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Vertex-degree-based topological indices over starlike trees

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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 $1 \leq i \leq j \leq n-1$. We find conditions on the numbers $\{\varphi_{ij}\}$ which are easy to verify, under which the extremal values of TI over the set of starlike trees can be calculated. As an application we find the extremal values of many well-known vertex-degree-based topological indices over Ω_n.

1. Introduction

A topological index is a molecular descriptor that is calculated based on the molecular graph of a chemical compound. These type of indices are playing a significant role in theoretical chemistry, specially in QSPR/QSAR research [5] and [15]. Among all topological indices, one of the most investigated recently is the so-called vertex-degree-based topological index, which is defined in terms of the degrees of the vertices of the molecular graph. For more details on vertex-degree-based topological indices and on their comparative study we refer to [4,6,7,10,14,16,22].

Given a graph G with n vertices, a vertex-degree-based topological index is defined from a set of real numbers $\{\varphi_{ij}\}$ $(1 \leq i \leq j \leq n-1)$ as

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

where $m_{ij}(G)$ is the number of edges between vertices of degree i and degree j. Different choices of $\{\varphi_{ij}\}$ give different topological indices. For instance, if $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ for every $1 \leq i \leq j \leq n-1$, then TI defined as in (1) is the well-known Randić index [23]. We illustrate in Table 1 how different choices of the numbers $\{\varphi_{ij}\}$ generate the list of the most important vertex-degree-based topological indices in chemical graph theory.

Our interest in this paper is to study the extremal values of the vertex-degree-based topological indices over the set of starlike trees. Recall that a starlike tree is a tree with exactly one vertex of degree greater than 2. This class of trees have appeared frequently in the mathematical-chemistry literature. For instance, the problem of extremal values of the Wiener index and the Hosoya index was studied in [13] and [12]. Higher-order connectivity indices were examined in [21]. In another direction, those starlike trees whose spectra is integral were characterized in [25], and in [17] it was shown that non-isomorphic starlike trees are not cospectral. The same occurs with respect to the Laplacian spectra [19]. For other results on starlike trees we refer to [3,11,20].

Our approach is completely general. Starting with an expression of a vertex-degree-based topological index of the form (1), we first solve the problem locally, finding the extremal values over the set $\Omega_{n,k}$ of starlike trees with n vertices and unique vertex of degree $k > 2$. This is a consequence of Theorem 2.1, where it is shown that the extremal values strongly

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Table 1
Well-known vertex-degree-based topological indices.

Index	$\{\varphi_{ij}\}$	Notation
Randić [23]	$\frac{1}{\sqrt{ij}}$	$\chi(G)$
Geometric–Arithmetic [24]	$\frac{2\sqrt{ij}}{i+j}$	$GA(G)$
Sum-connectivity [27]	$\frac{1}{\sqrt{i+j}}$	$SCI(G)$
Harmonic [26]	$\frac{2}{i+j}$	$HI(G)$
Augmented Zagreb [9]	$\left(\frac{ij}{i+j-2}\right)^3$	$AZI(G)$
First Zagreb [18]	$i+j$	$M_1(G)$
Albertson [1]	$\lvert i-j\rvert$	$Alb(G)$
Atom-bond-connectivity [8]	$\sqrt{\frac{i+j-2}{ij}}$	$ABC(G)$

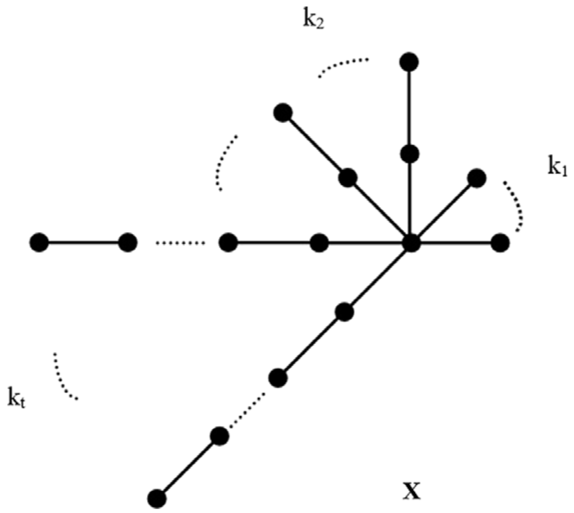

Fig. 1. Starlike tree.

depend on the number of branches of length 1. Then we consider the problem over $\Omega_n = \bigcup_{k=3}^{n-1} \Omega_{n,k}$, (i.e. the set of all starlike trees with n vertices), finding conditions on the numbers $\{\varphi_{ij}\}$ which are easy to verify, under which the extremal values of TI over the set of starlike trees can be calculated. As an application we find the extremal values of many well-known vertex-degree-based topological indices.

2. Vertex-degree-based topological indices over starlike trees

Let P_j denote the path of j vertices. By $S(n_1, \ldots, n_k)$ we denote the starlike tree which has a vertex u of degree $k > 2$ and has the property

$$S(n_1, \ldots, n_k) - u = P_{n_1} \cup P_{n_2} \cdots \cup P_{n_k}$$

where $1 \le n_1 \le n_2 \cdots \le n_k$. We say that the starlike tree $S(n_1, \ldots, n_k)$ has k branches, the lengths of which are $n_1, n_2, \ldots, n_k$, respectively. We denote by $\Omega_{n,k}$ the set of starlike trees with n vertices and k branches. From now on we assume that $n \ge k+1$, so that $\Omega_{n,k} \ne \emptyset$.

Let $X \in \Omega_{n,k}$. For $i \ge 1$ denote by k_i the number of branches of length i that X has. Let t be the length of the largest branch of X (see Fig. 1). The following formulas hold:

$$\left.\begin{aligned} k_1 + k_2 + \cdots + k_t &= k \\ k_1 + 2k_2 + \cdots + tk_t &= n-1 \end{aligned}\right\}. \tag{2}$$

In a first step we study the variation of a vertex-degree-based topological index over $\Omega_{n,k}$.

Theorem 2.1. *Let TI be a vertex-degree-based topological index as in (1) and $X \in \Omega_{n,k}$. Then*

$$TI(X) = k_1 P_k + kQ_k + (n-1)\varphi_{22}$$

where k_1 is the number of branches of length 1 *that* X *has and*

$$P_k = \varphi_{1k} + \varphi_{22} - \varphi_{12} - \varphi_{2k}$$
$$Q_k = \varphi_{12} + \varphi_{2k} - 2\varphi_{22}.$$

Proof. If $X \in \Omega_{n,k}$, then X has only vertices of degree 1, 2 and k. Hence expression (1) simplifies as

$$TI\,(X) = m_{1k}\varphi_{1k} + m_{12}\varphi_{12} + m_{2k}\varphi_{2k} + m_{22}\varphi_{22}. \tag{3}$$

Moreover, it is clear that

$$m_{1k} = k_1$$
$$m_{12} = m_{2k} = k_2 + \cdots + k_t$$
$$m_{22} = k_3 + 2k_4 + \cdots + (t-2)\,k_t.$$

Since

$$k_3 + 2k_4 + \cdots + (t-2)\,k_t + 2\,(k_3 + k_4 + \cdots + k_t) = 3k_3 + 4k_4 + \cdots + tk_t$$

then it follows from relations (2) that

$$m_{1k} = k_1$$
$$m_{12} = m_{2k} = k - k_1$$
$$m_{22} = n - 1 + k_1 - 2k.$$

Consequently by (3)

$$\begin{aligned} TI\,(X) &= k_1\varphi_{1k} + (k-k_1)\,(\varphi_{12}+\varphi_{2k}) + (n-1+k_1-2k)\,\varphi_{22} \\ &= k_1\,(\varphi_{1k}+\varphi_{22}-\varphi_{12}-\varphi_{2k}) + k\,(\varphi_{12}+\varphi_{2k}-2\varphi_{22}) + (n-1)\,\varphi_{22} \\ &= k_1P_k + kQ_k + (n-1)\,\varphi_{22}. \quad \blacksquare \end{aligned}$$

We can now find the extremal values of a vertex-degree-based topological index TI over the set $\Omega_{n,k}$.

Corollary 2.2. *Let TI be a vertex-degree-based topological index as in* (1). *If $P_k \geq 0$ (resp. $P_k \leq 0$), then*

1. *The maximal (resp. minimal) TI-value over $\Omega_{n,k}$ is attained in* $S\left(\underbrace{1,\ldots,1}_{k-1}, n-k\right)$.
2. *The minimal (resp. maximal) TI-value over $\Omega_{n,k}$ is attained in* $S\left(\underbrace{2,\ldots,2}_{k-1}, n+1-2k\right)$ *if $n \geq 2k+1$. If $n < 2k+1$, then the minimal (resp. maximal) TI-value is attained in* $S\left(\underbrace{1,\ldots,1}_{2k+1-n}, \underbrace{2,\ldots,2}_{n-1-k}\right)$.

Proof. By Theorem 2.1

$$TI\,(Y) - TI\,(X) = (k_1\,(Y) - k_1\,(X))\,P_k.$$

Hence if $P_k \geq 0$, then the maximal TI-value is attained in a starlike tree with maximal number of branches of length 1. This is clearly $S\left(\underbrace{1,\ldots,1}_{k-1}, n-k\right)$. On the other hand, the minimal TI-value is attained in starlike trees with minimal number of branches of length 1. If $n \geq 2k+1$, then $S = S\left(\underbrace{2,\ldots,2}_{k-1}, n+1-2k\right)$ satisfies $k_1\,(S) = 0$ and so has minimal TI-value. Otherwise $k+1 \leq n < 2k+1$, and in this case $S\left(\underbrace{1,\ldots,1}_{2k+1-n}, \underbrace{2,\ldots,2}_{n-1-k}\right)$ has minimal number of branches of length 1. This ends the proof when $P_k \geq 0$. The case $P_k \leq 0$ is similar. $\blacksquare$

Note that for $n \geq 2k+1$ any starlike tree of the form $S\,(n_1,\ldots,n_k)$ such that $n_1 + n_2 + \cdots + n_k = n-1$ and $n_i \geq 2$ for each $i = 1,\ldots,k$ satisfies $k_1\,(S) = 0$ and hence has minimal TI-value over $\Omega_{n,k}$.

Table 2
Sign of P_k for the well-known vertex-degree-based topological indices.

Index	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{2}{i+j}$	$\left(\frac{ij}{i+j-2}\right)^3$	$i+j$	$\lvert i-j\rvert$	$\sqrt{\frac{i+j-2}{ij}}$
Sign of P_k	$-$	$-$	$-$	$-$	$-$	0	0	$+$

From now on we denote by Ω_n the set of all starlike trees with n vertices. In other words,

$$\Omega_n = \bigcup_{k=3}^{n-1} \Omega_{n,k}.$$

It is our interest now to determine the extreme values of a vertex-degree-based topological of the form (1) over Ω_n. Locally, we can find the extremal values over $\Omega_{n,k}$, for every $k = 3, \ldots, n-1$, and this will depend on the sign of P_k, as we can see in Corollary 2.2. Surprisingly, all well-known vertex-degree-based topological indices have uniform sign, in other words, either $P_k \geq 0$ or $P_k \leq 0$ for all $k = 3, \ldots, n-1$, as we can see in Example 2.3.

Example 2.3. Table 2 shows the sign of P_k for the list of well-known vertex-degree-based topological indices. We write $+, -$ or 0 depending on if $P_k \geq 0$, $P_k \leq 0$ or $P_k = 0$ holds for all $k \geq 3$, respectively. For instance, if we consider the Randić index induced by the numbers $\varphi_{ij} = \frac{1}{\sqrt{ij}}$, then

$$\begin{aligned} P_k &= \varphi_{1k} + \varphi_{22} - \varphi_{12} - \varphi_{2k} \\ &= \frac{1}{\sqrt{k}} + \frac{1}{2} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2k}} \\ &= -\frac{1}{2\sqrt{k}}\left(\sqrt{2}\sqrt{k} + \sqrt{2} - \sqrt{k} - 2\right) \leq 0 \end{aligned}$$

for all $k \geq 2$.

Note that for the first Zagreb index M_1

$$\begin{aligned} P_k &= \varphi_{1k} + \varphi_{22} - \varphi_{12} - \varphi_{2k} \\ &= (k+1) + 4 - 3 - (k+2) = 0 \end{aligned}$$

for all $k \geq 3$.

For every $k = 3, \ldots, n-1$, let us denote by

$$U_k = S\left(\underbrace{1, \ldots, 1}_{k-1}, n-k\right)$$

and

$$V_k = \begin{cases} S\left(\underbrace{2, \ldots, 2}_{k-1}, n+1-2k\right) & \text{if } n \geq 2k+1 \\ S\left(\underbrace{1, \ldots, 1}_{2k+1-n}, \underbrace{2, \ldots, 2}_{n-1-k}\right) & \text{if } n < 2k+1. \end{cases}$$

Corollary 2.4. *Let TI be a vertex-degree-based topological index as in (1). Then*

1. *If $P_k \geq 0$ for all $3 \leq k \leq n-1$, then the maximal value of TI over Ω_n is $\max_{3\leq k\leq n-1} TI(U_k)$ and the minimal value is $\min_{3\leq k\leq n-1} TI(V_k)$;*
2. *If $P_k \leq 0$ for all $3 \leq k \leq n-1$, then the maximal value of TI over Ω_n is $\max_{3\leq k\leq n-1} TI(V_k)$ and the minimal value is $\min_{3\leq k\leq n-1} TI(U_k)$.*

Proof. Immediate consequence of Corollary 2.2. ∎

Consequently, the problem of finding the extremal values of *TI* over Ω_n reduces to finding the extremal values of *TI* over $\{U_k\}$ or $\{V_k\}$ $(k = 3, \ldots, n-1)$.

Note that $U_{n-1} = S\left(\underbrace{1, \ldots, 1}_{n-2}, 1\right)$ is the star tree on n vertices and $U_3 = S(1, 1, n-3)$ (see Fig. 2).

We will next give conditions on the numbers $\{\varphi_{ij}\}$ which are easy to verify, under which a topological index *TI* of the form (1) attains an extremal value in U_{n-1} (resp. U_3).

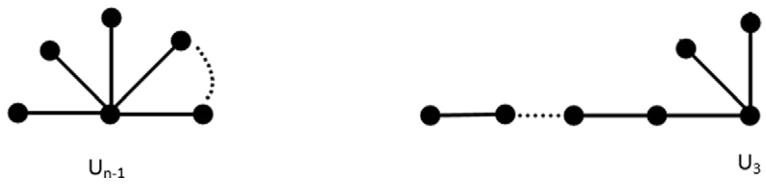

Fig. 2. Extremal starlike trees considered in Theorems 2.5 and 2.6.

Theorem 2.5. *Let TI be a vertex-degree-based topological index as in (1) such that $P_k \leq 0$ for all $3 \leq k \leq n-1$.*

1. *If $\varphi_{1,4} \leq \varphi_{22}$ and $\varphi_{1,k}$ is decreasing on k, then U_{n-1} has minimal TI-value over Ω_n.*
2. *If $\varphi_{1,4} \geq \varphi_{22}$, $\varphi_{1,k}$ is increasing on k and $\varphi_{2,k}$ is also increasing on k, then U_3 has minimal TI-value over Ω_n.*

Proof. 1. By Theorem 2.1, for each $3 \leq k \leq n-2$

$$\begin{aligned} TI\left(U_{n-1}\right) - TI\left(U_k\right) &= (n-1)\, P_{n-1} + (n-1)\, Q_{n-1} - (k-1)\, P_k - kQ_k \\ &= (n-1)\left(\varphi_{1,n-1} - \varphi_{22}\right) - k\left(\varphi_{1,k} - \varphi_{22}\right) + P_k. \end{aligned} \tag{4}$$

Since $k < n-1$ and $\varphi_{1,k}$ is decreasing on k, $\varphi_{1,n-1} - \varphi_{22} \leq \varphi_{1,4} - \varphi_{22} \leq 0$. It follows from (4) that

$$\begin{aligned} TI\left(U_{n-1}\right) - TI\left(U_k\right) &< k\left(\varphi_{1,n-1} - \varphi_{22}\right) - k\left(\varphi_{1,k} - \varphi_{22}\right) + P_k \\ &= k\left(\varphi_{1,n-1} - \varphi_{1,k}\right) + P_k \leq P_k \leq 0. \end{aligned}$$

Hence $TI\left(U_{n-1}\right) = \min_{3 \leq k \leq n-1} TI\left(U_k\right)$ and so by part 2 of Corollary 2.4 it follows that U_{n-1} has minimal TI-value over Ω_n.
2. By Theorem 2.1, for each $4 \leq k \leq n-1$

$$\begin{aligned} TI\left(U_k\right) - TI\left(U_3\right) &= (k-1)\, P_k + kQ_k - 2P_3 - 3Q_3 \\ &= (k-1)\left(\varphi_{1,k} - \varphi_{22}\right) - 2\left(\varphi_{1,3} - \varphi_{22}\right) + \left(\varphi_{2,k} - \varphi_{23}\right). \end{aligned} \tag{5}$$

Since $k > 3$ and $\varphi_{1,k}$ is increasing on k, $\varphi_{1,k} - \varphi_{22} \geq \varphi_{1,4} - \varphi_{22} \geq 0$. It follows from (5) and the fact that $\varphi_{2,k}$ is also increasing on k that

$$\begin{aligned} TI\left(U_k\right) - TI\left(U_3\right) &> 2\left(\varphi_{1,k} - \varphi_{22}\right) - 2\left(\varphi_{1,3} - \varphi_{22}\right) + \left(\varphi_{2,k} - \varphi_{23}\right) \\ &= 2\left(\varphi_{1,k} - \varphi_{1,3}\right) + \left(\varphi_{2,k} - \varphi_{23}\right) \geq 0. \end{aligned}$$

Hence $TI\left(U_3\right) = \min_{3 \leq k \leq n-1} TI\left(U_k\right)$ and so by part 2 of Corollary 2.4 it follows that U_3 has minimal TI-value over Ω_n. ■

Dually we have the following result:

Theorem 2.6. *Let TI be a vertex-degree-based topological index as in (1) such that $P_k \geq 0$ for all $3 \leq k \leq n-1$.*

1. *If $\varphi_{1,4} \geq \varphi_{22}$ and $\varphi_{1,k}$ is increasing on k, then U_{n-1} has maximal TI-value over Ω_n.*
2. *If $\varphi_{1,4} \leq \varphi_{22}$, $\varphi_{1,k}$ is decreasing on k and $\varphi_{2,k}$ is also decreasing on k, then U_3 has maximal TI-value over Ω_n.*

Proof. Similar to the proof of Theorem 2.5. ■

Example 2.7. Consider the augmented Zagreb index induced by the numbers $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$. We will see that this index satisfies the hypothesis of Theorem 2.5 part 1. We already checked in Example 2.3 that $P_k \leq 0$ for all $k \geq 3$. Moreover,

$$\varphi_{14} = \left(\frac{4}{3}\right)^3 \leq 8 = \varphi_{22}$$

and $\varphi_{1k} = \left(\frac{k}{k-1}\right)^3$ as a function of k has derivative $-3\frac{k^2}{(k-1)^4} \leq 0$ for all $k \geq 3$. Hence φ_{1k} is decreasing on k. It is easy to check that the Randić index, the geometric–arithmetic index, the sum-connectivity index, the harmonic index also satisfy the hypothesis of Theorem 2.5 part 1. Hence for all these indices, the star tree U_{n-1} has minimal value over Ω_n.

On the other hand, consider the atom-bond-connectivity index ABC determined by $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$. We know from Example 2.3 that $P_k \geq 0$ for all $k \geq 3$. Furthermore,

$$\varphi_{14} = \sqrt{\frac{3}{4}} \geq \frac{1}{\sqrt{2}} = \varphi_{22}$$

and $\varphi_{1k} = \sqrt{\frac{k-1}{k}}$ as a function of k has derivative $\frac{1}{2k^2\sqrt{\frac{1}{k}(k-1)}}$, which is clearly positive for all $k \geq 3$. Hence $\varphi_{1,k}$ is increasing on k. Similarly, the first Zagreb index M_1 and the Albertson index Alb satisfy the hypothesis of Theorem 2.6 part 1. Consequently, for these indices U_{n-1} has maximal value over Ω_n.

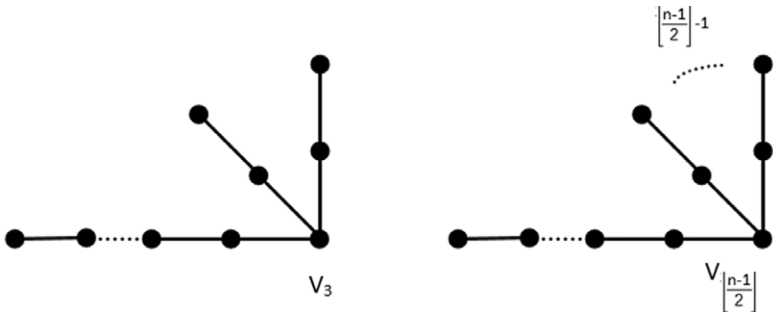

Fig. 3. Extremal starlike trees considered in Theorems 2.8 and 2.9.

We can also give conditions on the numbers $\{\varphi_{ij}\}$ which can be easily verified, under which a topological index TI of the form (1) attains an extremal value in V_3 (resp. $V_{\lfloor \frac{n-1}{2} \rfloor}$). Note that $V_3 = S(2, 2, n-5)$ and

$$V_{\lfloor \frac{n-1}{2} \rfloor} = S\left(\underbrace{2, \dots, 2}_{\lfloor \frac{n-1}{2} \rfloor - 1}, n + 1 - 2\left\lfloor \frac{n-1}{2} \right\rfloor\right) \text{ (see Fig. 3).}$$

Theorem 2.8. *Let TI be a vertex-degree-based topological index as in (1) such that $P_k \le 0$ for all $3 \le k \le n-1$.*

1. *If kQ_k is decreasing on k, then V_3 has maximal TI-value over Ω_n.*
2. *If kQ_k is increasing on k, $\varphi_{1,4} \le \varphi_{22}$, $\varphi_{1,k}$ is decreasing on k and $\varphi_{2,k}$ is also decreasing on k, then $V_{\lfloor \frac{n-1}{2} \rfloor}$ has maximal TI-value over Ω_n.*

Proof. 1. By Theorem 2.1, for every k such that $n \ge 2k+1$

$$TI(V_3) - TI(V_k) = 3Q_3 - kQ_k. \tag{6}$$

On the other hand, if k is such that $n < 2k+1$, then

$$\begin{aligned} TI(V_3) - TI(V_k) &= 3Q_3 - kQ_k - (2k+1-n)P_k \\ &\ge 3Q_3 - kQ_k \end{aligned} \tag{7}$$

since $2k+1-n > 0$ and $P_k \le 0$ for all $k = 3, \dots, n-1$. Hence for all $k = 3, \dots, n-1$

$$TI(V_3) - TI(V_k) \ge 3Q_3 - kQ_k.$$

Now, since kQ_k is decreasing on k, $kQ_k \le 3Q_3$ for all $3 \le k \le n-1$ and we conclude that $TI(V_3) \ge TI(V_k)$ for all $k = 3, \dots, n-1$. In other words, $TI(V_3) = \max_{3 \le k \le n-1} TI(V_k)$ and so by part 2 of Corollary 2.4, V_3 has maximal TI-value over Ω_n.

2. By Theorem 2.1, for every k such that $n \ge 2k+1$

$$TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) - TI(V_k) = \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - kQ_k. \tag{8}$$

Since kQ_k is increasing on k, $TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) \ge TI(V_k)$, for every k, such that $n \ge 2k+1$.

On the other hand, if k is such that $n < 2k+1$ then

$$\begin{aligned} TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) - TI(V_k) &= \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - kQ_k - (2k+1-n)P_k \\ &= \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - (n-1-k)Q_k - (2k+1-n)(\varphi_{1k} - \varphi_{22}) \\ &\ge \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - (n-1-k)Q_k \end{aligned} \tag{9}$$

since $2k+1-n > 0$ and $\varphi_{1k} \le \varphi_{14} \le \varphi_{22}$ for all $k = 3, \dots, n-1$. Now, since φ_{2k} is decreasing on k and $n-1-k < k$, we have that $Q_k \le Q_{n-1-k}$. Considering that kQ_k is increasing on k and the fact that $n-1-k \le \left\lfloor \frac{n-1}{2} \right\rfloor$ we obtain

Table 3
Extremal starlike trees of the well-known vertex-degree-based topological indices.

Index	$\frac{1}{\sqrt{ij}}$	$\frac{2\sqrt{ij}}{i+j}$	$\frac{1}{\sqrt{i+j}}$	$\frac{2}{i+j}$	$\left(\frac{ij}{i+j-2}\right)^3$	$i+j$	$\lvert i-j\rvert$	$\sqrt{\frac{i+j-2}{ij}}$
Maximal	V_3	V_3	V_3	V_3	V_3	U_{n-1}	U_{n-1}	U_{n-1}
Minimal	U_{n-1}	U_{n-1}	U_{n-1}	U_{n-1}	U_{n-1}	V_3	V_3	V_3

$$TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) - TI\left(V_k\right) \geq \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - (n-1-k)\, Q_{n-1-k} \geq 0.$$

Hence $TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) = \max_{3\leq k\leq n-1} TI\left(V_k\right)$ and so by part 2 of Corollary 2.4, $V_{\lfloor \frac{n-1}{2} \rfloor}$ has maximal TI-value over Ω_n. ■

The dual result of Theorem 2.8 is as follows:

Theorem 2.9. *Let TI be a vertex-degree-based topological index as in (1) such that $P_k \geq 0$ for all $3 \leq k \leq n-1$.*

1. *If kQ_k is increasing on k, then V_3 has minimal TI-value over Ω_n.*
2. *If kQ_k is decreasing on k, $\varphi_{1,4} \geq \varphi_{22}$, $\varphi_{1,k}$ is increasing on k and $\varphi_{2,k}$ is also increasing on k, then $V_{\lfloor \frac{n-1}{2} \rfloor}$ has minimal TI-value over Ω_n.*

Proof. 1. Using relations (6) and (7) and the fact that $2k+1-n > 0$ and $P_k \geq 0$ for all $k = 3, \ldots, n-1$, we deduce that

$$TI\left(V_3\right) - TI\left(V_k\right) \leq 3Q_3 - kQ_k$$

for all $k = 3, \ldots, n-1$. Now since $kQ_k \geq 3Q_3$ for all $3 \leq k \leq n-1$, it follows that $TI\left(V_3\right) \leq TI\left(V_k\right)$ for all $k = 3, \ldots, n-1$, and so $TI\left(V_3\right) = \min_{3\leq k\leq n-1} TI\left(V_k\right)$. Consequently, by part 1 of Corollary 2.4, V_3 has minimal TI-value over Ω_n.

2. Using relation (8) and the fact that kQ_k is decreasing on k, we obtain that $TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) \leq TI\left(V_k\right)$ for every k, such that $n \geq 2k+1$.

On the other hand, if k is such that $n < 2k+1$, then using relation (9), the fact that φ_{2k} and kQ_k are increasing on k and taking into account that $\varphi_{1k} \geq \varphi_{14} \geq \varphi_{22}$ for all $k = 3, \ldots, n-1$ we obtain

$$TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) - TI\left(V_k\right) \leq \left\lfloor \frac{n-1}{2} \right\rfloor Q_{\lfloor \frac{n-1}{2} \rfloor} - (n-1-k)\, Q_{n-1-k} \leq 0.$$

Hence $TI\left(V_{\lfloor \frac{n-1}{2} \rfloor}\right) = \min_{3\leq k\leq n-1} TI\left(V_k\right)$ and so by part 2 of Corollary 2.4, $V_{\lfloor \frac{n-1}{2} \rfloor}$ has minimal TI-value over Ω_n. ■

Example 2.10. The harmonic index satisfies the hypothesis of Theorem 2.8 since $P_k \leq 0$ for all $3 \leq k \leq n-1$ (Example 2.3) and

$$\begin{aligned}(k+1)\, Q_{k+1} - kQ_k &= (k+1)\left(\frac{2}{3} + \frac{2}{k+3} - \frac{4}{4}\right) - k\left(\frac{2}{3} + \frac{2}{k+2} - \frac{4}{4}\right) \\ &= -\frac{1}{3} + \frac{4}{(k+3)\,(k+2)} \leq 0\end{aligned}$$

for all $k \geq 3$. Similarly, it is easy to check that the Randić index, the geometric–arithmetic index, the sum-connectivity index and the augmented Zagreb index all satisfy the hypothesis of Theorem 2.8. Hence for all these indices, the star tree V_3 has maximal TI-value over Ω_n.

On the other hand, the Albertson index Alb satisfies the hypothesis of Theorem 2.9 since

$$(k+1)\, Q_{k+1} - kQ_k = (k+1)\, k - k(k-1) = 2k \geq 0$$

for all $k \geq 3$. Also the atom-bond-connectivity index ABC and the first Zagreb index M_1 satisfy the hypothesis of Theorem 2.9. Consequently, for these indices V_3 has the minimal value over Ω_n.

From Examples 2.7 and 2.10 we can complete the extremal starlike trees of the most important vertex-degree-based topological indices over Ω_n (see Table 3).

We end this section studying the extremal values of the general Randić index R_α [2] over Ω_n. Recall that R_α is determined by $\varphi_{ij} = (ij)^\alpha$, where α is a real number. Then

$$\begin{aligned}P_k &= \varphi_{1k} + \varphi_{22} - \varphi_{12} - \varphi_{2k} \\ &= k^\alpha + 4^\alpha - 2^\alpha - 2^\alpha k^\alpha \\ &= \left(k^\alpha - 2^\alpha\right)\left(1 - 2^\alpha\right) < 0\end{aligned}$$

for all $\alpha \neq 0$.

Note that for $\alpha \leq 0$, the general Randić satisfies the hypothesis of Theorem 2.5 part 1, since $\varphi_{1k} = k^\alpha$ is decreasing on k and $\varphi_{14} = (4)^\alpha = \varphi_{22}$. Hence, the star tree U_{n-1} has minimal value over Ω_n.

For the case $\alpha > 0$, the general Randić satisfies the hypothesis of Theorem 2.5 part 2, since both $\varphi_{1k} = k^\alpha$ and $\varphi_{2k} = 2^\alpha k^\alpha$ are increasing on k and $\varphi_{14} = (4)^\alpha = \varphi_{22}$. Hence, the tree U_3 has minimal value over Ω_n.

In order to find the maximal value of the general Randić over Ω_n, note that for the case $-1 \leq \alpha \leq 0$, it satisfies the hypothesis of Theorem 2.8 part 1, since $P_k \leq 0$ for all $3 \leq k \leq n-1$ and the difference

$$\begin{aligned}(k+1)Q_{k+1} - kQ_k &= (k+1)\left(2^\alpha + 2^\alpha (k+1)^\alpha - 2^{2\alpha+1}\right) - k\left(2^\alpha + 2^\alpha k^\alpha - 2^{2\alpha+1}\right) \\ &= 2^\alpha \left[(k+1)^{\alpha+1} - k^{\alpha+1} - 2^{\alpha+1} + 1\right] \qquad (10)\end{aligned}$$

is nonnegative. Hence, the star tree V_3 has maximal general Randić index over Ω_n.

For the case $\alpha < -1$, using relation (10) it is easy to check that kQ_k is increasing on k. Since in this case, $\varphi_{1,4} = 4^\alpha = \varphi_{22}$, $\varphi_{1,k} = k^\alpha$ is decreasing on k and $\varphi_{2,k} = 2^\alpha k^\alpha$ is also decreasing on k then, by Theorem 2.8 part 2, $V_{\left\lfloor \frac{n-1}{2} \right\rfloor}$ has maximal value over Ω_n.

For the case $\alpha > 0$, we have that kQ_k is also increasing on k, but we cannot apply Theorem 2.8 part 2 since $\varphi_{1,k}$ and $\varphi_{2,k}$ are increasing on k. In this case, we can only guarantee that

$$\max_{3 \leq k \leq n-1} R_\alpha (V_k) \geq R_\alpha \left(V_{\left[\frac{n-1}{2}\right]}\right)$$

and the maximal is attained in a tree of type V_k with $k \geq \left[\frac{n-1}{2}\right]$. For example, for $\alpha = 4$ and $n = 100$, it is easy to check computationally that the maximal value is attained in the tree V_{85}.

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