

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

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Abstract

The zeroth-order general Randić index (usually denoted by R_α^0) and variable sum exdeg index (denoted by SEI_a) of a graph G are defined as $R_\alpha^0(G) = \sum_{v \in V(G)} (d_v)^\alpha$ 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 α 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 \mathbb{PT}_{n,n_1} , $\mathbb{ST}_{n,k}$, $\mathbb{BT}_{n,b}$ be the collections of all n -vertex trees having n_1 pendent 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 \mathbb{PT}_{n,n_1} , $\mathbb{ST}_{n,k}$, $\mathbb{BT}_{n,b}$. The obtained extremal trees for the collection $\mathbb{ST}_{n,k}$ 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 vice 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 π -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_α^0 and is defined as:

$$R_\alpha^0(G) = \sum_{v \in V(G)} (d_v)^\alpha,$$

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where α is a real number other than 0 and 1. Indeed, R_α^0 reduces to first Zagreb index and zeroth-order Randić index for $\alpha = 2$ and $\alpha = -\frac{1}{2}$, respectively. The topological index R_α^0 has attracted a considerable attention from mathematicians, for example see the papers [1, 13, 18–20, 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 P , whose terminal vertices are branching or pendent, and all non-terminal vertices (if exist) of P have degree 2. The main purpose the present paper is to solve the problem of determining all the trees with extremum (maximum and minimum) zeroth-order general Randić index and variable sum exdeg index from the collection of all n -vertex trees having fixed (i) pendent vertices (ii) segments (iii) branching vertices, is solved. The number of segments of a tree T can be determined from the number of vertices of T with degree 2 and vise versa [17]. Hence, the obtained extremal trees for the collection $\mathbb{ST}_{n,k}$ are also extremal trees for the collection of all n -vertex trees having fixed number of vertices with degree 2.

Let G' be a graph obtained from another graph G by applying some graph transformation such that $V(G) = V(G')$. Throughout the paper, whenever such two graphs are under discussion, by the vertex degree d_u we always mean degree of the vertex u in G .

2 Zeroth-order general Randić index, variable sum exdeg index and pendent vertices of trees

Denote by $n_i(G)$ (or simply by n_i) the number of vertices of graph G having degree i . For $n \geq 6$, let \mathbb{PT}_{n,n_1} be the collection of all n -vertex trees with n_1 pendent vertices. Clearly, $2 \leq n_1 \leq n-1$. Both the collections $\mathbb{PT}_{n,2}$ and $\mathbb{PT}_{n,n-1}$ 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 \mathbb{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 $T \in \mathbb{PT}_{n,n_1}$ contains more than one branching vertex then there exist a tree $T' \in \mathbb{PT}_{n,n_1}$ such that $SEI_a(T) > SEI_a(T')$ for $0 < a < 1$ and*

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

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 $T' = T - vw + uw$ then Lagrange's mean value theorem guaranties the existence of numbers Θ_1, Θ_2 such that $d_v - 1 < \Theta_1 < d_v \leq d_u < \Theta_2 < d_u + 1$ and

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= d_v a^{d_v} - (d_v - 1) a^{d_v - 1} - [(d_u + 1) a^{d_u + 1} - d_u a^{d_u}] \\ &= a^{\Theta_1} (1 + \Theta_1 \ln a) - a^{\Theta_2} (1 + \Theta_2 \ln a) \end{aligned} \quad (1)$$

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 (2) implies that $SEI_a(T) > SEI_a(T')$ for $0 < a < 1$.

Again, by virtue of Lagrange's mean value theorem there exist numbers Θ_3, Θ_4 such that $d_v - 1 < \Theta_3 < d_v \leq d_u < \Theta_4 < d_u + 1$ and

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= (d_v)^\alpha - (d_v - 1)^\alpha - [(d_u + 1)^\alpha - (d_u)^\alpha] \\ &= \alpha(\Theta_3^{\alpha-1} - \Theta_4^{\alpha-1}) \\ &\begin{cases} < 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

This completes the proof. □

If $V(G) = \{v_1, v_2, \dots, v_n\}$ such that $d_{v_1} \geq d_{v_2} \geq \dots \geq d_{v_n}$ then the sequence $\pi = (d_{v_1}, d_{v_2}, \dots, d_{v_n})$ 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*

$$R_\alpha^0(T) \begin{cases} \leq 2^\alpha n + (n_1)^\alpha - (2^\alpha - 1)n_1 - 2^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ \geq 2^\alpha n + (n_1)^\alpha - (2^\alpha - 1)n_1 - 2^\alpha & \text{if } 0 < \alpha < 1. \end{cases}$$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(n_1, \underbrace{2, \dots, 2}_{n-n_1-1}, \underbrace{1, \dots, 1}_{n_1})$.

Proof. The result directly follows from Lemma 2.1. □

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*

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

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 Θ_1, Θ_2 such that $d_v < \Theta_1 < d_v + 1 \leq d_u - 1 < \Theta_2 < d_u$ and

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= d_u a^{d_u} - (d_u - 1)a^{d_u-1} - [(d_v + 1)a^{d_v+1} - d_v a^{d_v}] \\ &= a^{\Theta_2}(1 + \Theta_2 \ln a) - a^{\Theta_1}(1 + \Theta_1 \ln a) < 0. \end{aligned} \tag{2}$$

There also exist numbers Θ_3, Θ_4 such that $d_v < \Theta_3 < d_v + 1 \leq d_u - 1 < \Theta_4 < d_u$ and

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= (d_u)^\alpha - (d_u - 1)^\alpha - [(d_v + 1)^\alpha - (d_v)^\alpha] \\ &= \alpha(\Theta_4^{\alpha-1} - \Theta_3^{\alpha-1}) \\ &\begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

This completes the proof. □

Lemma 2.4. *[11] 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 $t = \lfloor \frac{n-2}{n-n_1} \rfloor + 1$.*

Theorem 2.5. If $T \in \mathbb{PT}_{n,n_1}$ and $t = \lfloor \frac{n-2}{n-n_1} \rfloor + 1$ then

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

and

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

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(\underbrace{t+1, \dots, t+1}_{n-(n-n_1)t-2}, \underbrace{t, \dots, t}_{(n-n_1)t-n_1+2}, \underbrace{1, \dots, 1}_{n_1})$.

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

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

For $n \geq 6$, let $\mathbb{BT}_{n,b}$ 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 $\mathbb{BT}_{n,0}$ contains only one graph, namely the path graph P_n .

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

$$SEI_a(T) \begin{cases} > SEI_a(T') & \text{if } a > 1, \\ < SEI_a(T') & \text{if } 0 < a < 1. \end{cases}$$

and

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

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

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= d_u a^{d_u} - (d_u - 1)a^{d_u-1} - (2a^2 - a) \\ &= a^{\Theta_2}(1 + \Theta_2 \ln a) - a^{\Theta_1}(1 + \Theta_1 \ln a) \\ &\begin{cases} > 0 & \text{if } a > 1, \\ < 0 & \text{if } 0 < a < 1, \end{cases} \end{aligned}$$

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

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= (d_u)^\alpha - (d_u - 1)^\alpha - (2^\alpha - 1) \\ &\begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

\square

Lemma 3.2. [6] If $T \in \mathbb{BT}_{n,b}$ has maximum degree 3 then $n_1 = b + 2$ and $n_2 = n - 2b - 2$.

Theorem 3.3. If $T \in \mathbb{BT}_{n,b}$ then

$$SEI_a(T) \begin{cases} \geq 2a^2n + (3a^3 - 4a^2 + a)b - 2a(2a - 1) & \text{if } a > 1, \\ \leq 2a^2n + (3a^3 - 4a^2 + a)b - 2a(2a - 1) & \text{if } 0 < a < 1 \end{cases}$$

and

$$R_\alpha^0(T) \begin{cases} \geq 2^\alpha n + (3^\alpha - 2^{\alpha+1} + 1)b - 2^{\alpha+1} + 2 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ \leq 2^\alpha n + (3^\alpha - 2^{\alpha+1} + 1)b - 2^{\alpha+1} + 2 & \text{if } 0 < \alpha < 1. \end{cases}$$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(\underbrace{3, \dots, 3}_b, \underbrace{2, \dots, 2}_{n-2b-2}, \underbrace{1, \dots, 1}_{b+2})$.

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*

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

and

$$SEI_a(T) \begin{cases} < SEI_a(T') & \text{if } a > 1, \\ > SEI_a(T') & \text{if } 0 < a < 1. \end{cases}$$

Proof. Let $u, v \in V(T)$ such that $d_u \geq d_v \geq 4$. Suppose $N_T(v) = \{v_1, v_2, \dots, v_{r-1}, v_r\}$ and let u be connected to v through v_r (it is possible that $u = v_r$). If $T' = T - \{vv_1, vv_2, \dots, vv_{r-3}\} + \{uv_1, uv_2, \dots, uv_{r-3}\}$ then

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= (d_v)^\alpha - 3^\alpha - [(d_u + d_v - 3)^\alpha - (d_u)^\alpha] \\ &= \alpha(d_v - 3)(\Theta_1^{\alpha-1} - \Theta_2^{\alpha-1}) \\ &\begin{cases} < 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ > 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

where $3 < \Theta_1 < d_v \leq d_u < \Theta_2 < d_u + d_v - 3$. Also, we have

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= d_v a^{d_v} - 3a^3 - [(d_u + d_v - 3)a^{d_u+d_v-3} - d_u a^{d_u}] \\ &= (d_v - 3) [a^{\Theta_3}(1 + \Theta_3 \ln a) - a^{\Theta_4}(1 + \Theta_4 \ln a)] \\ &\begin{cases} < 0 & \text{if } a > 1, \\ > 0 & \text{if } 0 < a < 1, \end{cases} \end{aligned}$$

where $3 < \Theta_3 < d_v \leq d_u < \Theta_4 < d_u + d_v - 3$. \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*

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

and

$$SEI_a(T) \begin{cases} < SEI_a(T') & \text{if } a > 1, \\ > SEI_a(T') & \text{if } 0 < a < 1. \end{cases}$$

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 $R_\alpha^0(T) - R_\alpha^0(T')$ and $SEI_a(T) - SEI_a(T')$. \square

Lemma 3.6. *[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 $(n - 2b + 1, \underbrace{3, \dots, 3}_{b-1}, \underbrace{1, \dots, 1}_{n-b})$.*

Theorem 3.7. *If $T \in \mathbb{BT}_{n,b}$ then*

$$R_\alpha^0(T) \begin{cases} \leq (n-2b+1)^\alpha + n + (3^\alpha - 1)b - 3^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ \geq (n-2b+1)^\alpha + n + (3^\alpha - 1)b - 3^\alpha & \text{if } 0 < \alpha < 1 \end{cases}$$

and

$$SEI_a(T) \begin{cases} \leq (n-2b+1)a^{n-2b+1} + na + (3a^3 - a)b - 3a^3 & \text{if } a > 1, \\ \geq (n-2b+1)a^{n-2b+1} + na + (3a^3 - a)b - 3a^3 & \text{if } 0 < a < 1. \end{cases}$$

The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(n-2b+1, \underbrace{3, \dots, 3}_{b-1}, \underbrace{1, \dots, 1}_{n-b})$.

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 $\mathbb{ST}_{n,k}$ the set of all n -vertex trees with k segments. Throughout this section we take $3 \leq k \leq n-2$ because $\mathbb{ST}_{n,1} = \{P_n\}$, $\mathbb{ST}_{n,n-1} = \{S_n\}$ and the set $\mathbb{ST}_{n,2}$ 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 [17]. Hence

$$k = |E(S(T))| = |V(S(T))| - 1 = n - n_2 - 1 \quad (3)$$

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 $\mathbb{ST}_{n,k}$ 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. [15] *For $n \geq 4$, if T is an n -vertex tree then*

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

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

Theorem 4.3. *If $T \in \mathbb{ST}_{n,k}$ then*

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

and

$$SEI_a(T) \leq 2a^2n + ka^k - (2a-1)ak - 2a^2$$

for $a > 1$. The equality sign in any of the above inequalities holds if and only if T has the degree sequence $(k, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_k)$.

Proof. By definition of the squeeze of a tree, zeroth-order general Randić index and variable sum exdeg index, we have

$$R_\alpha^0(T) = R_\alpha^0(S(T)) + 2^\alpha n_2 \quad (4)$$

and

$$SEI_a(T) = SEI_a(S(T)) + 2a^2 n_2. \quad (5)$$

From Equation (3), we have $n_2 = n - k - 1$ and hence from Equation (4) and Equation (5) it follow that

$$R_\alpha^0(T) = R_\alpha^0(S(T)) + 2^\alpha(n - k - 1) \quad (6)$$

and

$$SEI_a(T) = SEI_a(S(T)) + 2a^2(n - k - 1). \quad (7)$$

Since $S(T)$ has $n - n_2 = k + 1$ vertices. So, by Lemma 4.1 and Lemma 4.2, we have

$$SEI_a(S(T)) \leq ka^k + ka \quad \text{and} \quad R_\alpha^0(S(T)) \begin{cases} \leq k^\alpha + k & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ \geq k^\alpha + k & \text{if } 0 < \alpha < 1, \end{cases}$$

where $a > 1$ 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. \square

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 $T \in \mathbb{ST}_{n,k}$ has maximum degree greater than 4 then there exist $T' \in \mathbb{ST}_{n,k}$ such that*

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

and

$$SEI_a(T) \begin{cases} > SEI_a(T') & \text{if } a > 1, \\ < SEI_a(T') & \text{if } 0 < a < 1. \end{cases}$$

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

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

Let $P : v_0 v_1 \dots v_r v_{r+1}$ 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 $i \in \{1, 2, \dots, r\}$. 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 $T' = T^{(1)} - \{u_1 v_i, u_2 v_i\} + \{u_1 v_{r+1}, u_2 v_{r+1}\}$. Clearly, $T' \in \mathbb{ST}_{n,k}$. By virtue of Lagrange's mean value theorem there exists numbers Θ_1, Θ_2 such that $1 < \Theta_1 < 3 \leq d_{v_i} - 2 < \Theta_2 < d_{v_i}$ and

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= R_\alpha^0(T^{(1)}) - R_\alpha^0(T') = [(d_{v_i})^\alpha - (d_{v_i} - 2)^\alpha] - [3^\alpha - 1^\alpha] \\ &= 2\alpha(\Theta_2^{\alpha-1} - \Theta_1^{\alpha-1}) \\ &\begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

Also, there exists numbers Θ_3, Θ_4 such that $1 < \Theta_3 < 3 \leq d_{v_i} - 2 < \Theta_4 < d_{v_i}$ and

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= SEI_a(T^{(1)}) - SEI_a(T') \\ &= \left[d_{v_i} a^{d_{v_i}} - (d_{v_i} - 2) a^{(d_{v_i} - 2)} \right] - [3a^3 - a] \\ &= 2a^{\Theta_4} (1 + \Theta_4 \ln a) - 2a^{\Theta_3} (1 + \Theta_3 \ln a) \\ &\quad \begin{cases} > 0 & \text{if } a > 1, \\ < 0 & \text{if } 0 < a < 1. \end{cases} \end{aligned}$$

□

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

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

and

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

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

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

Suppose that the vertices $u, v \in V(T^{(1)})$ have degree 4. Let $P : v_0 v_1 \dots v_r v_{r+1}$ be the longest path in $T^{(1)}$ containing the vertices u, v . Let $u = v_i$ and $v = v_j$ for some $i, j \in \{1, 2, \dots, r\}$, $i \neq j$. There must exist two pendent vertices u_1, u_2 , not included in the path P such that $u_1 v_i, u_2 v_j \in E(T^{(1)})$. Let $T' = T^{(1)} - \{u_1 v_i, u_2 v_j\} + \{u_1 v_{r+1}, u_2 v_{r+1}\}$. Clearly, $T' \in \mathbb{ST}_{n,k}$ and

$$\begin{aligned} R_\alpha^0(T) - R_\alpha^0(T') &= R_\alpha^0(T^{(1)}) - R_\alpha^0(T') = 2(4^\alpha - 3^\alpha) - (3^\alpha - 1) \\ &\quad \begin{cases} > 0 & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ < 0 & \text{if } 0 < \alpha < 1. \end{cases} \end{aligned}$$

Also, we have

$$\begin{aligned} SEI_a(T) - SEI_a(T') &= SEI_a(T^{(1)}) - SEI_a(T') = a(8a^3 - 9a^2 + 1) \\ &\quad \begin{cases} > 0 & \text{if } a > 1, \\ < 0 & \text{if } \frac{1+\sqrt{33}}{16} < a < 1. \end{cases} \end{aligned}$$

□

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

$$\pi = \begin{cases} \left(\underbrace{4, \dots, 4}_{\frac{k-4}{2}}, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_{\frac{k+4}{2}} \right) & \text{if } k \text{ is even,} \\ \left(\underbrace{3, \dots, 3}_{\frac{k-1}{2}}, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_{\frac{k+3}{2}} \right) & \text{if } k \text{ is odd.} \end{cases}$$

Theorem 4.8. Let $T \in \mathbb{ST}_{n,k}$ where $3 \leq k \leq n - 2$.

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

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

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

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

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

where $g(n, k) = 2a^2n + \left(\frac{3a^3-4a^2+a}{2}\right)k$. 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 π given below:

$$\pi = \begin{cases} (4, \underbrace{3, \dots, 3}_{\frac{k-4}{2}}, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_{\frac{k+4}{2}}) & \text{if } k \text{ is even,} \\ (3, \underbrace{3, \dots, 3}_{\frac{k-1}{2}}, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_{\frac{k+3}{2}}) & \text{if } k \text{ is odd.} \end{cases}$$

Proof. From Lemma 4.5, Lemma 4.6 and Lemma 4.7, the desired result follows. □

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