MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **82** (2019) 715-732

ISSN 0340 - 6253

The Path and the Star as Extremal Values of Vertex–Degree–Based Topological Indices Among Trees

Roberto Cruz, Juan Rada

Instituto de Matemáticas, Universidad de Antioquia
Medellín, Colombia
roberto.cruz@udea.edu.co , pablo.rada@udea.edu.co

(Received March 2, 2019)

Abstract

We denote by $\mathcal{T}_n$ the set of trees with n vertices, $P_n \in \mathcal{T}_n$ is the path tree and $S_n \in \mathcal{T}_n$ is the star tree. Let φ be a vertex-degree-based topological index defined over $\mathcal{T}_n$. For any tree $T \in \mathcal{T}_n$, we find an expression of $\varphi(T)$ in terms of $\varphi(P_n)$ and a function f_φ associated to φ, in such a way that the derivatives of f_φ over a compact set gives information on when the path P_n is an extremal value of φ over $\mathcal{T}_n$, for $n \geq 3$. Similarly, we present results which give information on when the star S_n is an extremal value of φ over $\mathcal{T}_n$, for $n \geq 3$. As an application, we determine extremal trees for exponential vertex-degree-based topological indices.

1 Introduction

The problem of finding extremal graphs over a significant graph family with respect to important topological indices has attracted considerable attention in mathematical-chemistry literature (for motivation and chemical applications of the topological indices see [7, 23, 24, 30, 31]). We are mostly interested in vertex-degree-based (VDB for short) topological indices, which are defined as a sum, over all edges of a graph, of certain numbers that depend on the degrees of the end-vertices of each edge [5, 9, 13, 15, 19, 27].

A formal definition of a VDB topological index is as follows. Let $\mathcal{G}_n$ be the set of 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 $\{\varphi_{i,j}\}_{(i,j)\in K}$ 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 (1) were referred as bond incident degree indices in [32]. These indices were also considered in [21], and more recently in [2].

The most studied VDB topological indices are the First Zagreb index $\mathcal{M}_1$ [20], induced by numbers $\varphi_{i,j} = i+j$; the Second Zagreb index $\mathcal{M}_2$ [20], induced by $\varphi_{i,j} = ij$; the Randić index χ [29] induced by $\varphi_{i,j} = \frac{1}{\sqrt{ij}}$; the Harmonic index $\mathcal{H}$ [35], induced by $\varphi_{i,j} = \frac{2}{i+j}$; the Geometric-Arithmetic index $\mathcal{GA}$ [33], induced by $\varphi_{i,j} = \frac{2\sqrt{ij}}{i+j}$; the Sum-Connectivity index $\mathcal{SC}$ [34], induced by $\varphi_{i,j} = \frac{1}{\sqrt{i+j}}$; the Atom-Bond-Connectivity index $\mathcal{ABC}$ [10], induced by $\varphi_{i,j} = \sqrt{\frac{i+j-2}{ij}}$ and the Augmented Zagreb index $\mathcal{AZ}$ [12], induced by $\varphi_{i,j} = \left(\frac{ij}{i+j-2}\right)^3$.

Let $\mathcal{T}_n$ be the set of all trees with n vertices. It is well known that P_n (the path on n vertices) and S_n (the star on n vertices) are extremal trees with respect to most of the VDB topological indices mentioned above over $\mathcal{T}_n$, as we can see in Table 1 [3,8,11,12,25,33–35]. The problem of finding the minimal tree with respect to the $\mathcal{ABC}$ index and maximal tree

	$\mathcal{M}_1$	$\mathcal{M}_2$	χ	$\mathcal{H}$	$\mathcal{GA}$	$\mathcal{SC}$	$\mathcal{ABC}$	$\mathcal{AZ}$
min	P_n	P_n	S_n	S_n	S_n	S_n	?	S_n
max	S_n	S_n	P_n	P_n	P_n	P_n	S_n	?

Table 1. Extremal trees for well known VDB topological indices.

with respect to the $\mathcal{AZ}$ index are open and very difficult problems [1, 4, 14, 16–18, 26].

In this paper we give a general method to determine whether the path P_n or the star S_n are extremal trees of a VDB topological index φ over $\mathcal{T}_n$. Generally speaking, let φ be a vertex-degree-based topological index defined over $\mathcal{T}_n$. For any tree $T \in \mathcal{T}_n$, we find an expression of $\varphi(T)$ in terms of $\varphi(P_n)$ and a function f_φ associated to φ, in such a way that the derivatives of f_φ over a compact set gives information on when the path P_n is an extremal value of φ over $\mathcal{T}_n$, for $n \geq 3$. Similarly, we present results which give information on when the star S_n is an extremal value of φ over $\mathcal{T}_n$, for $n \geq 3$. As an application, we determine extremal trees for exponential vertex-degree-based topological indices. Recall that the exponential of φ is defined as the VDB topological index e^φ induced by numbers $\{e^{\varphi_{i,j}}\}_{(i,j)\in K}$ [28]. It was shown in [28] that these topological indices have good discrimination properties. Our results are summarized in Table 2.

	$e^{\mathcal{M}_1}$	$e^{\mathcal{M}_2}$	$e^{\mathcal{X}}$	$e^{\mathcal{H}}$	$e^{\mathcal{GA}}$	$e^{\mathcal{SC}}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{AZ}}$
min	P_n	P_n	S_n	S_n	S_n	S_n	?	S_n
max	S_n	?	?	P_n	P_n	P_n	S_n	?

Table 2. Results on extremal trees for exponential of well known VDB topological indices.

Using this technique we failed to find the minimal tree for $e^{\mathcal{ABC}}$ and the maximal tree for $e^{\mathcal{M}_2}$, $e^{\mathcal{X}}$ and $e^{\mathcal{AZ}}$.

2 VDB topological indices with the path as extremal tree

Let $T \in \mathcal{T}_n$, where $n \geq 3$. Since a tree is a connected acyclic graph, then $m_{1,1}(T) = 0$, $m_{i,j}(T) = 0$ for any $1 \leq i \leq j \leq n-1$ such that $i+j > n$ and $\sum_{1\leq i\leq j\leq n-1} m_{i,j}(T) = n-1$. Consider the subset L of K defined as

$$L = \{(i,j) \in K : i+j \leq n, (i,j) \neq (1,1)\}.$$

If φ is a VDB topological index induced by the numbers $\{\varphi_{i,j}\}_{(i,j)\in K}$ then, for every $T \in \mathcal{T}_n$,

$$\varphi(T) = \sum_{(i,j)\in K} m_{i,j}(T)\,\varphi_{i,j} = \sum_{(i,j)\in L} m_{i,j}(T)\varphi_{i,j}. \tag{2}$$

We define the function

$$f(i,j) = \frac{ij}{i+j}\left(\varphi_{i,j} + 2\varphi_{1,2} - 3\varphi_{2,2}\right)$$

over the set L. Note that

$$f(1,2) = f(2,2) = 2\left(\varphi_{1,2} - \varphi_{2,2}\right).$$

Recall that P_n denotes the path with n vertices. It is easy to see that

$$\varphi(P_n) = 2\varphi_{1,2} + (n-3)\varphi_{2,2}.$$

Theorem 2.1 *Let φ be a VDB topological index as in (2) and $T \in \mathcal{T}_n$. Then*

$$\varphi(T) = \varphi(P_n) + \sum_{(i,j)\in L} [f(i,j) - f(1,2)] \frac{i+j}{ij} m_{i,j}.$$

Proof. Since T is a connected acyclic graph, we have

$$\sum_{(i,j)\in L} \left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j} = n, \tag{3}$$

$$\sum_{(i,j)\in L} m_{i,j} = n-1. \tag{4}$$

Hence

$$\begin{aligned} \frac{3}{2} m_{1,2} + m_{2,2} &= n - \sum_{(i,j)\in L^*} \left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j} \\ m_{1,2} + m_{2,2} &= n - 1 - \sum_{(i,j)\in L^*} m_{i,j} \end{aligned}$$

where $L^* = L - \{(1,2),(2,2)\}$. It is easy to obtain

$$m_{1,2} = 2 + \sum_{(i,j)\in L^*} 2m_{i,j} - \sum_{(i,j)\in L^*} 2\left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j}, \tag{5}$$

$$m_{2,2} = n - 3 - \sum_{(i,j)\in L^*} 3m_{i,j} + \sum_{(i,j)\in L^*} 2\left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j}. \tag{6}$$

Replacing relations (5) and (6) in (2)

$$\begin{aligned} \varphi(T) &= \sum_{(i,j)\in L} m_{i,j}\varphi_{i,j} = m_{1,2}\varphi_{1,2} + m_{2,2}\varphi_{2,2} + \sum_{(i,j)\in L^*} m_{i,j}\varphi_{i,j} \\ &= 2\varphi_{1,2} + (n-3)\varphi_{2,2} + \sum_{(i,j)\in L^*} \left(\frac{1}{i} + \frac{1}{j}\right)(2\varphi_{2,2} - 2\varphi_{1,2}) m_{i,j} \\ &\quad + \sum_{(i,j)\in L^*} m_{i,j}(\varphi_{ij} + 2\varphi_{1,2} - 3\varphi_{2,2}) \\ &= \varphi(P_n) + \sum_{(i,j)\in L^*} \left(\frac{1}{i} + \frac{1}{j}\right) m_{i,j} \left[\frac{ij}{i+j}(\varphi_{i,j} + 2\varphi_{1,2} - 3\varphi_{2,2}) - 2(\varphi_{1,2} - \varphi_{2,2})\right] \\ &= \varphi(P_n) + \sum_{(i,j)\in L} [f(i,j) - f(1,2)] \frac{i+j}{ij} m_{i,j}. \end{aligned}$$

■

Corollary 2.2 *Let φ be a VDB topological index as in (2) and define*

$$f\left(i,j\right)=\frac{ij}{i+j}\left(\varphi_{i,j}+2\varphi_{1,2}-3\varphi_{2,2}\right)$$

for every $(i,j)\in L$.

1. *If $f(1,2)=f(2,2)=\max_{(i,j)\in L}f(i,j)$, then for every tree $T\in\mathcal{T}_n$*

$$\varphi\left(T\right)\leq\varphi\left(P_n\right).$$

2. *If $f(1,2)=f(2,2)=\min_{(i,j)\in L}f(i,j)$, then for every tree $T\in\mathcal{T}_n$*

$$\varphi\left(T\right)\geq\varphi\left(P_n\right).$$

Proof. First assume that $f(1,2)=f(2,2)=\max_{(i,j)\in L}f(i,j)$. Let $T\in\mathcal{T}_n$. By Theorem 2.1 and the fact that $f\left(i,j\right)\leq f\left(1,2\right)$ for all $(i,j)\in L$, we deduce $\varphi\left(T\right)\leq\varphi\left(P_n\right)$. The second affirmation can be proved similarly. ■

In order to find $\max_{(i,j)\in L}f(i,j)$ or $\min_{(i,j)\in L}f(i,j)$ for a given φ, we consider the extension of L to the compact set

$$\widehat{L}=\left\{(x,y)\in\mathbb{R}\times\mathbb{R}:1\leq x\leq y\leq n-1,\ x+y\leq n,\ y\geq 2\right\}.$$

If $\varphi:\widehat{L}\longrightarrow\mathbb{R}$ is a continuous and differentiable function then $f_\varphi:\widehat{L}\longrightarrow\mathbb{R}$ defined as

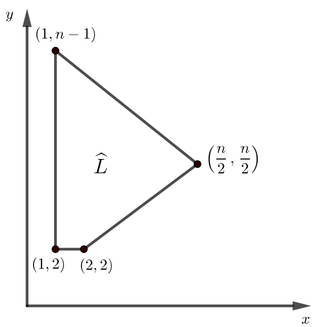

Figure 1. Compact set $\widehat{L}$.

$$f_\varphi\left(x,y\right)=\frac{xy}{x+y}\left[\varphi\left(x,y\right)+2\varphi\left(1,2\right)-3\varphi\left(2,2\right)\right],$$

is also continuous and differentiable function over $\widehat{L}$. Clearly,

$$\left.\begin{cases} \frac{\partial}{\partial y} f_\varphi(x,y) \le 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dx} f_\varphi(x,x) \le 0 & \forall x \in \left[2, \frac{n}{2}\right] \end{cases}\right\} \Longrightarrow \max_{(i,j)\in L} f_\varphi(i,j) = f_\varphi(1,2)$$

and

$$\left.\begin{cases} \frac{\partial}{\partial y} f_\varphi(x,y) \ge 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dx} f_\varphi(x,x) \ge 0 & \forall x \in \left[2, \frac{n}{2}\right] \end{cases}\right\} \Longrightarrow \min_{(i,j)\in L} f_\varphi(i,j) = f_\varphi(1,2)$$

Theorem 2.3 *The path P_n is the maximal tree over $\mathcal{T}_n$ with respect to the following exponential VDB topological indices:*

1. *The exponential of the Harmonic index $e^{\mathcal{H}}$;*
2. *The exponential of Geometric-Arithmetic index $e^{\mathcal{GA}}$;*
3. *The exponential of the Sum-Connectivity index $e^{\mathcal{SC}}$.*

Proof. 1. The exponential of the Harmonic index is induced by the numbers $\varphi_{i,j} = e^{\frac{2}{i+j}}$, and the associated function $f_{_{e^{\mathcal{H}}}}(x,y)$ is defined over $\widehat{L}$ as

$$f_{_{e^{\mathcal{H}}}}(x,y) = \frac{xy}{x+y}\left[e^{\frac{2}{x+y}} + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}}\right].$$

The derivative

$$\begin{aligned} \frac{\partial}{\partial y} f_{_{e^{\mathcal{H}}}}(x,y) &= \frac{x^2}{(x+y)^2}\left(e^{\frac{2}{x+y}} + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}} - \frac{y(x+y)}{x}\frac{2}{(x+y)^2}e^{\frac{2}{x+y}}\right) \\ &\le \frac{x^2}{(x+y)^2}\left[\left(1 - \frac{2}{x+y}\right)e^{\frac{2}{x+y}} + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}}\right] \\ &\le \frac{x^2}{(x+y)^2}\left[\left(1 - \frac{2}{3}\right)e^{\frac{2}{3}} + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}}\right] < 0 \end{aligned}$$

for all (x,y) in $\widehat{L}$, since $x \le y$ and $x+y \ge 3$ in $\widehat{L}$. On the other hand

$$\frac{d}{dx} f_{_{e^{\mathcal{H}}}}(x,x) = \frac{1}{2}\left(e^{\frac{1}{x}} + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}} - x\frac{1}{x^2}e^{\frac{1}{x}}\right) = \frac{1}{2}\left[e^{\frac{1}{x}}\left(1 - \frac{1}{x}\right) + 2e^{\frac{2}{3}} - 3e^{\frac{1}{2}}\right] < 0$$

for all $x \in \left[2, \frac{n}{2}\right]$. It follows that $f_{_{e^{\mathcal{H}}}}(1,2) = f_{_{e^{\mathcal{H}}}}(2,2) = \max_{(i,j)\in L} f_{_{e^{\mathcal{H}}}}(i,j)$ and we are done by Corollary 2.2.

2. The exponential of Geometric-Arithmetic index is induced by the numbers $\varphi_{i,j} = e^{\frac{2\sqrt{ij}}{i+j}}$ and the associated function $f_{_{e^{\mathcal{GA}}}}(x,y)$ is defined over $\widehat{L}$ as

$$f_{_{e^{\mathcal{GA}}}}(x,y) = \frac{xy}{x+y}\left[e^{\frac{2\sqrt{xy}}{x+y}} + 2e^{\frac{2\sqrt{2}}{3}} - 3e\right].$$

The derivative

$$\begin{aligned}
\frac{\partial}{\partial y} f_{e\mathcal{GA}}(x,y) &= \frac{x^2}{(x+y)^2}\left(e^{\frac{2\sqrt{xy}}{x+y}} + 2e^{\frac{2\sqrt{2}}{3}} - 3e + \frac{\sqrt{xy}\,(x-y)}{x\,(x+y)} e^{\frac{2\sqrt{xy}}{x+y}}\right) \\
&\leq \frac{x^2}{(x+y)^2}\left(e^{\frac{2\sqrt{xy}}{x+y}} + 2e^{\frac{2\sqrt{2}}{3}} - 3e\right) \\
&\leq \frac{x^2}{(x+y)^2}\left(e + 2e^{\frac{2\sqrt{2}}{3}} - 3e\right) < 0
\end{aligned}$$

for all (x, y) in $\widehat{L}$, since $x \leq y$ and $\frac{2\sqrt{xy}}{x+y} \leq 1$ in $\widehat{L}$. On the other hand

$$\frac{d}{dx} f_{e\mathcal{GA}}(x,x) = \frac{1}{2}\left(e + 2e^{\frac{2\sqrt{2}}{3}} - 3e\right) < 0,$$

for all $x \in \left[2, \frac{n}{2}\right]$. Then $f_{e\mathcal{GA}}(1,2) = f_{e\mathcal{GA}}(2,2) = \max_{(i,j)\in L} f_{e\mathcal{GA}}(i,j)$ and by Corollary 2.2, the maximal tree with respect to the exponential of Geometric-Arithmetic index is the path P_n.

3. The exponential of the Sum Connectivity index is induced by the numbers $\varphi_{i,j} = e^{\frac{1}{\sqrt{i+j}}}$, then

$$f_{e\mathcal{SC}}(x,y) = \frac{xy}{x+y}\left[e^{\frac{1}{\sqrt{x+y}}} + 2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}}\right].$$

The derivative

$$\begin{aligned}
\frac{\partial}{\partial y} f_{e\mathcal{SC}}(x,y) &= \frac{x^2}{(x+y)^2}\left[\left(1 - \frac{y}{2x\sqrt{x+y}}\right) e^{\frac{1}{\sqrt{x+y}}} + 2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}}\right] \\
&\leq \frac{x^2}{(x+y)^2}\left[\left(1 - \frac{1}{2\sqrt{x+y}}\right) e^{\frac{1}{\sqrt{x+y}}} + 2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}}\right] \\
&\leq \frac{x^2}{(x+y)^2}\left[\left(1 - \frac{1}{2\sqrt{3}}\right) e^{\frac{1}{\sqrt{3}}} + 2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}}\right] < 0
\end{aligned}$$

for all (x, y) in $\widehat{L}$, since $x \leq y$ and $x + y \geq 3$ in $\widehat{L}$. On the other hand,

$$\begin{aligned}
\frac{d}{dx} f_{e\mathcal{SC}}(x,x) &= \frac{1}{2}\left(e^{\frac{1}{\sqrt{2x}}} + 2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}} - \frac{x}{(2x)^{\frac{3}{2}}} e^{\frac{1}{\sqrt{2x}}}\right) \\
&= \frac{1}{2}\left(\frac{1}{2\sqrt{2x}} e^{\frac{1}{2x}} + +2e^{\frac{1}{\sqrt{3}}} - 3e^{\frac{1}{2}}\right) < 0
\end{aligned}$$

for all $x \geq 2$. It follows that $f_{e\mathcal{SC}}(1,2) = f_{e\mathcal{SC}}(2,2) = \max_{(i,j)\in L} f_{e\mathcal{SC}}(i,j)$ and we are done by Corollary 2.2. ■

Theorem 2.4 *The path P_n is the minimal tree over $\mathcal{T}_n$ with respect to the exponential of the First Zagreb index $e^{\mathcal{M}_1}$.*

Proof. For the exponential of the First Zagreb index $\varphi_{i,j} = e^{i+j}$ and the associated function $f_{e^{\mathcal{M}_1}}(x,y)$ is defined over $\widehat{L}$ as

$$f_{e^{\mathcal{M}_1}}(x,y) = \frac{xy}{x+y}\left[e^{x+y} + 2e^3 - 3e^4\right].$$

The derivative

$$\begin{aligned} \frac{\partial}{\partial y} f_{e^{\mathcal{M}_1}}(x,y) &= \frac{x^2}{(x+y)^2}\left(e^{x+y} + 2e^3 - 3e^4 + \frac{y(x+y)}{x}e^{x+y}\right) \\ &\geq \frac{x^2}{(x+y)^2}\left[e^{x+2}\left(3+\frac{4}{x}\right) + 2e^3 - 3e^4\right] > 0 \end{aligned}$$

for all $(x,y) \in \widehat{L}$ since $y \geq 2$. Moreover,

$$\frac{d}{dx} f_{e^{\mathcal{M}_1}}(x,x) = \frac{1}{2}\left[(1+2x)\, e^{2x} + 2e^3 - 3e^4\right] > 0,$$

for $x \geq 2$. Hence the minimum of $f_{e^{\mathcal{M}_1}}$ over L is $f_{e^{\mathcal{M}_1}}(2,2) = f_{e^{\mathcal{M}_1}}(1,2)$. By Corollary 2.2, the minimal tree with respect to the exponential of the First Zagreb index is the path P_n. ■

We will next show that the path P_n is the minimal tree over $\mathcal{T}_n$ with respect to the exponential of the Second Zagreb index $e^{\mathcal{M}_2}$. Unfortunately, the minimum value of $f_{e^{\mathcal{M}_2}}$ over $\widehat{L}$ is $f_{e^{\mathcal{M}_2}}(1,3)$, so we cannot apply Corollary 2.2. However, we can adapt the technique used by [22] in the study of the general Randić index. We will denote by $d_T(u)$ the degree of the vertex u of T.

Lemma 2.5 *Consider the trees T and T' with $n \geq 5$ vertices, as in Figure 2. If $p \geq 3$ then $e^{\mathcal{M}_2}(T) \geq e^{\mathcal{M}_2}(T')$.*

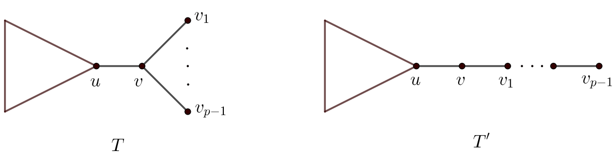

Figure 2. Trees used in the proof of Lemma 2.5.

Proof. Set $q = d_T(u)$. Then

$$\begin{aligned}\Delta &= e^{\mathcal{M}_2}(T) - e^{\mathcal{M}_2}(T') \\ &= \left(e^{pq} + (p-1)\,e^{p}\right) - \left(e^{2q} + (p-2)\,e^{4} + e^{2}\right) \\ &= \left(e^{pq} - e^{2q}\right) + (p-2)\left(e^{p} - e^{4}\right) + \left(e^{p} - e^{2}\right).\end{aligned}$$

If $p \geq 4$ then each of the summands above is non-negative, being the first and last strictly positive. Hence $\Delta > 0$.

Assume now that $p = 3$. Then

$$\Delta = e^{3q} - e^{2q} + 2e^{3} - e^{4} - e^{2}.$$

Note that $q \geq 2$ since $n \geq 5$. It is easy to see that

$$e^{3q} - e^{2q} \geq 2e^{3} - e^{4} - e^{2},$$

for all $q \geq 2$. Consequently, $\Delta > 0$. ∎

Lemma 2.6 *Assume that T is a tree with minimum $e^{\mathcal{M}_2}$ and $n \geq 5$ vertices. If v is a vertex of T adjacent to a leaf u of T, then $d_T(v) = 2$.*

Proof. Assume that $d_T(v) = d$ and let P be the largest path of T that contains v. Let s be an end-vertex of P and r a vertex in P adjacent to s. By Lemma 2.5, $d_T(r) = 2$. Let T' be the tree obtained from T by deleting the leaf u and adding an edge incident to s (see Figure 3). We consider two cases:

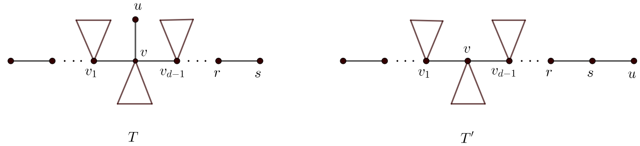

Figure 3. Trees used in the proof of Lemma 2.6.

1. $d_T(v) = d \geq 4$. If $q_1, \ldots, q_{d-1}$ are the degrees of the adjacent vertices to v different from u, then

$$\Delta = e^{\mathcal{M}_2}(T) - e^{\mathcal{M}_2}(T') = \sum_{i=1}^{d-1}\left(e^{dq_i} - e^{(d-1)q_i}\right) + e^{d} - e^{4} > 0.$$

This contradicts the minimality of T.

2. $d_T(v) = 3$. Let v_1 and v_2 be the adjacent vertices to v (different from u), such that $d_T(v_1) = p$ and $d_T(v_1) = q$. It follows from Lemma 2.5 that $p \geq 2$ and $q \geq 2$. Then

$$\Delta(p,q) = e^{\mathcal{M}_2}(T) - e^{\mathcal{M}_2}(T') = e^{3p} - e^{2p} + e^{3q} - e^{2q} + e^3 - e^4.$$

The derivatives of $\Delta(p,q)$ are

$$\begin{aligned} \frac{\partial}{\partial p}\Delta(p,q) &= 3e^{3p} - 2e^{2p} > 0, \\ \frac{\partial}{\partial q}\Delta(p,q) &= 3e^{3q} - 2e^{2q} > 0, \end{aligned}$$

Hence $\Delta(p,q) \geq \Delta(2,2) > 0$, which contradicts the fact that T is minimal. ■

Theorem 2.7 *The path P_n $(n \geq 5)$ is the minimal tree over $\mathcal{T}_n$ with respect to the exponential of the Second Zagreb index $e^{\mathcal{M}_2}$.*

Proof. Let T_0 be a tree with minimal $e^{\mathcal{M}_2}$-value over $\mathcal{T}_n$. By Lemma 2.6, $m_{1,j}(T_0) = 0$ for all $j \geq 3$. It follows from Theorem 2.1 that

$$\begin{aligned} e^{\mathcal{M}_2}(T_0) &= e^{\mathcal{M}_2}(P_n) + \sum_{(i,j)\in L}\left[f_{e^{\mathcal{M}_2}}(i,j) - f_{e^{\mathcal{M}_2}}(1,2)\right]\frac{i+j}{ij}m_{i,j}(T_0) \\ &= e^{\mathcal{M}_2}(P_n) + \sum_{(i,j)\in M}\left[f_{e^{\mathcal{M}_2}}(i,j) - f_{e^{\mathcal{M}_2}}(1,2)\right]\frac{i+j}{ij}m_{i,j}(T_0), \end{aligned} \tag{7}$$

where

$$M = \{(i,j) \in L : i \geq 2\}.$$

Let

$$\widehat{M} = \left\{(x,y) \in \widehat{L} : x \geq 2\right\}.$$

We will show that $\min_{(i,j)\in\widehat{M}} f_{e^{\mathcal{M}_2}}(i,j) = f_{e^{\mathcal{M}_2}}(2,2)$. Note that

$$f_{e^{\mathcal{M}_2}}(x,y) = \frac{xy}{x+y}\left(e^{xy} + 2e^2 - 3e^4\right).$$

The derivative

$$\begin{aligned} \frac{\partial}{\partial y}f_{e^{\mathcal{M}_2}}(x,y) &= \frac{x^2}{(x+y)^2}\left(e^{xy} + 2e^2 - 3e^4 + y(x+y)e^{xy}\right) \\ &\geq \frac{x^2}{(x+x)^2}\left[e^{x^2}\left(1+2x^2\right) + 2e^2 - 3e^4\right] > 0 \end{aligned}$$

for all $(x,y) \in \widehat{M}$. On the other hand

$$\frac{\partial}{\partial x} f_{{}_{e}\mathcal{M}_2}(x,x) = \frac{1}{2}\left[\left(1+2x^2\right)e^{x^2} + 2e^2 - 3e^4\right] > 0,$$

for all $x \geq 2$. Consequently, the minimum of $f_{{}_{e}\mathcal{M}_2}$ over $\widehat{M}$ is $f_{{}_{e}\mathcal{M}_2}(2,2) = f_{{}_{e}\mathcal{M}_2}(1,2)$.

Finally, if $T \in \mathcal{T}_n$ then by (7) we deduce

$$e^{\mathcal{M}_2}(T) \geq e^{\mathcal{M}_2}(T_0) \geq e^{\mathcal{M}_2}(P_n).$$

■

Remark 2.8 *Using Corollary 2.2 we can also obtain the known results given in Table 1 about the path as a maximal tree over $\mathcal{T}_n$, for the Randić, Harmonic, Geometric-Arithmetic and Sum-Connectivity indices.*

3 VDB topological indices with the star as extremal tree

Our concern in this section is when does the star S_n attain the minimal value of a VDB topological index φ over $\mathcal{T}_n$. If φ is a VDB topological index induced by the numbers $\{\varphi_{i,j}\}_{(i,j)\in K}$ then, as we mentioned in the previous section, for every $T \in \mathcal{T}_n$

$$\varphi(T) = \sum_{(i,j)\in L} m_{i,j}(T)\varphi_{i,j},$$

where

$$L = \{(i,j) \in K : i+j \leq n, (i,j) \neq (1,1)\}.$$

Consider the function

$$g(i,j) = \varphi_{i,j},$$

defined over the set L.

It is easy to see that

$$\varphi(S_n) = (n-1)\varphi_{1,n-1}.$$

Theorem 3.1 *Let φ be a VDB topological index as in (2) and T a tree with n vertices. Then*

$$\varphi(T) = \varphi(S_n) + \sum_{(i,j)\in L} \left[g(i,j) - g(1,n-1)\right] m_{i,j} \tag{8}$$

Proof. Using relation (4), we have

$$m_{1,n-1} = n - 1 - \sum_{(i,j)\in L^1} m_{i,j}, \tag{9}$$

where $L^1 = L - \{(1, n-1)\}$. Replacing (9) in (2)

$$\begin{aligned} \varphi(T) &= m_{1,n-1}\varphi_{1,n-1} + \sum_{(i,j)\in L^1} m_{i,j}\varphi_{i,j} \\ &= (n-1)\varphi_{1,n-1} + \sum_{(i,j)\in L^1} m_{i,j}(\varphi_{i,j} - \varphi_{1,n-1}) \\ &= \varphi(S_n) + \sum_{(i,j)\in L} [g(i,j) - g(1,n-1)]\, m_{i,j}. \end{aligned}$$

■

Corollary 3.2 *Let φ be a VDB topological index as in (2) and define*

$$g(i,j) = \varphi_{i,j}$$

for every $(i,j) \in L$.

1. *If $g(1,n-1) = \max_{(i,j)\in L} g(i,j)$, then for every tree $T \in \mathcal{T}_n$*

$$\varphi(T) \le \varphi(S_n).$$

2. *If $g(1,n-1) = \min_{(i,j)\in L} g(i,j)$, then for every tree $T \in \mathcal{T}_n$*

$$\varphi(T) \ge \varphi(S_n).$$

Proof. Let $T \in \mathcal{T}_n$. If $g(1,n-1) = \max_{(i,j)\in L} g(i,j)$, then by relation (8) and the fact that $g(i,j) \le g(1,n-1)$ for all $(i,j) \in L$, it follows that $\varphi(T) \le \varphi(S_n)$.

The second affirmation can be proved similarly. ■

We next use Corollary 3.2 to find extremal values of the exponentials of VDB topological indices over $\mathcal{T}_n$. In [6] we obtained that S_n is the minimal graph over $\mathcal{G}_n$, the set of graphs with n non-isolated vertices, for $e^{\mathcal{H}}, e^{\chi}$ and $e^{\mathcal{AZ}}$. In particular, S_n is the minimal tree over $\mathcal{T}_n$ for $e^{\mathcal{H}}, e^{\chi}$ and $e^{\mathcal{AZ}}$.

As in the previous section, we extend the function g to the compact set

$$\widehat{L} = \{(x,y) \in \mathbb{R}\times\mathbb{R} : 1 \le x \le y \le n-1,\ x+y \le n,\ y \ge 2\}.$$

Assume that

$$g_\varphi(x,y) = \varphi(x,y)$$

is a continuous and differentiable function over $\widehat{L}$. Clearly (see Figure 1),

$$\left.\begin{cases} \frac{\partial}{\partial x} g_\varphi(x,y) \le 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dy} g_\varphi(1,y) \ge 0 & \forall y \in [2, n-1] \end{cases}\right\} \Longrightarrow \max_{(i,j)\in L} g_\varphi(i,j) = g_\varphi(1, n-1),$$

and

$$\left.\begin{cases} \frac{\partial}{\partial x} g_\varphi(x,y) \ge 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dy} g_\varphi(1,y) \le 0 & \forall y \in [2, n-1] \end{cases}\right\} \Longrightarrow \min_{(i,j)\in L} g_\varphi(i,j) = g_\varphi(1, n-1).$$

Also,

$$\left.\begin{cases} \frac{\partial}{\partial y} g_\varphi(x,y) \ge 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dx} g_\varphi(x, n-x) \le 0 & \forall x \in \left[1, \frac{n}{2}\right] \end{cases}\right\} \Longrightarrow \max_{(i,j)\in L} g_\varphi(i,j) = g_\varphi(1, n-1),$$

and

$$\left.\begin{cases} \frac{\partial}{\partial y} g_\varphi(x,y) \le 0 & \forall (x,y) \in \widehat{L} \\ \frac{d}{dx} g_\varphi(x, n-x) \ge 0 & \forall x \in \left[1, \frac{n}{2}\right] \end{cases}\right\} \Longrightarrow \min_{(i,j)\in L} g_\varphi(i,j) = g_\varphi(1, n-1).$$

Theorem 3.3 *The star S_n is the minimal tree over $\mathcal{T}_n$ with respect to the exponential $e^{\mathcal{GA}}$ and the exponential $e^{\mathcal{SC}}$.*

Proof. 1. We associate to $e^{\mathcal{GA}}$ the function

$$g_{e^{\mathcal{GA}}}(x,y) = e^{\frac{2\sqrt{xy}}{x+y}},$$

defined over $\widehat{L}$. The derivative

$$\frac{\partial}{\partial x} g_{e^{\mathcal{GA}}}(x,y) = \frac{(y-x)\sqrt{xy}}{x(x+y)^2} e^{\frac{2\sqrt{xy}}{x+y}} \ge 0,$$

for all $(x,y) \in \widehat{L}$. On the other hand

$$\frac{d}{dy} g_{e^{\mathcal{GA}}}(1,y) = -\frac{y-1}{\sqrt{y}(y+1)^2} e^{\frac{2\sqrt{xy}}{x+y}} < 0$$

for all $y \in [2, n-1]$. Consequently, $g_{e^{\mathcal{GA}}}(1, n-1) = \min_{(i,j)\in L} g_{e^{\mathcal{GA}}}(i,j)$. The result follows by Corollary 3.2.

2. We associate to $e^{\mathcal{SC}}$ the function

$$g_{e^{\mathcal{SC}}}(x,y) = e^{\frac{1}{\sqrt{x+y}}},$$

defined over $\widehat{L}$. The derivative

$$\frac{\partial}{\partial y} g_{e\mathcal{SC}}(x,y) = -\frac{1}{2(x+y)^{\frac{3}{2}}} e^{\frac{1}{\sqrt{x+y}}} < 0$$

for all $(x,y) \in \widehat{L}$. On the other hand

$$\frac{d}{dx} g_{e\mathcal{SC}}(x, n-x) = 0$$

for all $x \in \left[1, \frac{n}{2}\right]$. It follows that $g_{e\mathcal{SC}}(1, n-1) = \min_{(i,j)\in L} g_{e\mathcal{SC}}(i,j)$. The result follows by Corollary 3.2. ■

Theorem 3.4 *The star S_n is the maximal tree over $\mathcal{T}_n$ with respect to $e^{\mathcal{ABC}}$.*

Proof. We associate to $e^{\mathcal{ABC}}$ the function

$$g_{e\mathcal{ABC}}(x,y) = e^{\sqrt{\frac{x+y-2}{xy}}},$$

for all $(x,y) \in \widehat{L}$. The derivative

$$\frac{\partial}{\partial x} g_{e\mathcal{ABC}}(x,y) = \frac{\sqrt{xy}}{2x^2 y} \frac{2-y}{\sqrt{(x+y-2)}} e^{\sqrt{\frac{x+y-2}{xy}}} \leq 0$$

for all $(x,y) \in \widehat{L}$. On the other hand

$$\frac{d}{dy} g_{e\mathcal{ABC}}(1,y) = \frac{1}{2y\sqrt{y(y-1)}} e^{\sqrt{\frac{y-1}{y}}} > 0$$

for all $y \in [2, n-1]$. It follows that $g_{e\mathcal{ABC}}(1, n-1) = \max_{(i,j)\in L} g_{e\mathcal{ABC}}(i,j)$. The result follows by Corollary 3.2. ■

Now we will show that S_n is the maximal tree with respect to $e^{\mathcal{M}_1}$ over $\mathcal{T}_n$. However, we cannot apply Corollary 3.2 since

$$g_{e\mathcal{M}_1}(1, n-1) \neq \max_{(i,j)\in L} g_{e\mathcal{M}_1}(i,j),$$

where

$$g_{e\mathcal{M}_1}(x,y) = e^{x+y}$$

for all $(x,y) \in \widehat{L}$. Instead we use the operations introduced in [8]. We denote by $N_T(u)$ the set of neighbors of u in the tree T.

Theorem 3.5 *The star S_n is the maximal tree over $\mathcal{T}_n$ with respect to the exponential $e^{\mathcal{M}_1}$.*

Proof. Let $T \in \mathcal{T}_n$ different from the star. Then T has at least one edge uv such that $d_T(v) = i \geq 2$ and $N_T(u) - \{v\} = \{w_1, \ldots, w_j\}$ are leaves, with $j \geq 1$. Let $T' = T - \{uw_1, \ldots, uw_j\} + \{vw_1, \ldots, vw_j\}$ (see Figure 4) and denote by $\{q_1, \ldots, q_{i-1}\}$ the degrees of the vertices adjacent to v in T different from u. Then

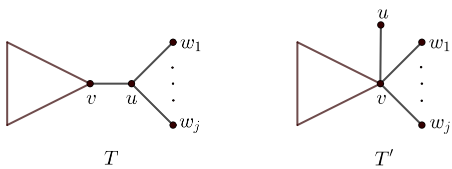

Figure 4. Trees used in the proof of Theorem 3.5.

$$\begin{aligned} e^{\mathcal{M}_1}(T') - e^{\mathcal{M}_1}(T) &= \sum_{l=1}^{i-1} \left[e^{q_l+i+j} - e^{q_l+i}\right] + (j+1)\, e^{i+j+1} - e^{i+j+1} - je^{j+2} \\ &> j\left(e^{i+j+1} - e^{j+2}\right) \geq 0. \end{aligned}$$

If $T' = S_n$ we are done, otherwise we repeat the operation until we reach the star S_n. ■

Remark 3.6 *Using Corollary 3.2 we can also obtain the known results given in Table 1 about the star as an extremal tree over $\mathcal{T}_n$, for the Harmonic, Augmented Zagreb, Geometric-Arithmetic, Sum-Connectivity and Atom-Bond-Connectivity indices.*

4 Open problems

As we mentioned in the Introduction, the problem of finding the minimal tree with respect to the $\mathcal{ABC}$ index and the maximal tree with respect to the $\mathcal{AZ}$ index are open and very difficult problems. Apparently the same occurs with the minimal of $e^{\mathcal{ABC}}$ and the maximal of $e^{\mathcal{AZ}}$. However, it is easy to see that the path P_n is not the minimal tree with respect to $e^{\mathcal{ABC}}$ neither the maximal tree with respect to $e^{\mathcal{AZ}}$. In fact, for each $k \geq 3$, let us denote by $T_{k,2}$ the Kragujevac tree [14] with a central vertex of degree k and k branches of type B_2 (see Figure 5). Note that $T_{k,2}$ has $n = 1 + 5k$ vertices.

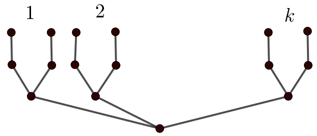

Figure 5. Kragujevac tree with k branches of type B_2.

Then

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

On the other hand, we still have no answer to the problem of finding the maximal value of the exponentials $e^{\mathcal{M}_2}$ and e^{χ} over $\mathcal{T}_n$.

References

[1] A. Ali, A. A. Bhatti, A note on augmented Zagreb index of cacti with fixed number of vertices and cycles, *Kuwait J. Sci.* **43** (2016) 11–17.

[2] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Appl. Math. Comput.* **238** (2018) 32–40.

[3] G. Caporossi, I. Gutman, P. Hansen, L. Pavlović, Graphs with maximum connectivity index, *Comput. Biol. Chem.* , **27** (2003) 85–90.

[4] X. Cheng, G. Hao, Extremal graphs with respect to generalized *ABC* index, *Discr. Appl. Math.* **243** (2018) 115–124.

[5] R. Cruz, T. Pérez, J. Rada, Extremal values of vertex–degree–based topological indices over graphs, *J. Appl. Math. Comput.* **48** (2015) 395–406.

[6] R. Cruz, J. Rada, Extremal graphs of exponential vertex–degree–based topological indices over graphs, submitted.

[7] J. Devillers, A. Balaban, *Topological Indices and Related Descriptors in QSAR and QSPR* , Gordon & Breach, Amsterdam, 1999.

[8] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[9] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex–degree–based molecular structure descriptors, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 613–626.

[10] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[11] B. Furtula, A. Graovac, D. Vukičević, Atom–bond connectivity index of trees, *Discr. Appl. Math.* **157** (2009) 2828–2835.

[12] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* **48** (2010) 370–380.

[13] B. Furtula, I. Gutman, M. Dehmer, On structure–sensitivity of degree–based topological indices, *Appl. Math. Comput.* **219** (2013) 8973–8978.

[14] B. Furtula, I. Gutman, M. Ivanović, D. Vukičević, Computer search for trees with minimal *ABC* index, *Appl. Math. Comput.* **219** (2012) 767–772.

[15] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[16] I. Gutman, B. Furtula, Trees with smallest atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 131–136.

[17] I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani, M. Zarrinderakht, The *ABC* conundrum, *Filomat* **27** (2015) 1075–1083.

[18] I. Gutman, B. Furtula, M. Ivanović, Notes on trees with minimal atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 467–482.

[19] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex–degree–based topological indices, *J. Serb. Chem. Soc.* **78** (2013) 805–810.

[20] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[21] B. Hollas, The covariance of topological indices that depend on the degree of a vertex, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 177–187.

[22] Y. Hu, X. Li, Y. Yu, Trees with maximum general Randić index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 129–146.

[23] L. Kier and L. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.

[24] L. Kier and L. Hall, *Molecular Connectivity in Structure–Activity Analysis*, Wiley, New York, 1986.

[25] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.

[26] W. Lin, A. Ali, L. Huang, Z. Wu, J. Chen, On trees with maximal augmented Zagreb index, *IEEE Access* **6** (2018) 69335–69341.

[27] J. Rada, R. Cruz, Vertex–degree–based topological indices over graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 603–616.

[28] J. Rada, Exponential vertex–degree–based topological indices and discrimination, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 29–41.

[29] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[30] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.

[31] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.

[32] D. Vukičević, J. Đurđević, Bond additive modeling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes, *Chem. Phys. Lett.* **515** (2011) 186–189.

[33] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[34] L. Zhong, The harmonic index for graphs, *Appl. Math. Lett.* **25** (2012) 561–566.

[35] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.