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VERTEX-DEGREE-BASED TOPOLOGICAL INDICES OVER TREES WITH TWO BRANCHING VERTICES

R. CRUZ[1], C. A. MARÍN[1], AND J. RADA[1]

Abstract. Given a graph G with n vertices, a vertex-degree-based topological index is defined from a set of real numbers $\{\varphi_{ij}\}$ as $TI(G) = \sum m_{ij}(G)\varphi_{ij}$, where $m_{ij}(G)$ is the number of edges between vertices of degree i and degree j, and the sum runs over all $1 \leq i \leq j \leq n-1$. Let $\Omega(n,2)$ denote the set of all trees with n vertices and 2 branching vertices. In this paper we give conditions on the number $\{\varphi_{ij}\}$ under which the extremal trees with respect to TI can be determined. As a consequence, we find extremal trees in $\Omega(n,2)$ for several well-known vertex-degree-based topological indices.

1. Introduction

Topological indices are molecular descriptors which play an important role in theoretical chemistry, especially in QSPR/QSAR research ([4,13] and [14]). Among all topological indices one of the most investigated are the so-called vertex-degree-based (VDB for short) topological indices, defined for a graph G with n vertices as

$$TI(G) = \sum_{1\leq i\leq j\leq n-1} m_{ij}\varphi_{ij}, \tag{1.1}$$

where m_{ij} is the number of edges of G joining a vertex of degree i with a vertex of degree j and $\{\varphi_{ij}\}$ is a set of real numbers. Several well-known VDB topological indices in the literature are obtained by different choices of the numbers $\{\varphi_{ij}\}$. For example, for the First Zagreb index $\varphi_{ij} = i + j$ [12] , for the Second Zagreb index $\varphi_{ij} = ij$ [12], for the Randić index $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ [21], for the Harmonic index $\varphi_{ij} = \frac{2}{i+j}$ [24], for the Geometric-Arithmetic $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [22], for the Sum-Connectivity index

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$\varphi_{ij} = \frac{1}{\sqrt{i+j}}$ [25], for the Atom-Bond-Connectivity index $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [5] and for the Augmented Zagreb index $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$ [6]. A more complete list thereof can be found in [7] and [8]. For recent results on VDB topological indices we refer to [1–3, 7, 8, 11, 18–20, 23].

Let $\Omega(n,i)$ denote the set of all trees with n vertices and i branching vertices. The problem of finding extremal values of a topological index over the set of trees with exactly one branching vertex (i.e., starlike trees) was solved for the Wiener index [10], the Hosoya index [9], the Randić index or more generally, for vertex-degree-based topological indices [1]. Moreover, the extremal values of the Hosoya index over trees with exactly 2 branching vertices can be deduced from [17]. See also [16] for the Wiener index. The double star $S_{p,q}$ is a tree with $p+q=n$ vertices with two branching vertices with degrees p and q respectively and $p+q-2$ pendant vertices. If $|p-q| \leq 1$ then the double star is said to be balanced. In [15] is reported that the balanced double star is the tree with the maximum general Randić index among all trees of order $n \geq 8$ for $\alpha \in [2, +\infty)$. Also, the double stars $S_{n-2,2}$ and $S_{n-3,3}$ are the trees with the second and the third minimum zeroth-order general Randić index for $0 < \alpha < 1$ and the second and the third maximum zeroth-order general Randić index for $\alpha < 0$ or $\alpha > 1$ respectively [15].

It is our interest in this paper to give a general criteria to decide which trees in $\Omega(n,2)$, minimize and maximize TI. We denote by $S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ the tree with two branching vertices of degrees $r+1, s+1 > 2$ connected by the path P_t, and in which the lengths of the pendant paths attached to the two branching vertices are $a_1,\ldots,a_r$ and $b_1,\ldots,b_s$ respectively (see Figure 1). Let $\Omega_1(n,2)$ be the set of all trees

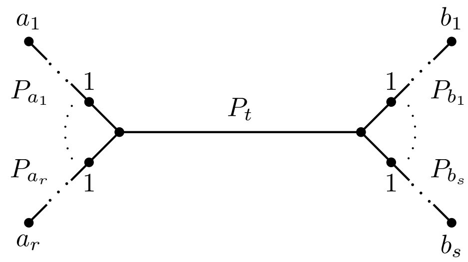

FIGURE 1. The tree $S(a_1,\ldots,a_r;\mathbf{t};b_1,\ldots,b_s)$ in $\Omega(n,2)$.

in $\Omega(n,2)$ in which each pendant path has length 1 and $\Omega^2(n,2)$ be the set of all trees in $\Omega(n,2)$ such that the branching vertices are connected by an edge. Note that

$$\Omega_1(n,2)=\left\{S(x;\mathbf{t};y)=S(\underbrace{1,\dots,1}_{x};\mathbf{t};\underbrace{1,\dots,1}_{y})\}\ :\ x+y+t=n\right\},$$

$$\Omega^2(n,2)=\left\{S(a_1,\dots,a_r;\mathbf{2};b_1,\dots,b_s)\}\ :\ \sum_{i=1}^{r}a_i+\sum_{j=1}^{s}b_j+2=n\right\}.$$

In sections 2 and 3 we consider the problem of finding extremal trees with respect to VDB index TI over $\Omega_1(n,2)$ and $\Omega^2(n,2)$ respectively. In Theorems 2.1 and 3.1 we give conditions on the number $\{\varphi_{ij}\}$ under which the trees with extremal TI values over $\Omega_1(n,2)$ and over $\Omega^2(n,2)$ respectively, can be determined.

Finally, in section 4 we show that under certain conditions on the number $\{\varphi_{ij}\}$, one of the extremal values of the VDB index TI over the class of trees with two branching vertices is attained in a tree of the class $\Omega_1(n,2)$ and the other one is attained in a tree of the class $\Omega^2(n,2)$ (see Theorem 4.1). As a consequence, in Corollary 4.1 we find extremal trees for the First Zagreb index, the Second Zagreb index, the Randić index, the Harmonic index and the Sum-Connectivity index. Also we find the maximal tree for the Atom-Bond-Connectivity index and the minimal tree for the Augmented Zagreb index.

2. Extremal Values of VDB Topological Indices Over $\Omega_1(n,2)$

First we consider the set of double stars $S(x;\mathbf{2};y)=S(\underbrace{1,\dots,1}_{x};\mathbf{2};\underbrace{1,\dots,1}_{y})$, where $2\le x\le n-4$, $x+y+2=n$ and $n\ge 6$. The value of the VDB index TI of double stars is

$$f_1(x)=TI\left(S(x;\mathbf{2};y)\right)=x\varphi_{1,x+1}+\varphi_{x+1,y+1}+y\varphi_{1,y+1}. \tag{2.1}$$

In the next proposition we give conditions on the numbers $\{\varphi_{ij}\}$ under which the extremal double stars with respect to VDB index TI can be determined.

Proposition 2.1. *Let TI be a VDB topological index defined as in* (1.1) *and assume that $f_1(x)$ is increasing* (*decreasing*) *for $2\le x\le\left\lfloor\frac{n-2}{2}\right\rfloor$, where $n\ge 6$. Then the double star with minimal* (*maximal*) *TI value is $S(2;\mathbf{2};n-4)$ and the double star with maximal* (*minimal*) *TI value is the balanced double star $S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right)$.*

Proof. It is sufficient to note that, for $2\le x\le\left\lfloor\frac{n-2}{2}\right\rfloor$ and $y=n-2-x$, $f_1(x)=f_1(y)$. Then, if $f_1(x)$ is monotone for $2\le x\le\left\lfloor\frac{n-2}{2}\right\rfloor$, then the extremal values of $f_1(x)$ are attained in $x=2$ and $x=\left\lfloor\frac{n-2}{2}\right\rfloor$. □

We apply the previous proposition in order to find extremal double stars with respect to well-known vertex-degree-based topological indices.

Corollary 2.1. *Among all double stars of order $n\ge 6$:*

(a) *the Randić index, the Sum-Connectivity index, the Geometric-Arithmetic index, the Harmonic index and the Augmented Zagreb index attain the minimal value in the double star* $S(2;\mathbf{2};n-4)$ *and the maximal value in the balanced double star* $S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right)$*;*

(b) *the First Zagreb index, the Second Zagreb index and the Atom Bond Connectivity index attain the maximal value in the double star* $S(2;\mathbf{2};n-4)$ *and the minimal value in the balanced double star* $S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right)$*.*

Proof. For each index in Corollary 2.1 it can be verified that the function $f_1(x)$ is continuous in $[2,n-4]$ and differentiable in $(2,n-4)$.

For all VDB topological indices in part 1 of Corollary 2.1, we obtain that $f_1'(x)>0$ if $2<x<\frac{n-2}{2}<y<n-4$. It implies that

$$f_1(2)=f_1(n-4)\leq f_1(x)\leq f_1\left(\frac{n-2}{2}\right),$$

for $2\leq x\leq n-4$ and the result follows.

On the other hand, for all VDB topological indices in part 2 of Corollary 2.1, we obtain that $f_1'(x)<0$ if $2<x<\frac{n-2}{2}<y<n-4$. It implies that

$$f_1(2)=f_1(n-4)\geq f_1(x)\geq f_1\left(\frac{n-2}{2}\right),$$

for $2\leq x\leq n-4$ and the result follows. □

Next we consider the set of trees of the form $S(x;\mathbf{3};y)=S(\underbrace{1,\ldots,1}_{x};\mathbf{3};\underbrace{1,\ldots,1}_{y})$, where $2\leq x\leq n-5$, $x+y+3=n$ and $n\geq 7$. The value of the VDB index TI of $S(x;\mathbf{3};y)$ is

$$f_2(x)=TI\left(S(x;\mathbf{3};y)\right)=x\varphi_{1,x+1}+\varphi_{2,x+1}+\varphi_{2,y+1}+y\varphi_{1,y+1}. \tag{2.2}$$

Conditions on the numbers $\{\varphi_{ij}\}$ under which the extremal trees of the form $S(x;\mathbf{3};y)$ with respect to VDB index TI can be determined are presented in the following

Proposition 2.2. *Let* TI *be a VDB topological index defined as in* (1.1) *and assume that* $f_2(x)$ *is increasing* (*decreasing*) *for* $2\leq x\leq\left\lfloor\frac{n-3}{2}\right\rfloor$ *where* $n\geq 7$*. Then the tree of the form* $S(x;\mathbf{3};y)$ *with minimal* (*maximal*) TI *value is* $S(2;\mathbf{3};n-5)$ *and the tree with maximal* (*minimal*) TI *value is* $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right)$*.*

Proof. The proof is similar to the proof of Proposition 2.1. □

The results of applying conditions in the previous proposition to the topological indices listed in Proposition 2.1 are presented in the next

Corollary 2.2. *Among all trees of order* $n\geq 7$ *of the form in* $S(x;\mathbf{3};y)$*:*

(a) *the Randić index, the Sum-Connectivity index, the Geometric-Arithmetic index and the Harmonic index attain the minimal value in* $S(2;\mathbf{3};n-5)$ *and the maximal value in* $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right)$*;*

(b) *the First Zagreb index, the Second Zagreb index, the Atom Bond Connectivity index and the Augmented Zagreb index attain the minimal value in* $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right)$ *and the maximal value in* $S(2;\mathbf{3};n-5)$.

Proof. For each index in Corollary 2.2 it can be verified that the function $f_2(x)$ is continuous in $[2,n-5]$ and differentiable in $(2,n-5)$.

For all VDB topological indices in part 1 of Corollary 2.2, we obtain that $f_2'(x)>0$ if $2<x<\frac{n-3}{2}<y<n-5$. It implies that

$$f_2(2)=f_2(n-5)\le f_2(x)\le f_2\left(\frac{n-3}{2}\right),$$

for $2\le x\le n-5$ and the result follows.

On the other hand, for all VDB topological indices in part 2 of Corollary 2.2, we obtain that $f_2'(x)<0$ if $2<x<\frac{n-3}{2}<y<n-5$. It implies that

$$f_2(2)=f_2(n-5)\ge f_2(x)\ge f_2\left(\frac{n-3}{2}\right),$$

for $2\le x\le n-5$ and the result follows. □

Now we find the extremal trees with respect to vertex-degree-based topological index TI over $\Omega_1(n,2)$. Let $4\le t\le n-4$, $2\le x\le n-t-2$, $x+y+t=n$, $n\ge 8$ and

$$\begin{aligned} f_3(x)=&TI\left(S(x;\mathbf{t};y)\right)-TI\left(S(x+1;\mathbf{t}-\mathbf{1};y)\right)\\ =&\left(\varphi_{2,x+1}-\varphi_{2,x+2}\right)+(x+1)\left(\varphi_{1,x+1}-\varphi_{1,x+2}\right)+\left(\varphi_{22}-\varphi_{1,x+1}\right). \end{aligned} \tag{2.3}$$

Theorem 2.1. *Let* TI *be a VDB topological index defined as in* (1.1) *and* $n\ge 8$.

(a) *If* $f_3(x)\le 0$ *for all* $2\le x\le n-6$, $f_2(x)$ *is decreasing for* $2\le x\le\left\lfloor\frac{n-3}{2}\right\rfloor$ *and* $f_1(x)$ *is decreasing for* $2\le x\le\left\lfloor\frac{n-2}{2}\right\rfloor$, *then the minimal tree in* $\Omega_1(n,2)$ *with respect to VDB index* TI *is*

$$\begin{cases} S(2;\mathbf{n-4};2), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}\le f_1\left(\frac{n-2}{2}\right),\\ S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}> f_1\left(\frac{n-2}{2}\right),\end{cases}$$

while the maximal tree is

$$\begin{cases} S(2;\mathbf{2};n-4), & \text{if } f_1(2)\ge f_2(2),\\ S(2;\mathbf{3};n-5), & \text{if } f_1(2)< f_2(2).\end{cases}$$

(b) *If* $f_3(x)\ge 0$ *for all* $2\le x\le n-6$, $f_2(x)$ *is increasing for* $2\le x\le\left\lfloor\frac{n-3}{2}\right\rfloor$ *and* $f_1(x)$ *is increasing for* $2\le x\le\left\lfloor\frac{n-2}{2}\right\rfloor$, *then the minimal tree in* $\Omega_1(n,2)$ *with respect to VDB index* TI *is*

$$\begin{cases} S(2;\mathbf{2};n-4), & \text{if } f_1(2)\le f_2(2),\\ S(2;\mathbf{3};n-5), & \text{if } f_1(2)> f_2(2),\end{cases}$$

while the maximal tree is

$$\begin{cases} S(2;\mathbf{n-4};2), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}\geq f_1\left(\frac{n-2}{2}\right), \\ S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}< f_1\left(\frac{n-2}{2}\right). \end{cases}$$

(c) *If $f_3(x)\geq 0$ for all $2\leq x\leq n-6$, $f_2(x)$ is decreasing for $2\leq x\leq\left\lfloor\frac{n-3}{2}\right\rfloor$ and $f_1(x)$ is increasing for $2\leq x\leq\left\lfloor\frac{n-2}{2}\right\rfloor$, then the minimal tree in $\Omega_1(n,2)$ with respect to VDB index TI is*

$$\begin{cases} S(2;\mathbf{2};n-4), & \text{if } f_1(2)\leq f_2\left(\frac{n-3}{2}\right), \\ S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right), & \text{if } f_1(2)> f_2\left(\frac{n-3}{2}\right), \end{cases}$$

while the maximal tree is

$$\begin{cases} S(2;\mathbf{n-4};2), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}\geq f_1\left(\frac{n-2}{2}\right), \\ S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right), & \text{if } 4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}< f_1\left(\frac{n-2}{2}\right). \end{cases}$$

Proof. (a) If $f_3(x)\leq 0$ for all $2\leq x\leq n-6$, $f_2(x)$ is decreasing for $2\leq x\leq\left\lfloor\frac{n-3}{2}\right\rfloor$ and $f_1(x)$ is decreasing for $2\leq x\leq\left\lfloor\frac{n-2}{2}\right\rfloor$, by relation (2.3) and Propositions 2.1 and 2.2 we obtain

$$\begin{aligned} f_2(2)=TI\left(S(2;\mathbf{3};n-5)\right)\geq f_2(x)=TI\left(S(x;\mathbf{3};y)\right)&\geq TI\left(S(x;\mathbf{t};y)\right)\\ &\geq TI\left(S(2;\mathbf{n-4};2)\right)=4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}, \end{aligned}$$

$$f_1(2)=TI\left(S(2;\mathbf{2};n-4)\right)\geq TI\left(S(x;\mathbf{2};y)\right)=f_1(x)\geq f_1\left(\frac{n-2}{2}\right),$$

and the part 1 is proved.

(b) The proof is obtained as in part 1 by reversing inequalities.

(c) If $f_3(x)\geq 0$ for all $2\leq x\leq n-6$, $f_2(x)$ is decreasing for $2\leq x\leq\left\lfloor\frac{n-3}{2}\right\rfloor$ and $f_1(x)$ is increasing for $2\leq x\leq\left\lfloor\frac{n-2}{2}\right\rfloor$, by relation (2.3) and Propositions 2.1 and 2.2 we obtain

$$\begin{aligned} f_2\left(\frac{n-3}{2}\right)&\leq f_2(x)=TI\left(S(x;\mathbf{3};y)\right)\leq TI\left(S(x;\mathbf{t};y)\right)\\ &\leq TI\left(S(2;\mathbf{n-4};2)\right)=4\varphi_{13}+2\varphi_{23}+(n-7)\varphi_{22}, \end{aligned}$$

$$f_1(2)=TI\left(S(2;\mathbf{2};n-4)\right)\leq TI\left(S(x;\mathbf{2};y)\right)=f_1(x)\leq f_1\left(\frac{n-2}{2}\right),$$

and the part 3 is proved. □

We apply the previous theorem in order to find extremal trees in $\Omega_1(n,2)$ with respect to well-known vertex-degree-based topological indices.

Corollary 2.3. *Among all trees in $\Omega_1(n,2)$ with $n\geq 8$:*

(a) *the Randić index, the Sum-Connectivity index, the Geometric-Arithmetic index and the Harmonic index index attain the minimal value in the tree $S(2;\mathbf{2};n-4)$ and the maximal value in the tree $S(2;\mathbf{n-4};2)$;*

(b) *the First Zagreb index, the Second Zagreb index and the Atom Bond Connectivity index attain the minimal value in the tree* $S(2;\mathbf{n-4};2)$ *and the maximal value in the tree* $S(2;\mathbf{2};n-4)$*;*

(c) *the Augmented Zagreb attains the minimal value in the tree* $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right)$ *and the maximal value in the tree* $S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right)$.

Proof. For all the indices in part 1 of Corollary 2.3 it can be verified that $f_3(x) \geq 0$ for all $2 \leq x \leq n-6$. Moreover, by the proofs Corollaries 2.1 and 2.2, the functions $f_1(x)$ and $f_2(x)$ are increasing. It is easy to verify that for all these indices

$$\begin{aligned} f_1(2) \leq & f_2(2), \\ 4\varphi_{13} + 2\varphi_{23} + (n-7)\varphi_{22} \geq & f_1\left(\frac{n-2}{2}\right), \end{aligned}$$

for all $n \geq 8$. Then, by Theorem 2.1 the minimal tree is $S(2;\mathbf{2};n-4)$ and the maximal tree is $S(2;\mathbf{n-4};2)$.

For all the indices in Part 2 of Corollary 2.3 it can be verified that $f_3(x) \leq 0$ for all $2 \leq x \leq n-6$. Moreover, by the proofs Corollaries 2.1 and 2.2, the functions $f_1(x)$ and $f_2(x)$ are decreasing. It is easy to verify that for all these indices

$$\begin{aligned} f_1(2) \geq & f_2(2), \\ 4\varphi_{13} + 2\varphi_{23} + (n-7)\varphi_{22} \leq & f_1\left(\frac{n-2}{2}\right), \end{aligned}$$

for all $n \geq 8$. Then, by Theorem 2.1 the minimal tree is $S(2;\mathbf{n-4};2)$ and the maximal tree is $S(2;\mathbf{2};n-4)$.

For the Augmented Zagreb index, it is easy to check that $f_3(x) > 0$ for all $x > 0$. By the proofs of Corollaries 2.1 and 2.2, the function $f_1(x)$ is increasing while the function $f_2(x)$ is decreasing. It can be verified that

$$\begin{aligned} f_1(2) \geq & f_2\left(\frac{n-3}{2}\right), \\ 4\varphi_{13} + 2\varphi_{23} + (n-7)\varphi_{22} \leq & f_1\left(\frac{n-2}{2}\right), \end{aligned}$$

for all $n \geq 8$,. By Theorem 2.1 the minimal tree is $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right))$ and the maximal tree is $S\left(\left\lfloor\frac{n-2}{2}\right\rfloor;\mathbf{2};\left\lceil\frac{n-2}{2}\right\rceil\right)$. □

3. Extremal Values of VDB Topological Indices Over $\Omega^2(n,2)$

In order to find the trees with extremal TI values over $\Omega^2(n,2)$ we compute the differences between TI indices of trees of the form $S(a_1,\dots,a_r;\mathbf{2};b_1,\dots,b_s)$, where $n \geq 8$.

Let $S(a_1,\dots,a_x,y) = S(a_1,\dots,a_x,\underbrace{1,\dots,1}_{y};\mathbf{2};b_1,\dots,b_{z-1})$, where $x,y \geq 0$, $x+y \geq 2$ and $z \geq 3$. In the case of $x \geq 1$, we assume that $a_i \geq 2$ for each $i = 1,\dots,x$.

For $x \geq 1$, $y \geq 1$ and $z \geq 3$ we have

$$\begin{aligned} f_4(x,y,z) =& TI\left(S(a_1,\ldots,a_x,y)\right) - TI\left(S(a_1,\ldots,a_x+1,y-1)\right) \\ =& \left(\varphi_{z,x+y+1} - \varphi_{z,x+y}\right) + x\left(\varphi_{2,x+y+1} - \varphi_{2,x+y}\right) \\ & + y\left(\varphi_{1,x+y+1} - \varphi_{1,x+y}\right) + \left(\varphi_{1,x+y} - \varphi_{22}\right). \end{aligned} \tag{3.1}$$

For $x \geq 0$, $y \geq 2$ and $z \geq 3$ we have

$$\begin{aligned} f_5(x,y,z) =& TI\left(S(a_1,\ldots,a_x,y)\right) - TI\left(S(a_1,\ldots,a_x,2,y-2)\right) \\ =& \left(\varphi_{z,x+y+1} - \varphi_{z,x+y}\right) + x\left(\varphi_{2,x+y+1} - \varphi_{2,x+y}\right) \\ & + y\left(\varphi_{1,x+y+1} - \varphi_{1,x+y}\right) + \left(2\varphi_{1,x+y} - \varphi_{12} - \varphi_{2,x+y}\right). \end{aligned} \tag{3.2}$$

For $x \geq 3$ and $z \geq 3$ we have

$$\begin{aligned} f_6(x,z) =& TI\left(S(a_1,\ldots,a_{x-1},a_x)\right) - TI\left(S(a_1,\ldots,a_{x-1}+a_x)\right) \\ =& \left(\varphi_{z,x+1} - \varphi_{z,x}\right) + x\left(\varphi_{2,x+1} - \varphi_{2,x}\right) + \left(\varphi_{2,x} + \varphi_{12} - 2\varphi_{22}\right). \end{aligned} \tag{3.3}$$

Let A and X be arbitrary connected graphs with at least two vertices. For each $i = 2,\ldots,n-3$, consider the path-coalescence graphs $AX_{i+1,i}$ and for $i = 2,\ldots,n-2$ the path-coalescence graphs $X_{n,i}$, depicted in Figure 2, where $n \geq 5$.

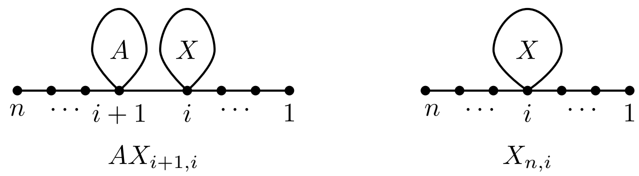

FIGURE 2. Path-coalescence graphs $AX_{i+1,i}$ and $X_{n,i}$.

Now we compute the difference between the vertex-degree-based topological index TI as in (1.1) of introduced path-coalescence graphs. Let x be the degree of the vertex i and y the degree of the vertex $i+1$ in $AX_{i+1,i}$. Similarly, x is the degree of the vertex x in $X_{n,i}$. For $3 \leq i \leq n-2$ we have:

$$TI\left(X_{n,i}\right) - TI\left(X_{n,2}\right) = \left(\varphi_{2x} - \varphi_{22}\right) + \left(\varphi_{12} - \varphi_{1x}\right) = f_7(x) \tag{3.4}$$

and for $3 \leq i \leq n-3$ we have

$$TI\left(AX_{i+1,i}\right) - TI\left(AX_{3,2}\right) = \left(\varphi_{2x} - \varphi_{22}\right) + \left(\varphi_{12} - \varphi_{1x}\right) = f_7(x). \tag{3.5}$$

Moreover, $TI\left(X_{n,i}\right)$ is constant for each $i \in \{3,\ldots,n-2\}$ and $TI\left(AX_{i+1,i}\right)$ is also constant for $i \in \{3,\ldots,n-3\}$.

Theorem 3.1. *Let TI be a VDB topological index defined as in* (1.1), *$f_7(x) \geq 0$ for all $x \geq 3$ and $n \geq 8$.*

(a) *If* $f_4(x,y,z) \leq 0$ *for all* $x \geq 1$, $y \geq 1$ *and* $z \geq 3$, $f_5(x,y,z) \leq 0$ *for all* $x \geq 0$, $y \geq 2$ *and* $z \geq 3$ *and* $f_6(x,z) \leq 0$ *for all* $x, z \geq 3$, *then the maximal tree in* $\Omega^2(n,2)$ *with respect to VDB index* TI *is*

$$\begin{cases} S(2,2;\mathbf{2};2,n-8), & \text{if } f_7(x) \geq 0 \text{ for all } x \geq 3, \\ S(1,1;\mathbf{2};1,n-5), & \text{if } f_7(x) < 0 \text{ for all } x \geq 3, \end{cases}$$

while the minimal tree is

$$\begin{cases} S\left(\left\lfloor \frac{n-2}{2} \right\rfloor; \mathbf{2}; \left\lceil \frac{n-2}{2} \right\rceil\right), & \text{if } f_1(x) \text{ is decreasing for } 2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor, \\ S(2;\mathbf{2};n-4), & \text{if } f_1(x) \text{ is increasing for } 2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor. \end{cases}$$

(b) *If* $f_4(x,y,z) \geq 0$ *for all* $x \geq 1$, $y \geq 1$ *and* $z \geq 3$, $f_5(x,y,z) \geq 0$ *for all* $x \geq 0$, $y \geq 2$ *and* $z \geq 3$ *and* $f_6(x,z) \geq 0$ *for all* $x, z \geq 3$, *then the minimal tree in* $\Omega^2(n,2)$ *with respect to VDB index* TI *is*

$$\begin{cases} S(2,2;\mathbf{2};2,n-8), & \text{if } f_7(x) \leq 0 \text{ for all } x \geq 3, \\ S(1,1;\mathbf{2};1,n-5), & \text{if } f_7(x) > 0 \text{ for all } x \geq 3, \end{cases}$$

while the maximal tree is

$$\begin{cases} S\left(\left\lfloor \frac{n-2}{2} \right\rfloor; \mathbf{2}; \left\lceil \frac{n-2}{2} \right\rceil\right), & \text{if } f_1(x) \text{ is increasing for } 2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor, \\ S(2;\mathbf{2};n-4), & \text{if } f_1(x) \text{ is decreasing for } 2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor. \end{cases}$$

Proof. If $f_4(x,y,z) \leq 0$ for all $x \geq 1$, $y \geq 1$ and $z \geq 3$, $f_5(x,y,z) \leq 0$ for all $x \geq 0$, $y \geq 2$ and $z \geq 3$ and $f_6(x,z) \leq 0$ for all $x, z \geq 3$, by relations (3.1), (3.2) and (3.3), we have

$$TI\left(S(a_1,\ldots,a_r;\mathbf{2};b_1,\ldots,b_s)\right) \leq TI\left(S(a_1,a_2;\mathbf{2};b_1,b_2)\right),$$

where $a_1, a_2, b_1, b_2 \geq 2$. By relations (3.4) and (3.5) we have that

$$TI\left(S(a_1,a_2;\mathbf{2};b_1,b_2)\right) \leq \begin{cases} TI\left(S(2,2;\mathbf{2};2,n-8)\right), & \text{if } f_7(x) \geq 0 \text{ for all } x \geq 3, \\ TI\left(S(1,1;\mathbf{2};1,n-5)\right), & \text{if } f_7(x) < 0 \text{ for all } x \geq 3. \end{cases}$$

On the other hand, by relations (3.1) and (3.2), we have

$$TI\left(S(a_1,\ldots,a_r;\mathbf{2};b_1,\ldots,b_s)\right) \geq TI\left(S(\underbrace{1,\ldots,1}_{p};\mathbf{2};\underbrace{1,\ldots,1}_{n-2-p})\right) = f_1(p),$$

where $p = \sum_{i=1}^{r} a_i$. The result follows from Proposition 2.1 and the part 1 is proved.

The proof of part 2 is similar by reversing inequalities. □

Corollary 3.1. *Among all trees in* $\Omega^2(n,2)$ *with* $n \geq 8$*:*

(a) *the Randić index, the Sum-Connectivity index and the Harmonic index attain the minimal value in the tree* $S(2;\mathbf{2};n-4)$ *and the maximal value in the tree* $S(2,2;\mathbf{2};2,n-8)$*;*

(b) *the First Zagreb index and the Second Zagreb index attain the minimal value in the tree* $S(1,1;\mathbf{2};1,n-5)$ *and the maximal value in the tree* $S(2;\mathbf{2};n-4)$*.*

Proof. For all the indices in part 1 of Corollary 3.1 it can be verified that $f_4(x,y,z) \leq 0$ for all $x \geq 1$, $y \geq 1$ and $z \geq 3$, $f_5(x,y,z) \leq 0$ for all $x \geq 0$, $y \geq 2$ and $z \geq 3$, $f_6(x,z) \leq 0$ for all $x,z \geq 3$ and $f_7(x) \geq 0$ for all $x \geq 3$. Moreover, by the proof of Corollary 2.1, the function $f_1(x)$ is increasing for $2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor$. Then, by part 1 of Theorem 3.1 the minimal tree is $S(2;\mathbf{2};n-4)$ and the maximal tree is $S(2,2;\mathbf{2};2,n-8)$.

For all the indices in part 2 of Corollary 3.1 it can be verified that $f_4(x,y,z) \geq 0$ for all $x \geq 1$, $y \geq 1$ and $z \geq 3$, $f_5(x,y,z) \geq 0$ for all $x \geq 0$, $y \geq 2$ and $z \geq 3$, $f_6(x,z) \geq 0$ for all $x,z \geq 3$ and $f_7(x) \geq 0$ for all $x \geq 3$. Moreover, by the proof of Corollary 2.1, the function $f_1(x)$ is decreasing for $2 \leq x \leq \left\lfloor \frac{n-2}{2} \right\rfloor$. Then, by part 2 of Theorem 3.1 the minimal tree is $S(1,1;\mathbf{2};1,n-5)$ and the maximal tree is $S(2;\mathbf{2};n-4)$. □

The Geometric-Arithmetic, Atom-Bond-Connectivity and Augmented Zagreb indices do not satisfy conditions in Theorems 3.1.

4. Extremal Values of VDB Topological Indices Over Trees with Two Branching Vertices

In this section we consider the problem of finding trees in $\Omega(n,2)$ with extremal TI values.

Let X and A be arbitrary connected graphs with at least two vertices. For each $i = 2,\ldots,n-1$, consider the path-coalescence graphs $AX_{n,i}$, depicted in Figure 3, where $n \geq 3$.

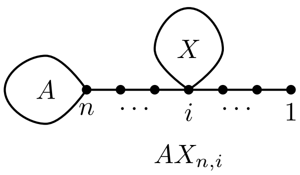

Figure 3. Path-coalescence graphs $AX_{n,i}$.

Now we compute the difference between the vertex-degree-based topological index TI as in (1.1) of introduced path-coalescence graphs. Let x be the degree of the vertex i and y the degree of the vertex n in $AX_{n,i}$. For $3 \leq i \leq n-2$ we have:

$$TI\left(AX_{n,n-1}\right) - TI\left(AX_{n,i}\right) = (\varphi_{xy} - \varphi_{2y}) + (\varphi_{22} - \varphi_{2x}) = f_8(x,y), \tag{4.1}$$

$$TI\left(AX_{n,i}\right) - TI\left(AX_{n,2}\right) = (\varphi_{2x} - \varphi_{22}) + (\varphi_{12} - \varphi_{1x}) = f_7(x). \tag{4.2}$$

Theorem 4.1. *Let TI be a VDB topological index defined as in* (1.1) *and $n \geq 8$.*

(a) *If $f_8(x,y) \geq 0$ and $f_7(x) \geq 0$ for all $x,y \geq 3$ then the tree with minimal value of the index TI over $\Omega(n,2)$ is the the tree with minimal value of the index TI over $\Omega_1(n,2)$ and the tree with maximal TI value over $\Omega(n,2)$ is the tree with maximal TI value over $\Omega^2(n,2)$.*

(b) *If* $f_8(x,y) \leq 0$ *and* $f_7(x) \leq 0$ *for all* $x, y \geq 3$ *then the tree with maximal value of the index* TI *over* $\Omega(n,2)$ *is the the tree with maximal value of the index* TI *over* $\Omega_1(n,2)$ *and the tree with minimal* TI *value over* $\Omega(n,2)$ *is the tree with minimal* TI *value over* $\Omega^2(n,2)$.

Proof. Consider a tree of the form $S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_s)$, with at least one of the parameters $a_1,\dots,a_r,b_1,\dots,b_s$ greater than 1. Assume that $b_s > 1$. If $f_8(x,y) \geq 0$ and $f_7(x) \geq 0$ for all $x, y \geq 3$, then applying relation (4.1) if $t = 2$ or relation (4.2) if $t > 2$ we obtain

$$TI\left(S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_{s-1},b_s)\right) \geq TI\left(S(a_1,\dots,a_r;\mathbf{t+1};b_1,\dots,b_{s-1},b_s-1)\right).$$

Now, applying repeatedly relation (4.2) we obtain

$$TI\left(S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_s)\right) \geq TI\left(S(\underbrace{1,\dots,1}_{r};\mathbf{t}';\underbrace{1,\dots,1}_{s})\right) = TI\left(S(r,\mathbf{t}',s)\right),$$

where $t' = t + \sum_{k=1}^{r}(a_k-1) + \sum_{k=1}^{s}(b_k-1) = n-r-s$. Then, the minimal tree with respect to the index TI is in $\Omega_1(n,2)$.

On the other hand, considering again a tree in $\Omega(n,2)$ with $t > 2$, we apply relation (4.1) if at least one of the parameters $a_1,\dots,a_r,b_1,\dots,b_s$ is greater than 1, or relation (4.2) otherwise. We obtain

$$TI\left(S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_s)\right) \leq TI\left(S(a_1,\dots,a_r;\mathbf{t-1};b_1,\dots,b_{s-1},b_s+1\right).$$

Now, applying repeatedly relation (4.1), we obtain

$$TI\left(S(a_1,\dots,a_r;\mathbf{t};b_1,\dots,b_s)\right) \leq TI\left(S(a_1,\dots,a_r;\mathbf{2};b_1,\dots,b_{s-1},b_s'\right),$$

where $b_s' = b_s + t - 2$. Then, the maximal tree with respect to the index TI is in $\Omega^2(n,2)$ and the part 1 is proved.

The proof of part 2 is similar. □

The conditions listed in Theorem 4.1 can be used to find extremal trees in the class $\Omega(n,2)$ for a specific VDB topological index. In the next corollary we apply the mentioned theorem to well-know vertex-degree-based topological indices.

Corollary 4.1. *Among all trees of order* $n \geq 8$ *and two branching vertices:*

(a) *the Randić index, the Sum-Connectivity index and the Harmonic index attain the minimal value in the tree* $S(2;\mathbf{2};n-4)$ *and the maximal value in the tree* $S(2,2;\mathbf{2};2,n-8)$;

(b) *the First Zagreb index and the Second Zagreb index attain the minimal value in the tree* $S(2;\mathbf{n-4};2)$ *and the maximal value in the tree* $S(2;\mathbf{2};n-4)$;

(c) *the Atom-Bond-Connectivity index attains its maximal value in the tree* $S(2;\mathbf{2};n-4)$;

(d) *the Augmented Zagreb index attains its minimal value in the tree* $S\left(\left\lfloor\frac{n-3}{2}\right\rfloor;\mathbf{3};\left\lceil\frac{n-3}{2}\right\rceil\right)$.

Proof. It is sufficient to check the signs of $f_8(x, y)$ and $f_7(x)$ for $x, y \geq 3$ for each index in Corollary 4.1 and apply Theorem 4.1, Corollary 2.3 and Corollary 3.1 . □

In the case of Atom-Bond-Connectivity and Augmented Zagreb indices, it was obtained that the function $f_4(x, y, z)$ takes possitive and negatives values for different choices of $x \geq 2$, $y \geq 1$ and $z \geq 3$. On the other hand, for the Geometric-Arithmetic index it was found that $f_8(x, y) \geq 0$ for all $x, y \geq 3$, however $f_7(x) \leq 0$ for x sufficiently large. It means that the conditions in Theorem 4.1 do not hold.

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[1]Instituto de Matematicas,
Universidad de Antioquia,
Medellín, Colombia

Email address: roberto.cruz@udea.edu.co
Email address: calberto.marin@udea.edu.co
Email address: pablo.rada@udea.edu.co