Math Comput 402:126139

Cruz R, Monsalve J, Rada J (2020) Trees with maximum exponential Randić index. Discrete Appl Math 283:634–643

Cruz R, Monsalve J, Rada J (2021) The balanced double star has maximum exponential second Zagreb index. J Comb Optim 41:544–552

Cruz R, Rada J (2019) The path and the star as extremal values of vertex-degree-based topological indices among trees. MATCH Commun Math Comput Chem 82:715–732

Cruz R, Rada J (2022) Extremal graphs for exponential VDB indices. Kragujev J Math 46:105–113
Cruz R, Rada J, Sanchez W (2022) Extremal unicyclic graphs with respect to vertex-degree-based topological indices. MATCH Commun Math Comput Chem 88:481–503
Das KC, Elumalai S, Balachandran S (2021) Open problems on the exponential vertex-degree-based topological indices of graphs. Discrete Appl Math 293:38–49
Das KC, Gutman I, Milovanović I, Milovanović E, Furtula B (2018) Degree-based energies of graphs. Linear Algebra Appl 554:185–204
Das KC, Mondal S (2023) On exponential geometric-arithmetic index of graphs. J Math Chem. https://doi.org/10.1007/s10910-023-01542-z
Das KC, Mondal S (2024) On EAZ index of unicyclic and bicyclic graphs, general graphs in terms of the number of cut edges. J Appl Math Comput. https://doi.org/10.1007/s12190-024-02086-4
Das KC, Mondal S, Huh D (2024) On the exponential augmented Zagreb index of graphs. J Appl Math Comput 70:839–865
Das KC, Vetrík T (2023) General Gutman index of a graph. MATCH Commun Math Comput Chem 89:583–603
Du Z, Dimitrov D (2020) The minimal-ABC trees with B_2-branches. Comput Appl Math 39:85
Eliasi M (2022) Unicyclic and bicyclic graphs with maximum exponential second Zagreb index. Discrete Appl Math 307:172–179
Furtula B, Graovac A, Vukicević D (2010) Augmented Zagreb index. J Math Chem 48:370–380
Ghanbari N (2022) On the Sombor characteristic polynomial and Sombor energy of a graph. Comput Appl Math 41:242
Gutman I, Das KC (2004) The first Zagreb index 30 years after. MATCH Commun Math Comput Chem 50:83–92
Hayat S, Arshad M, Gutman I (2023) Proofs to some open problems on the maximum Sombor index of graphs. Comput Appl Math 42:279
Hosseini SA, Mohar B, Ahmadi MB (2022) The evolution of the structure of ABC-minimal trees. J Comb Theory Ser B 152:415–452
Li F, Ye Q, Broersma H, Ye R (2021) Sharp upper bounds for augmented zagreb index of graphs with fixed parameters. MATCH Commun Math Comput Chem 85:257–274
Li F, Ye Q, Rada J (2019) The augmented Zagreb indices of fluoranthene-type benzenoid systems. Bull Malays Math Sci Soc 42:1119–1141
Liu H (2023) Comparison between Merrifield–Simmons index and some vertex-degree-based topological indices. Comput Appl Math 42:89
Liu H (2022) Extremal problems on Sombor indices of unicyclic graphs with a given diameter. Comput Appl Math 41:138
Liu H, Huang Y (2023) Sharp bounds on the symmetric division deg index of graphs and line graphs. Comput Appl Math 42:285
Maitreyi V, Elumalai S, Balachandran S, Liu H (2023) The minimum Sombor index of trees with given number of pendant vertices. Comp Appl Math 42:331
Rada J (2019) Exponential vertex-degree-based topological indices and discrimination. MATCH Commun Math Comput Chem 82:29–41
Stein WA (2015) Sage mathematics software (Version 6.8). The Sage Development Team, http://www.sagemath.org
Sun X, Gao Y, Du J, Xu L (2018) Augmented Zagreb index of trees and unicyclic graphs with perfect matchings. Appl Math Comput 335:75–81
Wang F, Wu B (2022) The reduced Sombor index and the exponential reduced Sombor index of a molecular tree. J Math Anal Appl 515:126442
Wiener H (1947) Structural determination of paraffin boiling points. J Am Chem Soc 69:17–20
Xu C, Horoldagva B, Buyantogtokh L (2023) The exponential second Zagreb index of (n, m)-graphs. Mediterr J Math 20:181–188