On the zeroth-order general Randić index, variable sum exdeg index and trees having vertices with prescribed degree

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February 20, 2018

Abstract

The zeroth-order general Randić index (usually denoted by \( R_0^\alpha \)) and variable sum exdeg index (denoted by \( SEI_a \)) of a graph \( G \) are defined as
\[
R_0^\alpha (G) = \sum_{v \in V(G)} (d_v)^\alpha
\]
and
\[
SEI_a (G) = \sum_{v \in V(G)} d_v a^{d_v}
\]
where \( d_v \) is degree of the vertex \( v \in V(G) \), \( a \) is a positive real number different from 1 and \( \alpha \) is a real number other than 0 and 1. A segment of a tree is a path \( P \), whose terminal vertices are branching or pendent, and all non-terminal vertices (if exist) of \( P \) have degree 2. For \( n \geq 6 \), let \( PT_{n,n_1}, ST_{n,k}, BT_{n,b} \) be the collections of all \( n \)-vertex trees having \( n_1 \) pendant vertices, \( k \) segments, \( b \) branching vertices, respectively. In this paper, all the trees with extremum (maximum and minimum) zeroth-order general Randić index and variable sum exdeg index are determined from the collections \( PT_{n,n_1}, ST_{n,k}, BT_{n,b} \). The obtained extremal trees for the collection \( ST_{n,k} \) are also extremal trees for the collection of all \( n \)-vertex trees having fixed number of vertices with degree 2 (because it is already known that the number of segments of a tree \( T \) can be determined from the number of vertices of \( T \) with degree 2 and vise versa).

1 Introduction

Let \( G = (V(G), E(G)) \) be a finite and simple graph, where \( V(G) \) and \( E(G) \) are the nonempty sets, known as vertex set and edge set respectively. For a vertex \( v \in V(G) \), degree of \( v \) is denoted by \( d_v \) and is defined as the number of vertices adjacent to \( v \). Undefined terminologies and notations can be found in [5, 8].

“A molecular descriptor is the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into an useful number or the result of some standardized experiment” [25]. A topological index is a type of molecular descriptor based on the molecular graph of chemical compounds [3]. In graph theoretic words, topological indices are numerical quantities which are invariant under graph isomorphism [4]. The Randić index [21] (devised in 1975 for measuring the branching of molecules) and first Zagreb index [12] (appeared in 1972 within the study of total \( \pi \)-electron energy of molecules) are among the most studied topological indices [10]. Kier and Hall [14] proposed the zeroth order Randić index. In 2005, general first Zagreb index (also known as the zeroth-order general Randić index) was introduced by Li and Zheng [15]. The zeroth-order general Randić index is denoted by \( R_0^\alpha \) and is defined as:
\[
R_0^\alpha (G) = \sum_{v \in V(G)} (d_v)^\alpha
\]
where $\alpha$ is a real number other than 0 and 1. Indeed, $R^0_\alpha$ reduces to first Zagreb index and zeroth-order Randić index for $\alpha = 2$ and $\alpha = -\frac{1}{2}$, respectively. The topological index $R^0_\alpha$ has attracted a considerable attention from mathematicians, for example see the papers [1][3][8][20][23][29], particularly the recent ones [7][22][24][26] and related reference listed therein.

Variable sum exdeg index, introduced by Vukičević [27] in 2011, is denoted by $SEI_a$ and is defined as:

$$SEI_a(G) = \sum_{v \in V(G)} d_v a^{d_v},$$

where $a$ is any positive real number such that $a \neq 1$. The topological index $SEI_a$ is very well correlated with octanol-water partition coefficient of octane isomers [27]. Detail about the chemical applicability and mathematical properties of this index can be found in the references [2][9][27][28][30].

A vertex having degree 1 is called pendent vertex and a vertex which have degree greater than 2 is named as branching vertex. A segment of a tree is a path subtree branching vertices, is solved. The number of segments of a tree is very well correlated with octanol-water partition coefficient of octane isomers [27]. Detail about the chemical applicability and mathematical properties of this index can be found in the references [2][9][27][28][30].

Denote by $\mathcal{PT}_{n,1}$ the collection of all $n$-vertex trees having fixed (i) pendent vertices (ii) segments (iii) branching vertices. Clearly, 2 $\leq n_1 \leq n - 1$. Both the collections $\mathcal{PT}_{n,2}$ and $\mathcal{PT}_{n,n-1}$ contain only one graph, namely, the path graph $P_n$ and star graph $S_n$, respectively. Thereby, in order to make the extremal problem well defined we always take $3 \leq n_1 \leq n - 2$.

The trees with extremum $SEI_a$ values from the collection $\mathcal{PT}_{n,n_1}$ have already been determined in [28] for $a > 1$. Thereby, in this section, we solve this problem concerning $SEI_a$ for $0 < a < 1$, which gives a partial solution of a problem posed in [28].

**Lemma 2.1.** If $T \in \mathcal{PT}_{n,n_1}$ contains more than one branching vertex then there exist a tree $T' \in \mathcal{PT}_{n,n_1}$ such that $SEI_a(T) > SEI_a(T')$ for $0 < a < 1$ and

$$R^0_\alpha(T) \begin{cases} < R^0_\alpha(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > R^0_\alpha(T') & \text{if } 0 < \alpha < 1. \end{cases}$$

**Proof.** Let $u,v \in V(T)$ be branching vertices such that $d_u \geq d_v$. Let $w$ be the neighbor of $v$ which does not lie on the unique $u-v$ path. Take $T' = T - uv + uw$ then Lagrange’s mean value theorem guaranties the existence of numbers $\Theta_1, \Theta_2$ such that $d_v - 1 < \Theta_1 < d_v \leq d_u < \Theta_2 < d_u + 1$ and

$$SEI_a(T) - SEI_a(T') = d_v a^{d_v} - (d_v - 1)a^{d_v - 1} - [(d_u + 1)a^{d_u + 1} - d_u a^{d_u}]$$

$$= a^{\Theta_1}(1 + \Theta_1 \ln a) - a^{\Theta_2}(1 + \Theta_2 \ln a)$$

(1)
From the inequalities $\Theta_1 < \Theta_2$ and $0 < a < 1$, it follows that
\[ a^{\Theta_1}(1 + \Theta_1 \ln a) > a^{\Theta_1}(1 + \Theta_2 \ln a) > a^{\Theta_2}(1 + \Theta_2 \ln a), \]
which together with Equation \((\ref{eq:inequality})\) implies that $SEI_a(T) > SEI_a(T')$ for $0 < a < 1$.

Again, by virtue of Lagrange’s mean value theorem there exist numbers $\Theta_3, \Theta_4$ such that $d_v - 1 < \Theta_3 < d_v < d_u < \Theta_4 < d_v + 1$ and
\[
R_0^0(T) - R_0^0(T') = (d_u)^\alpha - (d_v - 1)^\alpha - [(d_u + 1)^\alpha - (d_u)^\alpha] \\
= \alpha(\Theta_3^{\alpha-1} - \Theta_4^{\alpha-1}) \\
\begin{cases} < 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > 0 & \text{if } 0 < \alpha < 1. \end{cases}
\]

This completes the proof.

If $V(G) = \{v_1, v_2, \ldots, v_n\}$ such that $d_{v_1} \geq d_{v_2} \geq \cdots \geq d_{v_n}$ then the sequence $\pi = (d_{v_1}, d_{v_2}, \ldots, d_{v_n})$ is called degree sequence of $G$.

**Theorem 2.2.** If $T \in \mathbb{PT}_{n,n_1}$ then $SEI_a(T) \geq 2a^2n + (a^{n_1} - 2a^2 + a)n_1 - 2a^2$ for $0 < a < 1$ and
\[
R_0^0(T) \begin{cases} < 2^\alpha n + (n_1)^\alpha - (2^\alpha - 1)n_1 - 2^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > 2^\alpha n + (n_1)^\alpha - (2^\alpha - 1)n_1 - 2^\alpha & \text{if } 0 < \alpha < 1. \end{cases}
\]

The equality sign in any of the above inequalities holds if and only if $T$ has the degree sequence \((n_1, 2, \ldots, 2, 1, \ldots, 1)\) for all non-\(\Theta\)\(\alpha\)\(\Theta\).2.1

**Proof.** The result directly follows from Lemma \(\ref{lemma:degree_sequence}\). \(\square\)

**Lemma 2.3.** If $T \in \mathbb{PT}_{n,n_1}$ contains two non-pendent vertices $u, v$ such that $d_u \geq d_v + 2$ then there exist $T' \in \mathbb{PT}_{n,n_1}$ such that $SEI_a(T) < SEI_a(T')$ for $0 < a < 1$ and
\[
R_0^0(T) \begin{cases} < R_0^0(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > R_0^0(T') & \text{if } 0 < \alpha < 1. \end{cases}
\]

**Proof.** Let $w$ be the neighbor of $u$ which does not lie on the unique $u-v$ path. If $T' = T - uw + vw$ then there exist numbers $\Theta_1, \Theta_2$ such that $d_v < \Theta_1 < d_v + 1 \leq d_u - 1 < \Theta_2 < d_u$ and
\[
SEI_a(T) - SEI_a(T') = d_u a^{d_u} - (d_u - 1)a^{d_u-1} - [(d_u + 1)a^{d_u+1} - d_v a^{d_v}] \\
= \alpha^{\Theta_2}(1 + \Theta_2 \ln a) - a^{\Theta_1}(1 + \Theta_1 \ln a) < 0. \tag{2}
\]
There also exist numbers $\Theta_3, \Theta_4$ such that $d_v < \Theta_3 < d_v + 1 \leq d_u - 1 < \Theta_4 < d_u$ and
\[
R_0^0(T) - R_0^0(T') = (d_u)^\alpha - (d_v - 1)^\alpha - [(d_v + 1)^\alpha - (d_v)^\alpha] \\
= \alpha(\Theta_3^{\alpha-1} - \Theta_4^{\alpha-1}) \\
\begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases}
\]

This completes the proof. \(\square\)

**Lemma 2.4.** \(\square\) If $T \in \mathbb{PT}_{n,n_1}$ such that the inequality $|d_u - d_v| \leq 1$ holds for all non-pendent vertices $u, v \in V(T)$, then $n_t = (n - n_1)t - n_1 + 2$ and $n_{t+1} = n - (n - n_1)t - 2$ where $t = \left\lfloor \frac{n_2}{n-n_1} \right\rfloor + 1$.\(\square\)
Theorem 3.3. If $T \in PT_{n,n_1}$ and $t = \left\lfloor \frac{n-2}{n-n_1} \right\rfloor + 1$ then

$$SEI_a(T) \leq [(n-n_1)t - n_1 + 2]a^t + [n - (n-n_1)t - 2](t+1)a^{t+1} + n_1a \quad \text{for} \quad 0 < a < 1$$

and

$$R_a^0(T) \begin{cases} 
> [n - (n-n_1)t - n_1 + 2]a^t + [n - (n-n_1)t - 2](t+1)a^{t+1} + n_1a & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\
< [(n-n_1)t - n_1 + 2]a^t + [n - (n-n_1)t - 2](t+1)a^{t+1} + n_1a & \text{if } 0 < \alpha < 1.
\end{cases}$$

The equality sign in any of the above inequalities holds if and only if $T$ has the degree sequence $(t+1, \cdots, t+1, t, \cdots, t, 1, \cdots, 1)$.

Proof. From Lemma 2.3 and Lemma 2.4, the desired result follows. \qed

3 Zeroth-order general Randić index, variable sum exdeg index and branching vertices of trees

For $n \geq 6$, let $BT_{n,b}$ be the collection of all $n$-vertex trees with branching vertices $b$. It is known that $b \leq \frac{n}{2} - 1$ [16]. Throughout this section we take $1 \leq b \leq \frac{n}{2} - 1$ because the set $BT_{n,0}$ contains only one graph, namely the path graph $P_n$.

Lemma 3.1. If $T \in BT_{n,b}$ contains a vertex having degree greater than 3 then there is a tree $T' \in BT_{n,b}$ such that

$$SEI_a(T) > SEI_a(T') \quad \text{if } \alpha > 1,$$

$$< SEI_a(T') \quad \text{if } 0 < \alpha < 1.$$ 

and

$$R_a^0(T) \begin{cases} 
> R_a^0(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\
< R_a^0(T') & \text{if } 0 < \alpha < 1.
\end{cases}$$

Proof. Let $u \in V(T)$ be a vertex having degree greater than 3. Let $P = v_0v_1 \cdots v_{r+1}$ be a longest path in $T$ containing $u$, where $u = v_i$ for some $i \in \{1, 2, \cdots, r\}$. Let $w$ be a neighbor of $u$ different from both $v_{i-1}, v_{i+1}$. If $T' = T - uw + wv_{i+1}$ then

$$SEI_a(T) - SEI_a(T') = d_u a^{d_u} - (d_u - 1)a^{d_u-1} - (2a^2 - a)$$

$$= a^{\Theta_2(1 + \Theta_2 \ln a)} - a^{\Theta_1(1 + \Theta_1 \ln a)}$$

$$\begin{cases} 
> 0 & \text{if } \alpha > 1, \\
< 0 & \text{if } 0 < \alpha < 1,
\end{cases}$$

where $1 < \Theta_1 < 2 < d_u - 1 < \Theta_2 < d_u$. Also, we have

$$R_a^0(T) - R_a^0(T') = (d_u)^\alpha - (d_u - 1)^\alpha - (2^\alpha - 1)$$

$$\begin{cases} 
> 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\
< 0 & \text{if } 0 < \alpha < 1.
\end{cases}$$

Lemma 3.2. If $T \in BT_{n,b}$ has maximum degree 3 then $n_1 = b + 2$ and $n_2 = n - 2b - 2$.

Theorem 3.3. If $T \in BT_{n,b}$ then

$$SEI_a(T) \begin{cases} 
\geq 2a^2n + (3a^3 - 4a^2 + a)b - 2a(2a - 1) & \text{if } \alpha > 1, \\
\leq 2a^2n + (3a^3 - 4a^2 + a)b - 2a(2a - 1) & \text{if } 0 < \alpha < 1
\end{cases}$$
Proof. The result follows from Lemma 3.1 and Lemma 3.2 \[ \square \]

**Lemma 3.4.** If \( T \in \mathbb{BT}_{n,b} \) contains two or more vertices having degree greater than 3 then there exist \( T' \in \mathbb{BT}_{n,b} \) such that

\[
R_0^0(T) \begin{cases} < R_0^0(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > R_0^0(T) & \text{if } 0 < \alpha < 1. \end{cases}
\]

and

\[
SEI_\alpha(T) \begin{cases} < SEI_\alpha(T') & \text{if } a > 1, \\ > SEI_\alpha(T') & \text{if } 0 < a < 1. \end{cases}
\]

Proof. Let \( u, v \in V(T) \) such that \( d_u \geq d_v \geq 4 \). Suppose \( N_T(v) = \{v_1, v_2, \ldots, v_{r-1}, v_r\} \) and let \( u \) be connected to \( v \) through \( v_r \) (it is possible that \( u = v_r \)). If \( T' = T - \{uv_1, uv_2, \ldots, uv_{r-3}\} + \{uv, uv_2, \ldots, uv_r\} \) then

\[
R_0^0(T) - R_0^0(T') = (d_v)^{\alpha} - (d_u)^{\alpha} - [(d_u + d_v - 3)^{\alpha} - (d_u)^{\alpha}]
\]

\[
= \alpha(d_v - 3)(\Theta_1 - \Theta_2^{a-1})
\]

\[
\begin{cases} < 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > 0 & \text{if } 0 < \alpha < 1. \end{cases}
\]

where \( 3 < \Theta_1 < d_u < \Theta_2 < d_u + d_v - 3 \). Also, we have

\[
SEI_\alpha(T) - SEI_\alpha(T') = d_v a^{d_v - 3} - [(d_u + d_v - 3)^{d_u + d_v - 3} - d_u a^{d_u}]
\]

\[
= (d_v - 3)[a^{\Theta_3}(1 + \Theta_3 \ln a) - a^{\Theta_4}(1 + \Theta_4 \ln a)]
\]

\[
\begin{cases} < 0 & \text{if } a > 1, \\ > 0 & \text{if } 0 < a < 1, \end{cases}
\]

where \( 3 < \Theta_3 < d_v < \Theta_4 < d_u + d_v - 3 \). \[ \square \]

**Lemma 3.5.** If \( T \in \mathbb{BT}_{n,b} \) contains at least one vertex of degree 2 then there is \( T' \in \mathbb{BT}_{n,b} \) such that

\[
R_0^0(T) \begin{cases} < R_0^0(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > R_0^0(T) & \text{if } 0 < \alpha < 1. \end{cases}
\]

and

\[
SEI_\alpha(T) \begin{cases} < SEI_\alpha(T') & \text{if } a > 1, \\ > SEI_\alpha(T') & \text{if } 0 < a < 1. \end{cases}
\]

Proof. The assumption \( b \geq 1 \) implies that there exist two adjacent vertices \( u, v \in V(T) \) such that \( d_u \geq 3 \) and \( d_v = 2 \). Let \( N_T(v) = \{u, w\} \) and \( T' = T - vw + uw \). Now, the desired result easily follows by observing the differences \( R_0^0(T) - R_0^0(T') \) and \( SEI_\alpha(T) - SEI_\alpha(T') \). \[ \square \]

**Lemma 3.6.** If \( T \in \mathbb{BT}_{n,b} \) has no vertex of degree 2 and has at most one vertex of degree greater than 3 then \( T \) has the degree sequence \( (n-2b+1, 3, \ldots, 3, 1, \ldots, 1) \).
The equality sign in the inequality holds if and only if

Proof. The result follows from Lemma 3.4, Lemma 3.5 and Lemma 3.6.

4 Zeroth-order general Randić index, variable sum exdeg index and segments of trees

For \( n \geq 6 \), denote by \( \mathbb{S}T_{n,k} \) the set of all \( n \)-vertex trees with \( k \) segments. Throughout this section we take \( 3 \leq k \leq n-2 \) because \( \mathbb{S}T_{n,1} = \{P_n\}, \mathbb{S}T_{n,n-1} = \{S_n\} \) and the set \( \mathbb{S}T_{n,2} \) is empty.

Squeeze of an \( n \)-vertex tree \( T \) (is denoted by \( S(T) \)) is a tree obtained from \( T \) by replacing each segment with an edge \([7] \). Hence

\[
k = |E(S(T))| = |V(S(T))| - 1 = n - n_2 - 1
\]

(3)

By an even-prime vertex we mean a vertex with degree 2. From Equation (3) it is clear that the problem of finding extremal trees from the collection \( \mathbb{S}T_{n,k} \) is equivalent to the problem of finding extremal trees from the collection of all \( n \)-vertex trees with fixed even-prime vertices.

Lemma 4.1. [28] If \( T \) is an \( n \)-vertex tree then

\[
SEI_a(T) \leq (n - 1)a^{n-1} + (n - 1)a
\]

for \( a > 1 \) and \( n \geq 4 \). The equality sign in the inequality holds if and only if \( T \cong S_n \).

Lemma 4.2. [25] For \( n \geq 4 \), if \( T \) is an \( n \)-vertex tree then

\[
R_a^0(T) \begin{cases} 
\leq (n - 1)^a + (n - 1) & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\
\geq (n - 1)^a + (n - 1) & \text{if } 0 < \alpha < 1.
\end{cases}
\]

The equality sign in the inequality holds if and only if \( T \cong S_n \).

Theorem 4.3. If \( T \in \mathbb{S}T_{n,k} \) then

\[
R_a^0(T) \begin{cases} 
\leq 2^n n + k^a - (2^a - 1)k - 2^a & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\
\geq 2^n n + k^a - (2^a - 1)k - 2^a & \text{if } 0 < \alpha < 1,
\end{cases}
\]

and

\[
SEI_a(T) \leq 2^n a + k^a - (2a - 1)ak - 2^a
\]

for \( a > 1 \). The equality sign in any of the above inequalities holds if and only if \( T \) has the degree sequence \((k, 2, ..., 2, 1, ..., 1)\).
Proof. By definition of the squeeze of a tree, zeroth-order general Randić index and variable sum exdeg index, we have
\[ R_0^0(T) = R_0^0(S(T)) + 2\alpha n_2 \] (4)
and
\[ SEI_a(T) = SEI_a(S(T)) + 2\alpha^2 n_2. \] (5)
From Equation (3), we have \( n_2 = n - k - 1 \) and hence from Equation (4) and Equation (5) it follow that
\[ R_0^0(T) = R_0^0(S(T)) + 2\alpha (n - k - 1) \] (6)
and
\[ SEI_a(T) = SEI_a(S(T)) + 2\alpha^2 (n - k - 1). \] (7)
Since \( S(T) \) has \( n - n_2 = k + 1 \) vertices. So, by Lemma 4.1 and Lemma 4.2, we have
\[ SEI_a(S(T)) \leq ka^k + ka \quad \text{and} \quad R_0^0(S(T)) \leq k^\alpha + k \] if \( \alpha < 0 \) or \( \alpha > 1 \),
\[ R_0^0(S(T)) \geq k^\alpha + k \] if \( 0 < \alpha < 1 \),
where \( \alpha > 1 \) and the equality sign in any of the above inequalities holds if and only if \( S(T) \cong S_{k+1} \). Now, from Equation (6) and Equation (7) the desired result follows.

A caterpillar is a tree which results in a path graph by deletion of all pendent vertices and incident edges.

Lemma 4.4. [17] If \( T \) is an \( n \)-vertex non-caterpillar then there exist an \( n \)-vertex caterpillar \( T' \) such that \( T' \) and \( T \) have the same degree sequence (and same number of segments).

Lemma 4.5. If \( T \in \mathcal{ST}_{n,k} \) has maximum degree greater than 4 then there exist \( T' \in \mathcal{ST}_{n,k} \) such that
\[ R_0^0(T) > R_0^0(T') \] if \( \alpha < 0 \) or \( \alpha > 1 \),
\[ R_0^0(T) < R_0^0(T') \] if \( 0 < \alpha < 1 \)
and
\[ SEI_a(T) > SEI_a(T') \] if \( \alpha > 1 \),
\[ SEI_a(T) < SEI_a(T') \] if \( 0 < \alpha < 1 \).

Proof. Let \( \pi \) be the degree sequence of the tree \( T \). By Lemma 4.1 there must exist a caterpillar \( T^{(1)} \in \mathcal{ST}_{n,k} \) with degree sequence \( \pi \) (it is possible that \( T = T^{(1)} \)). Obviously,
\[ R_0^0(T) = R_0^0(T^{(1)}) \quad \text{and} \quad SEI_a(T) = SEI_a(T^{(1)}). \]
Let \( P : v_0v_1 \ldots v_rv_{r+1} \) be the longest path in \( T^{(1)} \) containing the vertex of degree greater than 4. Obviously, \( v_0 \) and \( v_{r+1} \) are pendent vertices. Let \( d_{v_i} \geq 5 \) for some \( i \in \{1,2,\ldots,r\} \). The assumption that \( T^{(1)} \) is a caterpillar implies that there exist two pendent vertices \( u_1, u_2 \) adjacent to \( v_i \), not included in the path \( P \). Let \( T' = T^{(1)} - \{u_1v_i, u_2v_i\} + \{u_1v_{r+1}, u_2v_{r+1}\} \). Clearly, \( T' \in \mathcal{ST}_{n,k} \). By virtue of Lagrange’s mean value theorem there exists numbers \( \Theta_1, \Theta_2 \) such that \( 1 < \Theta_1 < 3 \leq d_{v_i} - 2 < \Theta_2 < d_{v_i} \) and
\[ R_0^0(T) - R_0^0(T') = R_0^0(T^{(1)}) - R_0^0(T') = [(d_{v_i})^\alpha - (d_{v_i} - 2)^\alpha] - [3^\alpha - 1^\alpha] = 2\alpha(\Theta_2^{\alpha-1} - \Theta_1^{\alpha-1}) \]
\[ > 0 \quad \text{if} \quad \alpha < 0 \quad \text{or} \quad \alpha > 1, \]
\[ < 0 \quad \text{if} \quad 0 < \alpha < 1. \]
Also, there exists numbers $\Theta_3$, $\Theta_4$ such that $1 < \Theta_3 < 3 \leq d_{v_i} - 2 < \Theta_4 < d_{v_i}$ and

$$SEI_a(T) - SEI_a(T') = SEI_a(T^{(1)}) - SEI_a(T')$$

$$= [d_{v_i}a^{d_{v_i}} - (d_{v_i} - 2)a^{(d_{v_i}-2)}] - [3a^3 - a]$$

$$= 2a^{\Delta + 4}(1 + \Theta_3 \ln a) - 2a^{\Theta_4}(1 + \Theta_3 \ln a)$$

$$\begin{cases} > 0 & \text{if } a > 1, \\ < 0 & \text{if } 0 < a < 1. \end{cases}$$

\[ \square \]

**Lemma 4.6.** If $T \in \mathcal{S}_{n,k}$ has two or more vertices of degree 4 then there exist $T' \in \mathcal{S}_{n,k}$ such that

$$R^0_\alpha(T) \begin{cases} > R^0_\alpha(T') & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < R^0_\alpha(T') & \text{if } 0 < \alpha < 1 \end{cases}$$

and

$$SEI_a(T) \begin{cases} > SEI_a(T') & \text{if } a > 1, \\ < SEI_a(T') & \text{if } \frac{\alpha + \sqrt{33}}{16} < a < 1. \end{cases}$$

**Proof.** Let $\pi$ be degree sequence of the tree $T$. By Lemma 4.4 there must exist a caterpillar $T^{(1)} \in \mathcal{S}_{n,k}$ with degree sequence $\pi$ (it is possible that $T = T^{(1)}$). Obviously,

$$R^0_\alpha(T) = R^0_\alpha(T^{(1)}) \quad \text{and} \quad SEI_a(T) = SEI_a(T^{(1)}).$$

Suppose that the vertices $u, v \in V(T^{(1)})$ have degree 4. Let $P : v_0v_1 \ldots v_rv_{r+1}$ be the longest path in $T^{(1)}$ containing the vertices $u, v$. Let $u = v_i$ and $u = v_j$ for some $i, j \in \{1, 2, \ldots, r\}$, $i \neq j$. There must exist two pendant vertices $u_1, u_2$, not included in the path $P$ such that $u_1v_i, u_2v_j \in E(T^{(1)})$. Let $T' = T^{(1)} - \{u_1v_i, u_2v_j\} + \{u_1v_{r+1}, u_2v_{r+1}\}$. Clearly, $T' \in \mathcal{S}_{n,k}$ and

$$R^0_\alpha(T) - R^0_\alpha(T') = R^0_\alpha\left(T^{(1)}\right) - R^0_\alpha(T') = 2\left(4a^\alpha - 3a^\alpha\right) - (3a^\alpha - 1)$$

$$\begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases}$$

Also, we have

$$SEI_a(T) - SEI_a(T') = SEI_a\left(T^{(1)}\right) - SEI_a(T') = a(8a^3 - 9a^2 + 1)$$

$$\begin{cases} > 0 & \text{if } a > 1, \\ < 0 & \text{if } \frac{\alpha + \sqrt{33}}{16} < a < 1. \end{cases}$$

\[ \square \]

**Lemma 4.7.** [17] If $T$ is a tree satisfying $\Delta \leq 4$ and $n_4 \leq 1$ then the degree sequence $\pi$ of $T$ is given below

$$\pi = \begin{cases} (4, 3, \ldots, 3, 2, \ldots, 2, 1, \ldots, 1) & \text{if } k \text{ is even}, \\ \frac{4}{n-k-1} & \frac{4}{n-k-1} \\
\frac{4}{n-k-1} & \frac{4}{n-k-1} \\
\frac{4}{n-k-1} & \frac{4}{n-k-1} \\
\frac{4}{n-k-1} & \frac{4}{n-k-1} \\
\end{cases}$$

if $k$ is odd.
Theorem 4.8. Let \( T \in \mathcal{ST}_{n,k} \) where \( 3 \leq k \leq n-2 \).

\((i)\). If \( \alpha < 0 \) or \( \alpha > 1 \), then the following inequality holds:

\[
R_{\alpha}^0(\mathcal{T}) \geq \begin{cases} 
 f(n,k) + 4\alpha^2 - 2 \cdot 3\alpha - 2\alpha^2 + 2 & \text{if } k \text{ is even}, \\
 f(n,k) + \frac{3\cdot 3\alpha - 2\alpha^2 + 1}{2} & \text{if } k \text{ is odd},
\end{cases}
\]

where \( f(n,k) = 2^{\alpha}n + \left( \frac{3\cdot 3\alpha - 2\alpha^2 + 1}{2} \right) k \). If \( 0 < \alpha < 1 \) then the inequality is reversed.

\((ii)\). For \( a > 1 \), the following inequality holds:

\[
SEI_a(T) \geq \begin{cases} 
 g(n,k) + 4a^4 - 6a^3 - 2a^2 + 2a & \text{if } k \text{ is even}, \\
 g(n,k) + \frac{3a - 3a^2 - 4a^2}{2} & \text{if } k \text{ is odd},
\end{cases}
\]

where \( g(n,k) = 2a^2n + \left( \frac{3a - 4a^2 + a}{2} \right) k \). If \( \frac{1+\sqrt{33}}{16} < a < 1 \) then the inequality is reversed.

In each part, the bound is best possible and is attained if and only if \( T \) has the degree sequence \( \pi \) given below:

\[
\pi = \begin{cases} 
 (4,3,\ldots,3,2,\ldots,2,1,\ldots,1) & \text{if } k \text{ is even}, \\
 (3,\ldots,3,2,\ldots,2,1,\ldots,1) & \text{if } k \text{ is odd},
\end{cases}
\]

Proof. From Lemma 4.5, Lemma 4.6 and Lemma 4.7, the desired result follows. \(\square\)

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