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Extremal Unicyclic Graphs with Respect to Vertex–Degree–Based Topological Indices

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Abstract

In this paper we present a general criteria to decide when the cycle C_n on n vertices and $H_{n,1}$, the coalescence of the star S_{n-2} with the cycle C_3, are extremal unicyclic graphs of a vertex-degree-based (VDB) topological index. We show that many of the well known results on extremal values of VDB topological indices over unicyclic graphs can be obtained as particular cases of ours. Moreover, we obtain new results on extremal values of VDB topological indices, such as the generalized Geometric-Arithmetic indices, the generalized Atom-Bond-Connectivity indices, and its exponentials, among others.

1 Introduction

Let G be a simple graph with set of vertices $V(G)$ and set of edges $E(G)$. Given a vertex u of G, the open neighborhood of u, denoted by $N_G(u)$, is the set of vertices adjacent to u and the degree of u, denoted by $d_G(u) = d(u)$, is the cardinality of the set $N_G(u)$. If $u, v \in V(G)$ and $uv \in E(G)$, by $G - uv$ we denote the graph obtained from G by removing the edge uv. Similarly, if $uv \notin E(G)$, $G + uv$ denotes the graph obtained from G by adding the edge uv.

Recall that an unicyclic graph with n vertices is a connected graph with $m = n$ edges. We denote by $\mathcal{G}_{n,1}$ the set of unicyclic graphs with n vertices. This set of graphs are of great importance and have been widely studied in graphical indices, chemical graph theory and spectral graph theory, as we can see in the recent papers [1, 3–5, 7, 23, 24, 28–31, 37, 38, 41–44, 46].

A formal definition of a vertex-degree-based topological index (VDB topological index) is as follows. Let $\mathcal{G}_n$ be the set of simple graphs with n non-isolated vertices. Consider the set

$$K = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leq i \leq j \leq n-1\}$$

and for a graph $G \in \mathcal{G}_n$, denote by $m_{i,j}(G)$ the number of edges in G joining vertices of degree i and j. A VDB topological index over $\mathcal{G}_n$ is a function $\varphi : \mathcal{G}_n \longrightarrow \mathbb{R}$ induced by real numbers $\{\varphi_{ij}\}_{(i,j)\in K}$ defined as

$$\varphi(G) = \sum_{(i,j)\in K} m_{i,j}(G)\, \varphi_{i,j}, \tag{1}$$

for every $G \in \mathcal{G}_n$. We note that the topological indices of the form (2) were referred as bond incident degree indices in [34]. These indices were also considered in [26]. A list of well known VDB topological indices is presented in Table 1.

Index	Symbol	φ_{ij}
First Zagreb [22]	$\mathcal{M}_1$	$i+j$
Second Zagreb [22]	$\mathcal{M}_2$	ij
Sombor [21]	$\mathcal{SO}$	$\sqrt{i^2+j^2}$
Forgotten [19]	$\mathcal{F}$	i^2+j^2
Randić [33]	χ	$\frac{1}{\sqrt{ij}}$
Harmonic [47]	$\mathcal{H}$	$\frac{2}{i+j}$
Sum-Connectivity [45]	$\mathcal{SC}$	$\frac{1}{\sqrt{i+j}}$
Geometric-Arithmetic [35]	$\mathcal{GA}$	$\frac{2\sqrt{ij}}{i+j}$
Arithmetic-Geometric [27]	$\mathcal{AG}$	$\frac{i+j}{2\sqrt{ij}}$
Atom-Bond-Connectivity [16]	$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$
Augmented Zagreb [17]	$\mathcal{AZ}$	$\left(\frac{ij}{i+j-2}\right)^3$

Table 1. Some well-known VDB topological indices.

The exponential of the VDB topological index φ was introduced in [32] as the VDB topological index e^{φ} induced by the real numbers $\{e^{\varphi_{ij}}\}_{(i,j)\in K}$. These indices have nice discrimination properties and there are several recent papers solving the problem of finding extremal graphs with respect to the exponentials of some of the VDB topological indices listed in Table 1 (see [8–12]).

In the case of unicyclic graphs, for $G \in \mathcal{G}_{n,1}$, $m_{1,1}(G) = 0$ and $m_{x,y}(G) = 0$ for any $1 \leq x \leq y \leq n-1$ such that $x+y > n+1$. Then, the definition in (1) is rewritten as follows

$$\varphi(G) = \sum_{(x,y)\in P} m_{x,y}(G)\,\varphi(x,y), \tag{2}$$

where

$$P = \{(x,y) \in \mathbb{N}\times\mathbb{N} : 1 \le x \le y \le n-1, (x,y) \ne (1,1), x+y \le n+1\}.$$

When it is required, we consider $\varphi(x,y)$ as a symmetric, continuously differentiable function defined over the set $[1,+\infty)\times[1,+\infty)$.

We denote by C_n the cycle with n vertices and by $H_{n,1}$ the unicyclic graph obtained from the star S_n by adding an edge between two pendent vertices.

In this paper we find general conditions on the function $\varphi(x,y)$ in order to assure that the cycle C_n (see Section 2) and the graph $H_{n,1}$ (see Section 3) are extremal unicyclic graphs with respect to the VDB topological index φ.

Using results in Section 2, we recover known results about the cycle C_n as an extremal graph with respect to the First Zagreb [13], the Second Zagreb [13], the Sombor [8], the Forgotten [1], the Harmonic [25], the Sum-Connectivity [14], the Randić [6], the Geometric-Arithmetic [15] and the Arithmetic-Geometric [36] indices. As an application we prove that the cycle C_n is an extremal graph with respect to the exponentials of the mentioned VDB indices except for the case of the exponential of the Randic index.

In the case of the graph $H_{n,1}$, using the results in Section 3, we recover known results about this graph as an extremal graph with respect to the First Zagreb [13], the Sombor [8], the Forgotten [1], the Atom-Bond-Connectyivity [40] and the Augmented Zagreb [44] indices. As an application we prove that the graph $H_{n,1}$ is an extremal graph with respect to the exponentials of the First Zagreb, the Second Zagreb, the Sombor, the Forgotten, the Harmonic, the Sum-Connectivity, the Atom-Bond-Connectyivity and the Augmented Zagreb indices.

In summary, the results in Section 2 and Section 3 unify the theory of extreme values of VDB topological indices on unicyclic graphs, and also can be applied to deduce when C_n and $H_{n,1}$ are extremal graphs with respect to new VDB topological indices on unicyclic graphs.

Finally, in Section 4, we discuss some open problems.

2 VDB topological indices with the cycle as extremal unicyclic graph

We start this section considering VDB topological indices induced by the function $\varphi(x, y)$ which is monotone as a function of $x \in [1, +\infty)$ for each fixed value of $y \in [1, +\infty)$. In this case we find conditions on the function $\varphi(x, y)$ in order to assure that the cycle C_n is an extremal unicyclic graph with respect to the VDB topological index φ. These conditions are obtained by applying transformations used in [13] to a general VDB topological index.

For integer values of $x \geq 1$ and $y \geq 1$, we introduce the following functions associated to φ that will be used in sequel:

$$\begin{aligned}
f_1(x) &= 2\varphi(x+2,1) - \varphi(x+1,2) - \varphi(2,1), \\
f_2(x) &= \varphi(x+2,2) + \varphi(x+2,1) - \varphi(x+1,2) - \varphi(2,2), \\
f_3(x) &= 2\varphi(x+2,2) - \varphi(x+1,2) - 2\varphi(2,2) + \varphi(2,1), \\
f_4(x,y) &= \varphi(x,3) - \varphi(x,2) + \varphi(y,3) - \varphi(y,2) - \varphi(2,2) + \varphi(3,1), \\
f_5(x,y) &= \varphi(x,3) - \varphi(x,2) + \varphi(y,3) - \varphi(y,2) - 2\varphi(2,2) + \varphi(2,1) + \varphi(3,2).
\end{aligned}$$

For each integer value of $2 \leq x \leq y \leq 3$, the values of $f_4(x, y)$ and $f_5(x, y)$ for known VDB topological indices are presented in Table 2. The correspondent values for the exponentials of these indices are presented in Table 3.

	$\mathcal{M}_1$	$\mathcal{M}_2$	$\mathcal{SO}$	$\mathcal{F}$	$\mathcal{H}$	$\mathcal{SC}$	χ
$f_4(2,2)$	2	3	1.888	12	−0.200	−0.106	−0.106
$f_4(2,3)$	2	4	1.748	12	−0.167	−0.092	−0.089
$f_4(3,3)$	2	5	1.608	12	−0.133	−0.078	−0.072
$f_5(2,2)$	2	4	1.739	12	−0.133	−0.081	−0.068
$f_5(2,3)$	2	5	1.599	12	−0.100	−0.067	−0.051
$f_5(3,3)$	2	6	1.459	12	−0.067	−0.053	−0.034

Table 2. Values of $f_4(x, y)$ and $f_5(x, y)$ for known VDB topological indices.

Let $p \geq 3$, $1 \leq i < p$, $G \in \mathcal{G}_{n,1}$, $u \in V(G)$ and $G_{p,i} \in \mathcal{G}_{n+p-1,1}$ is obtained from G as depicted in Figure 1.

Proposition 2.1. *Let φ be a VDB topological index defined as in (2).*

1. *If $\varphi(x, y)$ is increasing as a function of x and $f_1(x) \geq 0$, $f_2(x) \geq 0$ and $f_3(x) \geq 0$ for each integer value of $x \geq 1$, then $\varphi(G_{p,i}) \geq \varphi(G_{p,1})$.*

2. *If $\varphi(x, y)$ is decreasing as a function of x and $f_1(x) \leq 0$, $f_2(x) \leq 0$ and $f_3(x) \leq 0$ for each integer value of $x \geq 1$, then $\varphi(G_{p,i}) \leq \varphi(G_{p,1})$.*

	$e^{\mathcal{M}_1}$	$e^{\mathcal{M}_2}$	$e^{\mathcal{SO}}$	$e^{\mathcal{F}}$	$e^{\mathcal{H}}$	$e^{\mathcal{SC}}$	$e^{\mathcal{X}}$
$f_4(2,2)$	187.63	663.15	46.47	8.98×10^5	−0.314	−0.170	−0.156
$f_4(2,3)$	348.83	8014.0	59.38	6.57×10^7	−0.253	−0.145	−0.121
$f_4(3,3)$	510.03	15365	72.28	1.30×10^8	−0.192	−0.120	−0.085
$f_5(2,2)$	246.93	999.28	52.09	1.32×10^6	−0.172	−0.122	−0.054
$f_5(2,3)$	408.13	8350.1	64.99	6.61×10^7	−0.111	−0.097	−0.018
$f_5(3,3)$	569.33	15701	77.90	1.31×10^8	−0.050	−0.072	0.018

Table 3. Values of $f_4(x,y)$ and $f_5(x,y)$ for the exponentials of known VDB topological indices.

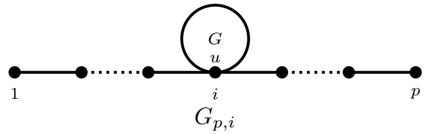

Figure 1. The unicyclic graph $G_{p,i}$.

Proof. Let $d_G(u) = x \geq 1$ and $N_G(u) = \{u_1, \ldots, u_x\}$. Since $G_{p,i} \in \mathcal{G}_{n,1}$, we may assume $d_G(u_x) = y \geq 2$. We prove part 1. The proof of the second part is similar.

If $p = 3$, then

$$\begin{aligned}\varphi(G_{3,2}) - \varphi(G_{3,1}) &= \sum_{j=1}^{x} [\varphi(x+2, d_G(u_j)) - \varphi(x+1, d_G(u_j))] \\ &\quad +2\varphi(x+2,1) - \varphi(x+1,2) - \varphi(2,1) \\ &\geq 2\varphi(x+2,1) - \varphi(x+1,2) - \varphi(2,1) = f_1(x).\end{aligned}$$

If $p > 3$ and $i = 2$, then

$$\begin{aligned}\varphi(G_{p,2}) - \varphi(G_{p,1}) &= \sum_{j=1}^{x} [\varphi(x+2, d_G(u_j)) - \varphi(x+1, d_G(u_j))] \\ &\quad +\varphi(x+2,2) - \varphi(2,2) + \varphi(x+2,1) - \varphi(x+1,2) \\ &\geq \varphi(x+2,2) - \varphi(2,2) + \varphi(x+2,1) - \varphi(x+1,2) = f_2(x).\end{aligned}$$

If $2 < i < \frac{p}{2}$, then

$$\begin{aligned}\varphi(G_{p,i}) - \varphi(G_{p,1}) &= \sum_{j=1}^{x} [\varphi(x+2, d_G(u_j)) - \varphi(x+1, d_G(u_j))] \\ &\quad +2\varphi(x+2,2) - \varphi(x+1,2) - 2\varphi(2,2) + \varphi(2,1) \\ &\geq 2\varphi(x+2,2) - \varphi(x+1,2) - 2\varphi(2,2) + \varphi(2,1) = f_3(x).\end{aligned}$$

∎

Proposition 2.2. *Let φ be a VDB topological index defined as in (2), $G_1 \in \mathcal{G}_{n,1}$ such that each vertex in the unique cycle of G_1 has degree 2 or 3. Let $w_1 \ldots w_k$ be a pendent path of G_1 such that $uw_1, vw_1 \in E(G_1)$ and $G_2 = G_1 - vw_1 + vw_k$ (see Figure 2).*

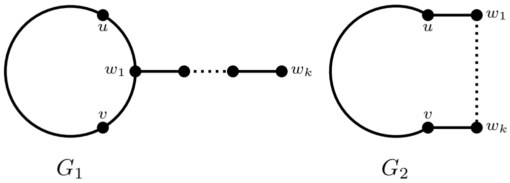

Figure 2. Graph used in Proposition 2.2.

1. *If $f_4(x,y) \geq 0$ and $f_5(x,y) \geq 0$ for each integer value of $2 \leq x \leq y \leq 3$, then $\varphi(G_1) \geq \varphi(G_2)$.*

2. *If $f_4(x,y) \leq 0$ and $f_5(x,y) \leq 0$ for each integer value of $2 \leq x \leq y \leq 3$, then $\varphi(G_1) \leq \varphi(G_2)$.*

Proof. Assume that $d_{G_1}(u) = x$ and $d_{G_1}(v) = y$. It is easy to see that if $k = 2$, $\varphi(G_1) - \varphi(G_2) = f_4(x,y)$ and, if $k > 2$, $\varphi(G_1) - \varphi(G_2) = f_5(x,y)$. ■

Theorem 2.3. *Let φ be a VDB topological index defined as in (2).*

1. *If $\varphi(x,y)$ is increasing as a function of x, $f_1(x) \geq 0$, $f_2(x) \geq 0$, $f_3(x) \geq 0$ for each integer value of $x \geq 1$ and $f_4(x,y) \geq 0$, $f_5(x,y) \geq 0$ for each integer value of $2 \leq x \leq y \leq 3$, then $\varphi(G) \geq \varphi(C_n)$ for any $G \in \mathcal{G}_{n,1}$.*

2. *If $\varphi(x,y)$ is decreasing as a function of x, $f_1(x) \leq 0$, $f_2(x) \leq 0$, $f_3(x) \leq 0$ for each integer value of $x \geq 1$ and $f_4(x,y) \leq 0$, $f_5(x,y) \leq 0$ for each integer value of $2 \leq x \leq y \leq 3$, then $\varphi(G) \leq \varphi(C_n)$ for any $G \in \mathcal{G}_{n,1}$.*

Proof. We prove part 1. The proof of the second part is similar.

Let $G \in \mathcal{G}_{n,1}$. Since $f_1(x) \geq 0$, $f_2(x) \geq 0$, $f_3(x) \geq 0$ for each integer value of $x \geq 1$, by Proposition 2.1, $\varphi(G) \geq \varphi(G')$, where G' is a unicyclic graph with all the vertices in the cycle having degree 2 or 3, and each of such vertices of degree 3 is attached to a path. Finally, by Proposition 2.2, the fact that $f_4(x,y) \geq 0$, $f_5(x,y) \geq 0$ for each integer value of $2 \leq x \leq y \leq 3$ implies $\varphi(G) \geq \varphi(C_n)$. ■

In the next two corollaries we recover known results about the cycle as an extremal unicyclic graph for several VDB topological indices [1, 6, 8, 13, 14, 25].

Corollary 2.4. *The cycle C_n is the minimal graph over $\mathcal{G}_{n,1}$ with respect to $\mathcal{M}_1, \mathcal{M}_2, \mathcal{SO}$, and $\mathcal{F}$.*

Proof. For each of these indices we check that conditions in part 1 of Theorem 2.3 hold. Specifically we check that $\varphi(x, y)$ is increasing as a function of x and $f_1(x) \geq 0$, $f_2(x) \geq 0$, $f_3(x) \geq 0$ for each integer value of $x \geq 1$. The conditions $f_4(x, y) \geq 0$, $f_5(x, y) \geq 0$ for each integer value of $2 \leq x \leq y \leq 3$ can be checked in Table 2.

1. The First Zagreb index $\mathcal{M}_1$ is induced by the function $\varphi(x, y) = x + y$, which is increasing as a function of x for each fixed value of $y \geq 1$. We have

$$f_1(x) = f_2(x) = f_3(x) = x.$$

2. The Second Zagreb index $\mathcal{M}_2$ is induced by the function $\varphi(x, y) = xy$, which is increasing as a function of x for each fixed value of $y \geq 1$. We have

$$f_1(x) = 0, f_2(x) = x, f_3(x) = 2x.$$

3. The Sombor index $\mathcal{SO}$ is induced by the function $\varphi(x, y) = \sqrt{x^2 + y^2}$ which is increasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 1$ we have

$$\begin{aligned} f_1(x) &= 2\sqrt{x^2+4x+5} - \sqrt{x^2+2x+5} - \sqrt{5} > \sqrt{x^2+4x+5} - \sqrt{5} > 0, \\ f_2(x) &= \sqrt{x^2+4x+5} - \sqrt{x^2+2x+5} + \sqrt{x^2+4x+8} - 2\sqrt{2} > 0, \\ f_3(x) &= 2\sqrt{x^2+4x+8} - \sqrt{x^2+2x+5} - 4\sqrt{2} + \sqrt{5} \\ &> \sqrt{x^2+4x+8} - 4\sqrt{2} + \sqrt{5} > \sqrt{13} - 4\sqrt{2} + \sqrt{5} > 0. \end{aligned}$$

4. The Forgotten index $\mathcal{F}$ is induced by the function $\varphi(x, y) = x^2 + y^2$ which is increasing as a function of x for each fixed value of $y \geq 1$. We have

$$f_1(x) = f_2(x) = f_3(x) = x(x+6).$$ ■

Corollary 2.5. *The cycle C_n is the maximal graph over $\mathcal{G}_{n,1}$ with respect to $\mathcal{H}, \mathcal{SC}$, and χ.*

Proof. For each of these indices we check that conditions in part 2 of Theorem 2.3 hold. Specifically we check that $\varphi(x,y)$ is decreasing as a function of x and $f_1(x) \le 0$, $f_2(x) \le 0$, $f_3(x) \le 0$ for each integer value of $x \ge 1$. The conditions $f_4(x,y) \le 0$, $f_5(x,y) \le 0$ for each integer value of $2 \le x \le y \le 3$ can be checked in Table 2.

1. The Harmonic index $\mathcal{H}$ is induced by the function $\varphi(x,y) = \frac{2}{x+y}$which is decreasing as a function of x for each fixed value of $y \ge 1$. We have

$$f_1(x) = -\frac{2x}{3(x+3)}, f_2(x) = -\frac{x}{2(x+4)}, f_3(x) = -\frac{x(x+1)}{3(x^2+7x+12)}.$$

2. The Sum-Connectivity index $\mathcal{SC}$ is induced by the function $\varphi(x,y) = \frac{1}{\sqrt{x+y}}$ which is decreasing as a function of x for each fixed value of $y \ge 1$. We have

$$f_1(x) = -\frac{\sqrt{x+3}-\sqrt{3}}{\sqrt{3}\sqrt{x+3}}, f_2(x) = -\frac{\sqrt{x+4}-2}{2\sqrt{x+4}},$$

$$f_3(x) = -\frac{\left(3-\sqrt{3}\right)\sqrt{x+3}\sqrt{x+4}+3\sqrt{x+4}-6\sqrt{x+3}}{3\sqrt{x+3}\sqrt{x+4}}.$$

3. The Randić index χ is induced by the function $\varphi(x,y) = \frac{1}{\sqrt{xy}}$ which is decreasing as a function of x for each fixed value of $y \ge 1$. We have

$$\begin{aligned} f_1(x) &= -\frac{\sqrt{2}\sqrt{x+2}+\sqrt{2}\sqrt{x+1}\sqrt{x+2}-4\sqrt{x+1}}{2\sqrt{x+1}\sqrt{x+2}}, \\ f_2(x) &= -\frac{\sqrt{2}\sqrt{x+2}-\sqrt{2}\sqrt{x+1}+\sqrt{x+1}\sqrt{x+2}-2\sqrt{x+1}}{2\sqrt{x+1}\sqrt{x+2}}, \\ f_3(x) &= -\frac{\sqrt{2}\sqrt{x+2}-2\sqrt{2}\sqrt{x+1}+2\sqrt{x+1}\sqrt{x+2}-\sqrt{2}\sqrt{x+1}\sqrt{x+2}}{2\sqrt{x+1}\sqrt{x+2}}. \end{aligned}$$

■

We can use Theorem 2.3 to prove that new VDB topological indices attain their maximal value in C_n.

Theorem 2.6. *The cycle C_n is the minimal graph over $\mathcal{G}_{n,1}$ with respect to $e^{\mathcal{M}_1}, e^{\mathcal{M}_2}, e^{\mathcal{SO}}$, and $e^{\mathcal{F}}$.*

Proof. For each of these indices we check that conditions in part 1 of Theorem 2.3 hold. Specifically we check that $\varphi(x,y)$ is increasing as a function of x and $f_1(x) \ge 0$, $f_2(x) \ge 0$, $f_3(x) \ge 0$ for each integer value of $x \ge 1$. The conditions $f_4(x,y) \ge 0$, $f_5(x,y) \ge 0$ for each integer value of $2 \le x \le y \le 3$ can be checked in Table 3.

1. The exponential of the First Zagreb index $e^{\mathcal{M}_1}$ is induced by the function $\varphi(x,y) = e^{x+y}$ which is increasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 1$ we have
$$f_1(x) = e^{x+3} - e^3, f_2(x) = e^{x+4} - e^4,$$
$$f_3(x) = 2e^{x+4} - e^{x+3} + e^3 - 2e^4 \geq e^{x+4} + e^3 - 2e^4 \geq e^5 + e^3 - 2e^4 > 0.$$

2. The exponential of the Sombor index $e^{\mathcal{SO}}$ is induced by the function $\varphi(x,y) = e^{\sqrt{x^2+y^2}}$ which is increasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 1$ we have
$$\begin{aligned} f_1(x) &= 2e^{\sqrt{x^2+4x+5}} - e^{\sqrt{x^2+2x+5}} - e^{\sqrt{5}} \geq e^{\sqrt{x^2+4x+5}} - e^{\sqrt{5}} > 0, \\ f_2(x) &= e^{\sqrt{x^2+4x+5}} + e^{\sqrt{x^2+4x+8}} - e^{\sqrt{x^2+2x+5}} - e^{2\sqrt{2}} \geq e^{\sqrt{x^2+4x+8}} - e^{2\sqrt{2}} > 0, \\ f_3(x) &= 2e^{\sqrt{x^2+4x+8}} - e^{\sqrt{x^2+2x+5}} - 2e^{2\sqrt{2}} + e^{\sqrt{5}} \geq e^{\sqrt{x^2+4x+8}} - 2e^{2\sqrt{2}} + e^{\sqrt{5}} \\ &\geq e^{\sqrt{13}} - 2e^{2\sqrt{2}} + e^{\sqrt{5}} > 0. \end{aligned}$$

3. The exponential of the Forgotten index $e^{\mathcal{F}}$ is induced by the function $\varphi(x,y) = e^{x^2+y^2}$ which is increasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 1$ we have
$$\begin{aligned} f_1(x) &= 2e^{x^2+4x+5} - e^{x^2+2x+5} - e^5 \geq e^{x^2+4x+5} - e^5 > 0, \\ f_2(x) &= e^{x^2+4x+5} + e^{x^2+4x+8} - e^{x^2+2x+5} - e^8 \geq e^{x^2+4x+8} - e^8 > 0, \\ f_3(x) &= 2e^{x^2+4x+8} - e^{x^2+2x+5} - 2e^8 + e^5 \geq e^{x^2+4x+8} - 2e^8 + e^5 \\ &\geq e^{13} - 2e^8 + e^5 > 0. \end{aligned}$$

4. The exponential of the Second Zagreb index $e^{\mathcal{M}_2}$ is induced by $\varphi(x,y) = e^{xy}$ which is increasing as a function of x for each fixed value of $y \geq 1$. Note that
$$f_1(x) = e^{x+2}(2 - e^x) - e^2 < 0$$
for $x \geq 1$. First we show directly that $e^{\mathcal{M}_2}(G_{3,2}) \geq e^{\mathcal{M}_2}(G_{3,1})$. Let $d_G(u) = x \geq 1$ and $N_G(u) = \{u_1, \ldots, u_x\}$. Since $G_{3,2} \in \mathcal{G}_{n,1}$, we may assume $d_G(u_x) = y \geq 2$.
$$\begin{aligned} e^{\mathcal{M}_2}(G_{3,2}) - e^{\mathcal{M}_2}(G_{3,1}) &= \sum_{j=1}^{x} \left[e^{(x+2)d_G(u_j)} - e^{(x+1)d_G(u_j)}\right] + 2e^{x+2} - e^{2x+2} - e^2 \\ &\geq e^{(x+2)y} - e^{(x+1)y} + 2e^{x+2} - e^{2x+2} - e^2. \end{aligned}$$

It is easy to check that $e^{(x+2)y} - e^{(x+1)y}$ is increasing as a function of y, then

$$\begin{aligned} e^{\mathcal{M}_2}\left(G_{3,2}\right) - e^{\mathcal{M}_2}\left(G_{3,1}\right) &\geq e^{2x+4} + 2e^{x+2} - 2e^{2x+2} - e^2 \\ &\geq 2e^{x+2} - e^2 > 0. \end{aligned}$$

Using the same arguments in the proof of part 1 of Theorem 2.3, to prove the result we need to verify the following conditions:

$$\begin{aligned} f_2\left(x\right) &= e^2 e^{2x+2} - e^{2x+2} + e^{x+2} - e^4 \\ &\geq e^{2x+2} + e^{x+2} - e^4 > 0, \\ f_3\left(x\right) &= 2e^2 e^{2x+2} - e^{2x+2} + e^2 - 2e^4 \\ &\geq 2e^{2x+2} + e^2 - 2e^4 > 0. \end{aligned}$$

■

Theorem 2.7. *The cycle C_n is the maximal graph over $\mathcal{G}_{n,1}$ with respect to $e^{\mathcal{H}}$ and $e^{\mathcal{SC}}$.*

Proof. For each of these indices we check that conditions in part 2 of Theorem 2.3 hold. Specifically we check that $\varphi\left(x,y\right)$ is decreasing as a function of x and $f_1\left(x\right) \leq 0$, $f_2\left(x\right) \leq 0$, $f_3\left(x\right) \leq 0$ for each integer value of $x \geq 1$. The conditions $f_4\left(x,y\right) \leq 0$, $f_5\left(x,y\right) \leq 0$ for each integer value of $2 \leq x \leq y \leq 3$ can be checked in Table 3.

1. The exponential of the Harmonic index $e^{\mathcal{H}}$ is induced by the function $\varphi\left(x,y\right) = e^{\frac{2}{x+y}}$ which is decreasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 3$ we have

$$f_1\left(x\right) = e^{\frac{2}{x+3}} - e^{\frac{2}{3}} < 0, f_2\left(x\right) = e^{\frac{2}{x+4}} - e^{\frac{1}{2}} < 0,$$

$$f_3\left(x\right) = 2e^{\frac{2}{x+4}} - e^{\frac{2}{x+3}} + e^{\frac{2}{3}} - 2e^{\frac{1}{2}} \leq e^{\frac{2}{x+4}} + e^{\frac{2}{3}} - 2e^{\frac{1}{2}} \leq e^{\frac{2}{7}} + e^{\frac{2}{3}} - 2e^{\frac{1}{2}} < 0,$$

and, by direct calculation, we obtain that $f_1\left(1\right)$, $f_1\left(2\right)$, $f_2\left(1\right)$, $f_2\left(2\right)$, $f_3\left(1\right)$ and $f_3\left(2\right)$ are negative.

2. The exponential of the Sum-Connectivity index $e^{\mathcal{SC}}$ is induced by the function $\varphi\left(x,y\right) = e^{\frac{1}{\sqrt{x+y}}}$ which is decreasing as a function of x for each fixed value of $y \geq 1$. For $x \geq 2$ we have

$$f_1\left(x\right) = e^{\frac{1}{\sqrt{x+3}}} - e^{\frac{1}{\sqrt{3}}} < 0, f_2\left(x\right) = e^{\frac{1}{\sqrt{x+4}}} - e^{\frac{1}{2}} < 0,$$

$$f_3\left(x\right) = 2e^{\frac{1}{\sqrt{x+4}}} - e^{\frac{1}{\sqrt{x+3}}} + e^{\frac{1}{\sqrt{3}}} - 2e^{\frac{1}{2}} \leq e^{\frac{1}{\sqrt{x+4}}} + e^{\frac{1}{\sqrt{3}}} - 2e^{\frac{1}{2}} \leq e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{\sqrt{3}}} - 2e^{\frac{1}{2}} < 0,$$

and, by direct calculation, we obtain that $f_1\left(1\right)$, $f_2\left(1\right)$ and $f_3\left(1\right)$ are negative. ■

Next we show that for those vertex-degree-based topological indices induced by functions that are not monotone as a function of $x \in [1, +\infty)$, for each fixed value of $y \in [1, +\infty)$, the cycle C_n is a extremal unicyclic graph when $\varphi(2,2)$ is an extremal value of the function $\varphi(x,y)$ over P.

Theorem 2.8. *Let $G \in \mathcal{G}_{n,1}$ and φ is a VDB topological index as in (2).*

If $\varphi(x,y) \geq \varphi(2,2)$ for each $(x,y) \in P$ then $\varphi(G) \geq \varphi(2,2)\, n = \varphi(C_n)$.

If $\varphi(x,y) \leq \varphi(2,2)$ for each $(x,y) \in P$ then $\varphi(G) \leq \varphi(2,2)\, n = \varphi(C_n)$.

Proof. We prove the first part. The second part is proven similarly by reversing inequalities.

For any $G \in \mathcal{G}_{n,1}$, the value of $\varphi(G)$ is

$$\varphi(G) = \sum_{(x,y)\in P} \varphi(x,y)\, m_{x,y} \geq \varphi(2,2) \sum_{(x,y)\in P} m_{x,y} = \varphi(2,2)\, n = \varphi(C_n). \qquad \blacksquare$$

Let $\mathcal{GA}_\alpha$ be the generalized Geometric-Arithmetic index induced by the function $\varphi(x,y) = \left(\dfrac{2\sqrt{xy}}{x+y}\right)^\alpha$. Note that for $\alpha = 1$ we recover the usual Geometric-Arithmetic index and for $\alpha = -1$ we recover the usual Arithmetic-Geometric index. The exponential of the generalized Geometric-Arithmetic index $e^{\mathcal{GA}_\alpha}$ is induced by the function $\psi(x,y) = e^{\left(\frac{2\sqrt{xy}}{x+y}\right)^\alpha}$.

Theorem 2.9. *For $\alpha > 0$ ($\alpha < 0$) the cycle C_n is the maximal (minimal) unicyclic graph with respect to $\mathcal{GA}_\alpha$ and with respect to $e^{\mathcal{GA}_\alpha}$.*

Proof. Let $\varphi(x,y) = \left(\frac{2\sqrt{xy}}{x+y}\right)^\alpha$ and $\psi(x,y) = e^{\left(\frac{2\sqrt{xy}}{x+y}\right)^\alpha}$. We have

$$\begin{aligned}
\frac{\partial}{\partial y}\varphi(x,y) &= \alpha 2^{\alpha-1} \frac{(x-y)\sqrt{xy}}{y(x+y)^2} \left(\frac{\sqrt{xy}}{x+y}\right)^{\alpha-1}, \\
\frac{\partial}{\partial y}\psi(x,y) &= \alpha 2^{\alpha-1} \frac{(x-y)\sqrt{xy}}{y(x+y)^2} \left(\frac{\sqrt{xy}}{x+y}\right)^{\alpha-1} e^{\left(\frac{2\sqrt{xy}}{x+y}\right)^\alpha} \\
\varphi(x,x) &= \varphi(2,2) = 1, \\
\psi(x,x) &= \psi(2,2) = e.
\end{aligned}$$

For $\alpha > 0$, $\frac{\partial}{\partial y}\varphi(x,y) \leq 0$ and $\frac{\partial}{\partial y}\psi(x,y) \leq 0$ for each $(x,y) \in P$. Then $\varphi(1,y) \leq \varphi(1,2) = \left(\frac{2}{3}\sqrt{2}\right)^\alpha < \varphi(2,2)$ and for $x \geq 2$, $\varphi(x,y) \leq \varphi(x,x) = \varphi(2,2)$. It means that the condition of the second part of Theorem 2.8 holds. Analogously, for the function $\psi(x,y)$ we have: $\psi(1,y) \leq \psi(1,2) = e^{\left(\frac{2}{3}\sqrt{2}\right)^\alpha} < \psi(2,2)$ and for $x \geq 2$, $\psi(x,y) \leq \psi(x,x) = \psi(2,2)$. On the other hand, for $\alpha < 0$ the condition of the first part of Theorem 2.8 holds for each of the functions $\varphi(x,y)$ and $\psi(x,y)$. $\blacksquare$

3 VDB topological indices with $H_{n,1}$ as extremal unicyclic graph

We begin this section with a lemma proved by Ali and Dimitrov in [2] that provides conditions on the function $\varphi(x, y)$ in order to assure that the graph $H_{n,1}$ is an extremal unicyclic graph with respect to the VDB topological index φ. This lemma is used for VDB topological indices induced by a function $\varphi(x, y)$ which is monotone in both variables on the interval $[1, +\infty)$.

Lemma 3.1. *[2] Let the function $\varphi(x, y)$, associated to the VDB topological index φ, be defined in $[1, \infty) \times [1, \infty)$. Let*

$$\begin{aligned}\Delta_1(\varphi) &= \varphi(x+t, y) - \varphi(x, y) + \varphi(c-t, y) - \varphi(c, y),\\ \Delta_2(\varphi) &= \varphi(x+t, c-t) - \varphi(x, c),\end{aligned}$$

where $x \geq c > t \geq 1$, $c \geq 2$ and $y \geq 1$.

1. *Let G be the connected graph with n vertices and m edges with maximum value of the VDB topological index φ and both expressions $\Delta_1(\varphi)$ and $\Delta_2(\varphi)$ are non-negatives. Furthermore, if one of the following two conditions holds:*

   (a) The function φ is increasing in both variables on the interval $[1, \infty)$ and at least one of the expressions $\Delta_1(\varphi)$ and $\Delta_2(\varphi)$ is positive,

   (b) The function φ is strictly increasing in both variables on the interval $[1, \infty)$,

   then the maximum vertex degree in G is $n-1$.

2. *Let G be the connected graph with n vertices and m edges with minimum value of the VDB topological index φ and both expressions $\Delta_1(\varphi)$ and $\Delta_2(\varphi)$ are non-positives. Furthermore, if one of the following two conditions holds:*

   (a) The function φ is decreasing in both variables on the interval $[1, \infty)$ and at least one of the expressions $\Delta_1(\varphi)$ and $\Delta_2(\varphi)$ is negative,

   (b) The function φ is strictly decreasing in both variables on the interval $[1, \infty)$,

   then the maximum vertex degree in G is $n-1$.

In the next corollary, using Lemma 3.1, we recover known results about $H_{n,1}$ as an extremal unicyclic graph for several VDB topological indices [1,8,13].

Corollary 3.2. *The graph $H_{n,1}$ is the maximal graph over $\mathcal{G}_{n,1}$ with respect to $\mathcal{M}_1, \mathcal{SO}$, and $\mathcal{F}$.*

Proof. For each of these indices we show that the corresponding function $\varphi(x,y)$ is strictly increasing in both variables and check the conditions $\Delta_1(\varphi) \geq 0$ and $\Delta_2(\varphi) \geq 0$. Then, by Lemma 3.1, the maximal graph over $\mathcal{G}_{n,1}$ with respect to the corresponding index has maximum degree $n-1$ and the unique graph in $\mathcal{G}_{n,1}$ with maximum degree $n-1$ is $H_{n,1}$.

1. The First Zagreb index $\mathcal{M}_1$ is induced by the function $\varphi(x,y) = x + y$, which is strictly increasing in both variables in $[1,\infty)$. It is easy to see that

$$\Delta_1(\mathcal{M}_1) = 0, \Delta_2(\mathcal{M}_1) = 0.$$

2. The Sombor index $\mathcal{SO}$ is induced by the function $\varphi(x,y) = \sqrt{x^2+y^2}$, which is strictly increasing in both variables in $[1,\infty)$. By the Mean Value Theorem, there exist c_1 and x_1, with $c - t < c_1 < c \leq x < x_1 < x + t$, such that

$$\begin{aligned} \Delta_1(\mathcal{SO}) &= \sqrt{(x+t)^2+y^2} - \sqrt{x^2+y^2} + \sqrt{(c-t)^2+y^2} - \sqrt{c^2+y^2} \\ &= \frac{x_1 t}{\sqrt{x_1^2+y^2}} - \frac{c_1 t}{\sqrt{c_1^2+y^2}}. \end{aligned}$$

It is easy to see that the function $\frac{x}{\sqrt{x^2+y^2}}$ is increasing as a function of x, then $\Delta_1(\mathcal{SO}) \geq 0$. Also,

$$\Delta_2(\mathcal{SO}) = \sqrt{(x+t)^2+(c-t)^2} - \sqrt{x^2+c^2} = \frac{2t(t+x-c)}{\sqrt{(x+t)^2+(c-t)^2}+\sqrt{x^2+c^2}} > 0.$$

3. The Forgotten index $\mathcal{F}$ is induced by the function $\varphi(x,y) = x^2+y^2$, which is strictly increasing in both variables in $[1,\infty)$. We obtain

$$\Delta_1(\mathcal{F}) = 2t(t+x-c) > 0, \Delta_2(\mathcal{F}) = 2t(t+x-c) > 0. \qquad \blacksquare$$

We cannot apply the Lemma 3.1 to the Second Zagreb index because the condition $\Delta_2(\varphi) \geq 0$ fails. In the case of the Randić, the Harmonic and the Sum Connectivity indices, we neither can apply the Lemma 3.1 because condition $\Delta_1(\varphi) \leq 0$ fails in each case.

Theorem 3.3. *The graph $H_{n.1}$ is the maximal graph over $\mathcal{G}_{n,1}$ with respect to $e^{\mathcal{M}_1}$, $e^{\mathcal{SO}}$, and $e^{\mathcal{F}}$.*

Proof. For each of these indices we show that the corresponding function $\varphi(x,y)$ is strictly increasing in both variables and check the conditions $\Delta_1(\varphi) \geq 0$ and $\Delta_2(\varphi) \geq 0$. Then, by Lemma 3.1, the maximal graph over $\mathcal{G}_{n,1}$ with respect to the corresponding index has maximum degree $n-1$ and the unique graph in $\mathcal{G}_{n,1}$ with maximum degree $n-1$ is $H_{n,1}$.

1. The exponential of the First Zagreb index $e^{\mathcal{M}_1}$is induced by the function $\varphi(x,y) = e^{x+y}$ which is strictly increasing in both variables in $[1,\infty)$. By the Mean Value Theorem, there exist c_1 and x_1, with $c-t < c_1 < c \leq x < x_1 < x+t$, such that

$$\begin{aligned} \Delta_1\left(e^{\mathcal{M}_1}\right) &= e^{x+y+t} - e^{x+y} + e^{c-t+y} - e^{c+y} = te^{y}\left(e^{x_1} - e^{c_1}\right) \geq 0. \\ \Delta_2\left(e^{\mathcal{M}_1}\right) &= e^{x+c} - e^{x+c} = 0. \end{aligned}$$

2. The exponential of the Sombor index $e^{\mathcal{SO}}$ is induced by the function $\varphi(x,y) = e^{\sqrt{x^2+y^2}}$ which is strictly increasing in both variables in $[1,\infty)$. Similarly, by the Mean Value Theorem, there exist c_1 and x_1, with $c-t < c_1 < c \leq x < x_1 < x+t$, such that

$$\begin{aligned} \Delta_1\left(e^{\mathcal{SO}}\right) &= e^{\sqrt{(x+t)^2+y^2}} - e^{\sqrt{x^2+y^2}} + e^{\sqrt{(c-t)^2+y^2}} - e^{\sqrt{c^2+y^2}} \\ &= \frac{x_1 t}{\sqrt{x_1^2+y^2}} e^{\sqrt{x_1^2+y^2}} - \frac{c_1 t}{\sqrt{c_1^2+y^2}} e^{\sqrt{c_1^2+y^2}}. \end{aligned}$$

It is easy to see that the function $\frac{x}{\sqrt{x^2+y^2}} e^{\sqrt{x^2+y^2}}$ is increasing as a function of x, then $\Delta_1\left(e^{\mathcal{SO}}\right) \geq 0$.

$$\Delta_2\left(e^{\mathcal{SO}}\right) = e^{\sqrt{(x+t)^2+(c-t)^2}} - e^{\sqrt{x^2+c^2}} = e^{\sqrt{x^2+c^2+2t(x+t-c)}} - e^{\sqrt{x^2+c^2}} \geq 0.$$

3. The exponential of the Forgotten index $e^{\mathcal{F}}$ is induced by the function $\varphi(x,y) = e^{x^2+y^2}$ which is strictly increasing in both variables in $[1,\infty)$. Similarly, by the Mean Value Theorem, there exist c_1 and x_1, with $c-t < c_1 < c \leq x < x_1 < x+t$, such that

$$\begin{aligned} \Delta_1\left(e^{\mathcal{F}}\right) &= e^{(x+t)^2+y^2} - e^{x^2+y^2} + e^{(c-t)^2+y^2} - e^{c^2+y^2} = 2t\left(x_1 e^{x_1^2+y^2} - c_1 e^{c_1^2+y^2}\right) \geq 0 \\ \Delta_2\left(e^{\mathcal{F}}\right) &= e^{(x+t)^2+(c-t)^2} - e^{x^2+c^2} = e^{x^2+c^2}\left(e^{2t(x+t-c)} - 1\right) \geq 0. \end{aligned}$$

■

As in the case of Second Zagreb index, we cannot apply the Lemma 3.1 to the exponential of the Second Zagreb index because the condition $\Delta_2(\varphi) \geq 0$ fails. In the case of the exponentials of the Randić, the Harmonic and Sum connectivity indices, we neither can apply the Lemma 3.1 because condition $\Delta_1(\varphi) \leq 0$ fails in each case as it occurs in the case of the Randić, the Harmonic and the Sum connectivity indices.

In order to prove that the graph $H_{n,1}$ is the minimal unicyclic graph with respect to the exponentials of the Harmonic and the Sum-Connectivity index, we generalize the method used in [14] for the general Sum-Connectivity index.

Proposition 3.4. *Let φ be a VDB topological index defined as (2) and G be a connected graph with $uv \in E(G)$, where $d_G(u), d_G(v) \geq 2$ and $N_G(u) \cap N_G(v) = \emptyset$. Let G' be the graph obtained from G by deleting the edge uv, identifying vertices u and v in one vertex denoted by w in G', and attaching a pendant vertex to w.*

1. *If $\varphi(x,y)$ is increasing as a function of x and $\varphi(x,y) \leq \varphi(x+1, y-1)$ for $y > 1$, then $\varphi(G) \leq \varphi(G')$.*
2. *If $\varphi(x,y)$ is decreasing as a function of x and $\varphi(x,y) \geq \varphi(x+1, y-1)$ for $y > 1$, then $\varphi(G) \geq \varphi(G')$.*

Proof. We prove part 1. The proof of the second part is similar.

$$\begin{aligned}
\varphi(G) - \varphi(G') &= \sum_{a \in N_G(u)} \varphi(d_G(u), d_G(a)) - \varphi(d_G(u) + d_G(v) - 1, d_G(a)) \\
&\quad + \sum_{b \in N_G(v)} \varphi(d_G(v), d_G(b)) - \varphi(d_G(u) + d_G(v) - 1, d_G(b)) \\
&\quad + \varphi(d_G(u), d_G(v)) - \varphi(d_G(u) + d_G(v) - 1, 1) < 0.
\end{aligned}$$

■

Let $C^3_{p,q,r} \in \mathcal{G}_{n,1}$, where $p \geq q \geq r \geq 0$ and $p+q+r = n-3$, be a unicyclic graph obtained from 3-cycle C_3 with $V(C_3) = \{u, v, w\}$, adding p, q and r pendent vertices to the vertices u, v and w, respectively (see Figure 3). Note that $C^3_{n-3,0,0} = H_{n,1}$.

Theorem 3.5. *Let φ be a VDB topological index defined as (2), $G \in \mathcal{G}_{n,1}$, and for $x \geq y$, $g(x,y) = x\varphi(x+2, 1) + \varphi(x+2, y)$.*

1. *If $\varphi(x,y)$ is increasing as a function of x, $\varphi(x,y) \leq \varphi(x+1, y-1)$ for $y > 1$ and $g(x+1, y) - g(x,y)$ is increasing as a function of x for each value of $y \geq 2$, then $\varphi(G) \leq \varphi(H_{n,1})$.*

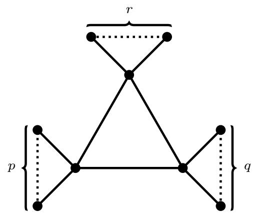

Figure 3. Unicyclic graph $C^3_{p,q,r}$.

2. *If* $\varphi(x,y)$ *is decreasing as a function of* x, $\varphi(x,y) \geq \varphi(x+1, y-1)$ *for* $y > 1$ *and* $g(x+1,y) - g(x,y)$ *is decreasing as a function of* x *for each value of* $y \geq 2$, *then* $\varphi(G) \geq \varphi(H_{n,1})$.

Proof. We prove part 1. The proof of the second part is similar.

Since $\varphi(x,y)$ is increasing as a function of x and $\varphi(x,y) \leq \varphi(x+1,y-1)$ for $y > 1$, the maximal graph in $\mathcal{G}_{n,1}$ with respect to the VDB topological index φ is a graph of the form $C^3_{p,q,r}$. We need to prove that $\varphi\left(C^3_{p,q,r}\right) \leq \varphi(H_{n,1})$. To do this it is sufficient to prove that $\varphi\left(C^3_{p+1,q-1,r}\right) \geq \varphi\left(C^3_{p,q,r}\right)$ for $q \geq 1$.

$$\begin{aligned}
\Delta_3(\varphi) &= \varphi\left(C^3_{p+1,q-1,r}\right) - \varphi\left(C^3_{p,q,r}\right) \\
&= [(p+1)\varphi(p+3,1) - p\varphi(p+2,1)] - [q\varphi(q+2,1) - (q-1)\varphi(q+1,1)] \\
&\quad + [\varphi(p+3,r+2) - \varphi(p+2,r+2)] - [\varphi(q+2,r+2) - \varphi(q+1,r+2)] \\
&\quad + [\varphi(p+3,q+1) - \varphi(p+2,q+2)] \\
&= [(p+1)\varphi(p+3,1) + \varphi(p+3,r+2) - p\varphi(p+2,1) - \varphi(p+2,r+2)] \\
&\quad - [q\varphi(q+2,1) + \varphi(q+2,r+2) - (q-1)\varphi(q+1,1) - \varphi(q+1,r+2)] \\
&\quad + [\varphi(p+3,q+1) - \varphi(p+2,q+2)] \\
&= [g(p+1,r+2) - g(p,r+2)] - [g(q,r+2) - g(q-1,r+2)] \\
&\quad + [\varphi(p+3,q+1) - \varphi(p+2,q+2)] \\
&\geq 0.
\end{aligned}$$

■

As an application of the previous theorem, we obtain that the graph $H_{n,1}$ is the minimal graph over $\mathcal{G}_{n,1}$with respect to the exponential of the Harmonic and the Sum-Connectivity indices.

Theorem 3.6. *The graph $H_{n,1}$ is the minimal graph over $\mathcal{G}_{n,1}$ with respect to $e^{\mathcal{H}}$ and $e^{\mathcal{SC}}$.*

Proof. For each of these indices we check that conditions in part 2 of Theorem 3.5 hold. Then, the minimal graph over $\mathcal{G}_{n,1}$ with respect to the corresponding index is $H_{n,1}$.

1. The exponential of the Harmonic index $e^{\mathcal{H}}$ is induced by the function $\varphi(x,y) = e^{\frac{2}{x+y}}$ which is decreasing as a function of x. We also have that $\varphi(x,y) - \varphi(x+1, y-1) = 0$. Finally, the derivative

$$\begin{aligned} \frac{\partial^2}{\partial x^2} g(x,y) &= -\frac{4(2x+9)}{(x+3)^4} e^{\frac{2}{x+3}} + \frac{4(x+y+3)}{(x+y+2)^4} e^{\frac{2}{x+y+2}} \\ &< \left(\frac{4(x+y+3)}{(x+y+2)^4} - \frac{4(2x+9)}{(x+3)^4} \right) e^{\frac{2}{x+3}} \\ &< 4e^{\frac{2}{x+3}} \frac{(x+y+3)-(2x+9)}{(x+3)^4} \\ &= 4e^{\frac{2}{x+3}} \frac{y-x-6}{(x+3)^4} < 0, \end{aligned}$$

which implies that $g(x+1,y) - g(x,y)$ is decreasing.

2. The exponential of the Sum-Connectivity index $e^{\mathcal{SC}}$ is induced by the function $\varphi(x,y) = e^{\frac{1}{\sqrt{x+y}}}$ which is decreasing as a function of x. We also have that $\varphi(x,y) - \varphi(x+1,y-1) = 0$. Finally, the derivative

$$\begin{aligned} \frac{\partial^2}{\partial x^2} g(x,y) &= e^{\frac{1}{\sqrt{x+3}}} \left(\frac{x\left(1+3\sqrt{x+3}\right) - 4(x+3)^{\frac{3}{2}}}{4(x+3)^3} \right) \\ &\quad + e^{\frac{1}{\sqrt{x+y+2}}} \frac{1+3\sqrt{x+y+2}}{4(x+y+2)^3} \\ &< e^{\frac{1}{\sqrt{x+3}}} \left(\frac{4x\sqrt{x+3} - 4(x+3)^{\frac{3}{2}}}{4(x+3)^3} \right) + e^{\frac{1}{\sqrt{x+y+2}}} \frac{4\sqrt{x+y+2}}{4(x+y+2)^3} \\ &= e^{\frac{1}{\sqrt{x+3}}} \frac{-3\sqrt{x+3}}{(x+3)^3} + e^{\frac{1}{\sqrt{x+y+2}}} \frac{\sqrt{x+y+2}}{(x+y+2)^3} \\ &< e^{\frac{1}{\sqrt{x+3}}} \left(\frac{\sqrt{x+y+2} - 3\sqrt{x+3}}{(x+3)^3} \right) \\ &< e^{\frac{1}{\sqrt{x+3}}} \left(\frac{\sqrt{2x+2} - 3\sqrt{x+3}}{(x+3)^3} \right) < 0, \end{aligned}$$

which implies that $g(x+1,y) - g(x,y)$ is decreasing.

■

We cannot apply Proposition 3.4 to the exponential of the Randić index because the condition $\varphi(x,y) \geq \varphi(x+1,y-1)$ does not hold.

Our next result is useful to prove that the graph $H_{n,1}$ is an extremal graph over $\mathcal{G}_{n,1}$ for VDB topological indices induced by functions $\varphi(x,y)$ that behave similarly to the function that induces the Atom-Bond-Connectivity index.

Theorem 3.7. *Let φ be a VDB topological index defined as (2).*

1. *If $\varphi(1,y)$ is decreasing for $y \geq 2$, $\varphi(1,2) = \varphi(2,y) \leq \varphi(3,3)$ for $2 \leq y \leq n-1$ and for $y \geq 3$ fixed, $\varphi(x,y)$ is increasing for $x \geq 3$, then $\varphi(G) \geq \varphi(H_{n,1})$ for any $G \in \mathcal{G}_{n,1}$.*

2. *If $\varphi(1,y)$ is increasing for $y \geq 2$, $\varphi(1,2) = \varphi(2,y) \geq \varphi(3,3)$ for $2 \leq y \leq n-1$ and for $y \geq 3$ fixed, $\varphi(x,y)$ is decreasing for $x \geq 3$, then $\varphi(G) \leq \varphi(H_{n,1})$ for any $G \in \mathcal{G}_{n,1}$.*

Proof. We prove part 1. The proof of the second part is similar. Let $G \in \mathcal{G}_{n,1}$

$$\begin{aligned}
\varphi(G) &= \sum_{(x,y)\in P} m_{x,y}\varphi(x,y) = \sum_{y=2}^{n-1} m_{1,y}\varphi(1,y) + \sum_{2\leq x\leq y\leq n+1-x} m_{x,y}\varphi(x,y) \\
&\geq \varphi(1,n-1)\sum_{y=2}^{n-1} m_{1,y} + \varphi(2,n-1) \sum_{2\leq x\leq y\leq n+1-x} m_{x,y} \\
&= n_1\varphi(1,n-1) + (n-n_1)\varphi(2,n-1),
\end{aligned}$$

where n_1 is the number of vertices with degree 1. Note that the previous expression is decreasing as a function of n_1 and the maximal value of n_1 over the set of unicyclic graphs with n vertices is $n-3$. Then,

$$\begin{aligned}
\varphi(G) &\geq (n-3)\varphi(1,n-1) + 3\varphi(2,n-1) \\
&= (n-3)\varphi(1,n-1) + \varphi(2,2) + 2\varphi(2,n-1) = \varphi(H_{n,1}).
\end{aligned}$$

■

Let $\mathcal{ABC}_\alpha$ be the generalized Atom Bond Connectivity index [39] induced by the function $\varphi(x,y) = \left(\frac{x+y-2}{xy}\right)^\alpha$. Note that for $\alpha = \frac{1}{2}$ we recover the usual Atom Bond Connectivity index and for $\alpha = -3$ we recover the Augmented Zagreb index. The exponential of the generalized Atom Bond Connectivity index $e^{\mathcal{ABC}_\alpha}$ is induced by the function $\psi(x,y) = e^{\left(\frac{x+y-2}{xy}\right)^\alpha}$.

Theorem 3.8. *For $\alpha < 0$ ($\alpha > 0$) the graph $H_{n,1}$ is the minimal (maximal) unicyclic graph with respect to $\mathcal{ABC}_\alpha$ and $e^{\mathcal{ABC}_\alpha}$.*

Proof. Let $\varphi(x,y) = \left(\frac{x+y-2}{xy}\right)^\alpha$ and $\psi(x,y) = e^{\left(\frac{x+y-2}{xy}\right)^\alpha}$. We have

$$\begin{aligned}
\frac{\partial}{\partial y}\varphi(1,y) &= \alpha\frac{(y-1)^{\alpha-1}}{y^{\alpha+1}}, \\
\varphi(2,y) &= \left(\frac{1}{2}\right)^\alpha, \\
\frac{\partial}{\partial x}\varphi(x,y) &= -\alpha(y-2)\frac{(x+y-2)^{\alpha-1}}{x^{\alpha+1}y^\alpha}, \\
\frac{\partial}{\partial y}\psi(1,y) &= \alpha\frac{(y-1)^{\alpha-1}}{y^{\alpha+1}}e^{\left(\frac{y-1}{y}\right)^\alpha}, \\
\psi(2,y) &= e^{\left(\frac{1}{2}\right)^\alpha}, \\
\frac{\partial}{\partial x}\psi(x,y) &= -\alpha(y-2)\frac{(x+y-2)^{\alpha-1}}{x^{\alpha+1}y^\alpha}e^{\left(\frac{x+y-2}{xy}\right)^\alpha}.
\end{aligned}$$

The proof follows from Theorem 3.7 since for $\alpha < 0$ the conditions of the first part of the theorem hold and for $\alpha > 0$ the conditions of the second part of theorem hold for both the generalized Atom-Bond-Connectivity index $\mathcal{ABC}_\alpha$ and its exponential $e^{\mathcal{ABC}_\alpha}$. ■

4 Open problems

As we already mentioned, the minimal unicyclic graph with respect to the $\mathcal{ABC}$ index is not known. The same occurs with the maximal unicyclic graph with respect to the $\mathcal{AZ}$ index. In the case of the exponentials of these indices, it seems to occur the same situation. Next we show that the cycle C_n is not the minimal unicyclic graph with respect to $e^{\mathcal{ABC}}$ neither the maximal unicyclic graph with respect to $e^{\mathcal{AZ}}$. In fact, for each $k \geq 3$, we construct a unicyclic graph $T_{k,2}+e$ with $n = 1+5k$ vertices, by adding an edge joining two leaves to the Kragujevac tree $T_{k,2}$ [18] with a central vertex of degree k and k branches of type B_2 (see Figure 4). The Kragujevac tree $T_{k,2}$ was used in [12] to show that the path is not the minimal tree with respect to $e^{\mathcal{ABC}}$ neither the maximal tree with respect to $e^{\mathcal{AZ}}$. For any VDB topological index φ, we obtain

$$\varphi(T_{k,2}+e) - \varphi(C_{5k+1}) = k\varphi(3,k) + (2k-2)\varphi(1,2) + 2k\varphi(2,3) - (5k-2)\varphi(2,2).$$

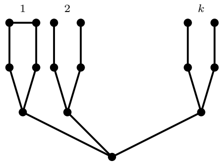

Figure 4. Unicyclic graph $T_{k,2}+e$.

Then

$$\begin{aligned}
\Delta\left(e^{\mathcal{ABC}}\right) &= e^{\mathcal{ABC}}\left(T_{k,2}+e\right)-e^{\mathcal{ABC}}\left(C_{5k+1}\right)\\
&= ke^{\sqrt{\frac{k+1}{3k}}}+(2k-2)\,e^{\sqrt{\frac{1}{2}}}+2ke^{\sqrt{\frac{1}{2}}}-(5k-2)\,e^{\sqrt{\frac{1}{2}}}\\
&= k\left(e^{\sqrt{\frac{1}{3}+\frac{1}{3k}}}-e^{\sqrt{\frac{1}{2}}}\right)<0\\
\Delta\left(e^{\mathcal{AZ}}\right) &= e^{\mathcal{AZ}}\left(T_{k,2}+e\right)-e^{\mathcal{AZ}}\left(C_{5k+1}\right)\\
&= ke^{\left(\frac{3k}{k+1}\right)^3}+(2k-2)\,e^{8}+2ke^{8}-(5k-2)\,e^{8}\\
&= k\left(e^{\left(\frac{3k}{k+1}\right)^3}-e^{8}\right)>0.
\end{aligned}$$

Although we proved in Section 2 that the cycle is an extremal unicyclic graph with respect to the exponentials of the Geometric-Arithmetic and Arithmetic-Geometric indices, using the techniques in Section 3 we could not prove that the graph $H_{n,1}$ is an extremal unicyclic graph with respect to these indices.

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