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Research Article

A note on the maximal inverse sum indeg index of trees

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Abstract

The inverse sum indeg index (ISI index) of a graph G is defined as $ISI(G) = \sum_{v_iv_j\in E(G)}(d(v_i)d(v_j))(d(v_i)+d(v_j))^{-1}$, where $d(v_i)$ is the degree of a vertex v_i. It is known that the star S_n uniquely minimizes the ISI index among trees of order n. However, characterizing trees of order n with the maximal ISI index (optimal trees, for convenience) appears to be difficult. Chen, Li, and Lin in [*Appl. Math. Comput.* **392** (2021) #125731] gave some structural properties and three conjectures regarding an optimal tree. In this paper, the trees within a set $\mathcal{TS}_n$ of trees of order n are investigated, where $\mathcal{TS}_n$ is defined in the main text and it is the set to which the optimal tree is conjectured to belong. Several structural properties associated with an optimal tree are presented. The findings of the present paper imply that if the second part of Conjecture 4.3 of the mentioned paper holds, then its remaining two conjectures are also valid.

Keywords: graph; inverse sum indeg index; optimal tree.

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1. Introduction

All graphs considered in this paper are finite, undirected, and simple. Let G be a such graph with vertex set $V(G) = \{v_0, v_1, \ldots, v_{n-1}\}$ and edge set $E(G)$. For $v_i \in V(G)$, let $N(v_i)$ be the set of neighbors of v_i, and $d_i = d_G(v_i)$ (or $d(v_i)$ for short) be the degree of a vertex v_i. Then $d(v_i) = |N(v_i)|$, and $\Delta = \Delta(G) = \max_{0\le i\le n-1} d(v_i)$ is the maximum degree of G. A vertex of degree 1 is said to be a pendent vertex. For an edge $e = uv \in E(G)$, if either $d(u) = 1$ or $d(v) = 1$, then e is a pendent edge. Let $P = u_0u_1\ldots u_\ell$, $\ell \ge 1$, be a path of G with $d(u_0) \ge 3$, $d(u_i) = 2$ for $1 \le i \le \ell-1$, and $d(u_\ell) \ne 2$. If $d(u_\ell) \ge 3$ (respectively, $d(u_\ell) = 1$), then P is said to be an internal path (respectively, a pendent path) of G.

The inverse sum indeg index (ISI index in short) of a graph G is defined [15] as

$$ISI(G) = \sum_{v_iv_j\in E(G)} f(d(v_i), d(v_j)),$$

where $f(x, y) = \frac{xy}{x+y}$ for $x, y \ge 1$. This recently developed topological index was shown to have a nice predicting ability for the total surface area of octane isomers [15]. Some extremal values of the ISI index have been determined by Sedlar et al. [14] for connected graphs, chemical trees, chemical graphs, graphs with given maximum degree, minimum degree, or number of pendent vertices, and trees with k leaves. An and Xiong [3] later obtained the extremal ISI index among graphs with prescribed matching number, vertex connectivity, or independence number. Recently, Jiang et al. [9] completely characterized the structure of chemical trees with the maximal ISI index. For more results concerning ISI index, we refer to [1–9, 11–14].

For trees, it was proven in [14] that the star uniquely has the minimal ISI index. However, the characterization of trees having maximal ISI index is an open problem [14]. Let $\mathcal{T}_n$ be the set of trees of order n. A tree with maximal ISI index in $\mathcal{T}_n$ is referred to as an n-vertex optimal tree. In 2021, some structural properties of an n-vertex optimal tree were observed and proven by Chen et al. [5]. Their main findings can be summarized as follows.

Proposition 1.1 (see [5]).

(i). *An optimal tree has no internal paths of length at least* 2.

(ii). *An optimal tree has no pendent paths of length at least* 3.

(iii). *An optimal tree contains at most one pendent path of length* 2.

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Additionally, Chen et al. [5] proposed the following three conjectures regarding an n-vertex optimal tree (corresponding to Conjectures 4.2, 4.3, and 4.4 in [5]).

Conjecture 1.1 (see [5]). *If T is an n-vertex optimal tree and $n \geq 20$, then T has no vertices of degree 2 (or equivalent, no pendent paths of length 2).*

Conjecture 1.2 (see [5]). *The n-vertex optimal tree is unique. Moreover, if $n \geq 20$, then it is formed from a star $S_{\Delta+1}$ with a few pendent edges attached to some vertices of $S_{\Delta+1}$.*

Conjecture 1.3 (see [5]). *If T is an n-vertex optimal tree, then $ISI(T) < 2n - 2$.*

In 2022, Lin et al. [10] investigated Conjectures 1.1 and 1.3, and Conjecture 1.3 has been proven for general trees in it. They also got a better upper bound than Conjecture 1.3.

Lemma 1.1 (see [10]). *Let $n \geq 2$ and T an n-vertex tree with maximum degree Δ. Then, $ISI(T) < 2n - 2 - \Delta$.*

In this paper, we consider a special class $\mathcal{TS}_n$ of trees (as defined in Section 2). Some structural properties of optimal trees over $\mathcal{TS}_n$ are presented. These results show that if the second part of Conjecture 1.2 holds, then both Conjectures 1.1 and 1.3 are also valid.

2. Main results

Let $n \geq 20$. For a tree $T \in \mathcal{TS}_n$ we introduce the following notation illustrated by Figure 2.1. The central vertex is denoted by v_0, its neighbors by $v_1, \ldots, v_\Delta$. Additional pendent vertices are attached to vertices $v_1, \ldots, v_m$, where $m \leq \Delta$, and the number of pendent vertices attached to v_i is denoted by p_i for $i = 1, \ldots, m$. Notice that $n = 1 + \Delta + \sum_{i=1}^{m} p_i$. Further, as for the degrees of vertices in T it holds that $d_T(v_0) = \Delta$, $2 \leq d_T(v_i) = p_i + 1 \leq \Delta$ for $i = 1, 2, \ldots, m$, and for all other vertices of T it holds that their degree equals one.

Without loss of generality, we assume that $p_1 \geq p_2 \geq \cdots \geq p_{m-1} \geq p_m$.

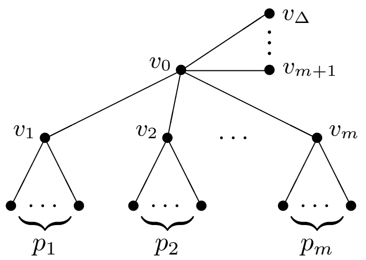

Figure 2.1: A tree $T \in \mathcal{TS}_n$.

We say that $T \in \mathcal{TS}_n$ is an optimal tree over $\mathcal{TS}_n$, if T achieves the maximum ISI index among all trees in $\mathcal{TS}_n$. In this section, some structural properties of optimal trees over $\mathcal{TS}_n$ are presented. Based on these properties, we can infer that if the second part of Conjecture 1.2 holds, then both Conjectures 1.1 and 1.3 are also valid.

Lemma 2.1. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. Then $\Delta \geq 5$.*

Proof. Note that

$$n = 1 + \Delta + \sum_{i=1}^{m} p_i \leq 1 + \Delta + m(\Delta - 1) \leq 1 + \Delta + \Delta(\Delta - 1) = \Delta^2 + 1.$$

Hence, $\Delta \geq 5$. □

Lemma 2.2. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then $m \geq 2$.*

Proof. Suppose to the contrary that $m = 1$. Let $T' = T - v_0 v_\Delta + v_2 v_\Delta$. Then $T' \in \mathcal{TS}_n$, and

$$\begin{aligned} ISI(T) - ISI(T') =& f(\Delta, p_1 + 1) + (\Delta - 1) f(\Delta, 1) - f(\Delta - 1, p_1 + 1) - (\Delta - 3) f(\Delta - 1, 1) - f(\Delta - 1, 2) - f(2, 1) \\ =& \frac{\Delta(p_1 + 1)}{\Delta + p_1 + 1} + \frac{(\Delta - 1)\Delta}{\Delta + 1} - \frac{(\Delta - 1)(p_1 + 1)}{\Delta + p_1} - \frac{(\Delta - 3)(\Delta - 1)}{\Delta} - \frac{2(\Delta - 1)}{\Delta + 1} - \frac{2}{3} \end{aligned}$$

$$= -\frac{A\cdot\Delta + 9p_1(p_1+1)}{3\Delta(\Delta+1)(\Delta+p_1)(\Delta+p_1+1)},$$

where $A = 2\Delta^3 + \Delta^2(4p_1-5) - \Delta\left(p_1^2+18p_1+1\right) - \left(10p_1^2-5p_1-6\right)$. In the following, we will prove $A>0$; that is, there is a tree $T' \in \mathcal{TS}_n$ such that $ISI(T) < ISI(T')$, a contradiction. Note that $n = 1+\Delta+p_1 \geq 20$. If $p_1 = 1$, then $\Delta \geq 18$, and

$$A = 2\Delta^3 - \Delta^2 - 20\Delta + 1 > 0.$$

If $2 \leq p_1 \leq 4$, then $\Delta \geq 19 - p_1$, and

$$\begin{aligned}\frac{\partial A}{\partial \Delta} &= 6\Delta^2 + 2\Delta(4p_1-5) - \left(p_1^2+18p_1+1\right)\\ &\geq 6(19-p_1)^2 + 2(19-p_1)(4p_1-5) - \left(p_1^2+18p_1+1\right)\\ &= -3p_1^2 - 84p_1 + 1975 > 0,\end{aligned}$$

that is, A is an increasing function on Δ. So,

$$A \geq A\Big|_{\Delta=19-p_1} = 3p_1^3 - 54p_1^2 - 868p_1 + 11900 > 0.$$

If $p_1 \geq 5$, noting that $\Delta \geq p_1+1$, we have

$$\begin{aligned}\frac{\partial A}{\partial \Delta} &= 6\Delta^2 + 2\Delta(4p_1-5) - \left(p_1^2+18p_1+1\right)\\ &\geq 6(p_1+1)^2 + 2(p_1+1)(4p_1-5) - \left(p_1^2+18p_1+1\right)\\ &= 13p_1^2 - 8p_1 - 5 > 0,\end{aligned}$$

that is, A is an increasing function on Δ. So,

$$A \geq A\Big|_{\Delta=p_1+1} = 5p_1^3 - 20p_1^2 - 14p_1 + 2 > 0.$$

This completes the proof of the lemma. □

Lemma 2.3. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then $p_{m-1} \geq 2$.*

Proof. Suppose to the contrary that $p_{m-1} = 1$. Then $p_m = 1$. Let $T' = T - v_m v_{m1} + v_{m-1}v_{m1}$, where v_{m1} is the unique child of v_m. Then $T' \in \mathcal{TS}_n$, and

$$\begin{aligned}ISI(T) - ISI(T') &= 2f(\Delta,2) + 2f(2,1) - f(\Delta,1) - f(\Delta,3) - 2f(3,1)\\ &= \frac{4\Delta}{\Delta+2} + \frac{4}{3} - \frac{\Delta}{\Delta+1} - \frac{3\Delta}{\Delta+3} - \frac{3}{2}\\ &= -\frac{\Delta^3 - 6\Delta^2 + 11\Delta + 6}{2(\Delta+1)(\Delta+2)(\Delta+3)}.\end{aligned}$$

By Lemma 2.1, $\Delta \geq 5$. Thus, $ISI(T) < ISI(T')$, which is a contradiction. □

Lemma 2.4. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then*

$$\Delta < \frac{p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4 + \sqrt{B}}{2(p_1+p_m+4)},$$

where

$$\begin{aligned}B = &\left(p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4\right)^2\\ &+ 2(p_1+p_m+4)\left(p_1^3p_m^2 + 3p_1^3p_m + p_1^2p_m^3 + 10p_1^2p_m^2 + 13p_1^2p_m + 5p_1p_m^3\right.\\ &\left.+21p_1p_m^2 + 2p_1p_m + 4p_m^3 + 8p_m^2 - 4p_1^2 - 18p_1 - 18p_m - 16\right).\end{aligned}$$

Proof. Let $T' = T - v_m v_{m1} + v_1 v_{m1}$ where $v_{m1} \in N(v_m)$ with $d_T(v_{m1}) = 1$. Then $T' \in \mathcal{TS}_n$, and

$$\begin{aligned} ISI(T) - ISI(T') =& p_1 f(p_1+1,1) + f(p_1+1,\Delta) + p_m f(p_m+1,1) + f(p_m+1,\Delta) \\ & - (p_1+1) f(p_1+2,1) - f(p_1+2,\Delta) - (p_m-1) f(p_m,1) - f(p_m,\Delta) \\ =& \frac{p_1(p_1+1)}{p_1+2} + \frac{\Delta(p_1+1)}{\Delta+p_1+1} + \frac{p_m(p_m+1)}{p_m+2} + \frac{\Delta(p_m+1)}{\Delta+p_m+1} - \frac{(p_1+1)(p_1+2)}{p_1+3} \\ & - \frac{\Delta(p_1+2)}{\Delta+p_1+2} - \frac{(p_m-1)p_m}{p_m+1} - \frac{\Delta p_m}{\Delta+p_m} \\ =& \frac{-(p_1-p_m+1)(A_1\cdot\Delta^2+A_2)}{(p_1+2)(p_1+3)(p_m+1)(p_m+2)(\Delta+p_1+1)(\Delta+p_1+2)(\Delta+p_m)(\Delta+p_m+1)}, \end{aligned}$$

where

$$\begin{aligned} A_1 =& 2\Delta^2(p_1+p_m+4) - 2\Delta\left(p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4\right) \\ & - \left(p_m^3(p_1^2+5p_1+4) + p_m^2(p_1^3+10p_1^2+21p_1+8) + p_m(3p_1^3+13p_1^2+2p_1-18) - 2(2p_1^2+9p_1+8)\right), \\ A_2 =& 2\Delta(p_1+p_m+2)(p_1+p_m+4)(2p_1p_m+p_1+3p_m+1) + 2p_m(p_1+1)(p_1+2)(p_m+1)(p_1+p_m+4). \end{aligned}$$

Note that $p_1 - p_m + 1 > 0$, and $A_2 > 0$. So, the necessary condition of $ISI(T) - ISI(T') > 0$ is $A_1 < 0$. Denote

$$A_1 = 2\Delta^2 a_2 - 2\Delta a_1 - a_0,$$

where

$$\begin{aligned} a_2 &= p_1 + p_m + 4 > 0, \\ a_1 &= p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4 > 0, \\ a_0 &= p_m^3(p_1^2+5p_1+4) + p_m^2(p_1^3+10p_1^2+21p_1+8) + p_m(3p_1^3+13p_1^2+2p_1-18) - 2(2p_1^2+9p_1+8). \end{aligned}$$

It is easy to see that a_0 is increasing in p_m. Then

$$a_0 \geq a_0\Big|_{p_m=1} = 4p_1^3 + 20p_1^2 + 10p_1 - 22 > 0.$$

So, exactly one of the two zero points of A_1 is positive, and its positive zero point is

$$\hat{\Delta} = \frac{2a_1 + \sqrt{4a_1^2 + 8a_2a_0}}{4a_2} = \frac{p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4 + \sqrt{B}}{2(p_1+p_m+4)},$$

where

$$\begin{aligned} B =& \left(p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4\right)^2 \\ & + 2(p_1+p_m+4)\left(p_1^3p_m^2 + 3p_1^3p_m + p_1^2p_m^3 + 10p_1^2p_m^2 + 13p_1^2p_m + 5p_1p_m^3\right. \\ & \left. + 21p_1p_m^2 + 2p_1p_m + 4p_m^3 + 8p_m^2 - 4p_1^2 - 18p_1 - 18p_m - 16\right). \end{aligned}$$

Note that A_1 is a quadratic function with the positive leading coefficient with respect to Δ. Then $A_1 < 0$ if $0 < \Delta < \hat{\Delta}$, and $A_1 > 0$ if $\Delta > \hat{\Delta}$. Recall that $A_1 > 0$ implies $ISI(T') > ISI(T)$, which is a contradiction with T being optimal. Hence, it must hold that $A_1 < 0$, which implies $\Delta < \hat{\Delta}$ as claimed. □

Lemma 2.5. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, and $p_1 \geq p_m + 2$, then*

$$\Delta > \frac{p_1^2(p_m+1)(p_m+4) + p_1(p_m+3)(3p_m+2) - 2(p_m+2)}{p_1+p_m+4}.$$

Proof. Let $T' = T - v_1v_{11} + v_mv_{11}$ where $v_{11} \in N(v_1)$ with $d_T(v_{11}) = 1$. Then $T' \in \mathcal{TS}_n$, and

$$\begin{aligned}ISI(T) - ISI(T') =& p_1f(p_1+1,1) + p_mf(p_m+1,1) + f(p_1+1,\Delta) + f(p_m+1,\Delta) - (p_1-1)f(p_1,1)\\ &- (p_m+1)f(p_m+2,1) - f(p_1,\Delta) - f(p_m+2,\Delta)\\ =& \frac{p_1(p_1+1)}{p_1+2} + \frac{p_m(p_m+1)}{p_m+2} + \frac{(p_1+1)\Delta}{\Delta+p_1+1} + \frac{(p_m+1)\Delta}{\Delta+p_m+1} - \frac{p_1(p_1-1)}{p_1+1}\\ &- \frac{(p_m+1)(p_m+2)}{p_m+3} - \frac{p_1\Delta}{\Delta+p_1} - \frac{(p_m+2)\Delta}{\Delta+p_m+2}\\ =& \frac{(p_1-p_m-1)(S-L)}{(p_1+1)(p_1+2)(p_m+2)(p_m+3)(\Delta+p_1)(\Delta+p_1+1)(\Delta+p_m+1)(\Delta+p_m+2)},\end{aligned}$$

where

$$\begin{aligned}S =& 2\Delta^4(p_1+p_m+4) - 2\Delta^3\left[p_1^2(p_m+1)(p_m+4) + p_1(p_m+3)(3p_m+2) - 2(p_m+2)\right],\\ L =& \Delta^2\left[p_1^3(p_m+1)(p_m+4) + p_1^2(p_m(p_m+3)(p_m+7)+8) + p_1(p_m-1)(p_m(3p_m+16)+18)\right.\\ &\left.-2(p_m(2p_m+9)+8)\right] - 2\Delta(p_1+p_m+2)(p_1+p_m+4)(p_1(2p_m+3)+p_m+1)\\ &- 2p_1(p_1+1)(p_m+1)(p_m+2)(p_1+p_m+4).\end{aligned}$$

Firstly, we will show that $L > 0$. Denote $L = \Delta^2 b_2 - 2\Delta b_1 - b_0$, where

$$\begin{aligned}b_2 &= p_1^3(p_m+1)(p_m+4) + p_1^2(p_m(p_m+3)(p_m+7)+8) + p_1(p_m-1)(p_m(3p_m+16)+18) - 2(p_m(2p_m+9)+8),\\ b_1 &= (p_1+p_m+2)(p_1+p_m+4)(p_1(2p_m+3)+p_m+1),\\ b_0 &= 2p_1(p_1+1)(p_m+1)(p_m+2)(p_1+p_m+4).\end{aligned}$$

Note that $\Delta \geq p_1+1$ and $p_1 \geq p_m+2 \geq 3$. Then

$$\begin{aligned}b_2 \geq& (p_m+2)^3(p_m+1)(p_m+4) + (p_m+2)^2(p_m(p_m+3)(p_m+7)+8)\\ &+ (p_m+2)(p_m-1)(p_m(3p_m+16)+18) - 2(p_m(2p_m+9)+8)\\ =& 2\left(p_m^5 + 14p_m^4 + 65p_m^3 + 124p_m^2 + 86p_m + 6\right) > 0,\\ \frac{\partial L}{\partial \Delta} =& 2\Delta b_2 - 2b_1 \geq 2(p_1+1)b_2 - 2b_1\\ =& 2p_m^3(p_1^3+4p_1^2+p_1-1) + 2p_m^2(p_1^4+11p_1^3+19p_1^2-8p_1-11)\\ &+ 2p_m(5p_1^4+24p_1^3+4p_1^2-58p_1-32) + 2(4p_1^4+9p_1^3-29p_1^2-64p_1-24) > 0,\end{aligned}$$

that is, L is an increasing function on Δ. Thus,

$$\begin{aligned}L \geq& L\Big|_{\Delta=p_1+1}\\ =& p_m^3(p_1^4+5p_1^3+p_1^2-5p_1-2) + p_m^2(p_1^5+12p_1^4+24p_1^3-26p_1^2-57p_1-18)\\ &+ p_m(5p_1^5+27p_1^4+p_1^3-149p_1^2-174p_1-46) + (4p_1^5+10p_1^4-46p_1^3-162p_1^2-142p_1-32)\\ \geq& (p_1^4+5p_1^3+p_1^2-5p_1-2) + (p_1^5+12p_1^4+24p_1^3-26p_1^2-57p_1-18)\\ &+ (5p_1^5+27p_1^4+p_1^3-149p_1^2-174p_1-46) + (4p_1^5+10p_1^4-46p_1^3-162p_1^2-142p_1-32)\\ =& 10p_1^5+50p_1^4-16p_1^3-336p_1^2-378p_1-98 > 0.\end{aligned}$$

Since $p_1 - p_m - 1 > 0$, and T is optimal, we have $S > 0$, and so

$$\Delta > \frac{p_1^2(p_m+1)(p_m+4) + p_1(p_m+3)(3p_m+2) - 2(p_m+2)}{p_1+p_m+4}.$$

□

Theorem 2.1. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then $p_1 \leq p_m + 1$; that is, $|p_i - p_j| \leq 1$ for $i, j \in \{1, 2, \ldots, m\}$.*

Proof. Suppose to the contrary that $p_1 \geq p_m + 2$. By Lemmas 2.5 and 2.4,

$$\Delta > \frac{p_1^2(p_m+1)(p_m+4) + p_1(p_m+3)(3p_m+2) - 2(p_m+2)}{p_1+p_m+4},$$

and

$$\Delta < \frac{p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4 + \sqrt{B}}{2(p_1+p_m+4)},$$

where B is defined in Lemma 2.4. Denote

$$X = p_1^2(p_m+1)(p_m+4) + p_1(p_m+3)(3p_m+2) - 2(p_m+2),$$
$$Y = p_1^2p_m^2 + 3p_1^2p_m + 5p_1p_m^2 + 11p_1p_m + 4p_m^2 + 6p_m - 2p_1 - 4 + \sqrt{B}.$$

Then

$$Y - 2X = -\left[p_1^2\left(p_m^2+7p_m+8\right) + p_1\left(p_m^2+11p_m+14\right) - 4p_m^2 - 10p_m - 4\right] + \sqrt{B}.$$

Denote

$$Z = \left[p_1^2\left(p_m^2+7p_m+8\right) + p_1\left(p_m^2+11p_m+14\right) - 4p_m^2 - 10p_m - 4\right]^2 - B.$$

Then

$$\begin{aligned} Z =& 2\left[p_1^4\left(4p_m^3+27p_m^2+53p_m+32\right) - p_1^3\left(4p_m^4+10p_m^3-51p_m^2-167p_m-116\right)\right. \\ & -p_1^2\left(21p_m^4+119p_m^3+170p_m^2-30p_m-98\right) - p_1\left(29p_m^4+173p_m^3+302p_m^2+100p_m-24\right) \\ & \left. -4p_m^4 - 8p_m^3 + 50p_m^2 + 152p_m + 64\right]. \end{aligned}$$

Since

$$\frac{\partial^4 Z}{\partial p_1^4} = 48(4p_m^3+27p_m^2+53p_m+32) > 0,$$

we have that $\frac{\partial^3 Z}{\partial p_1^3}$ is increasing in p_1. Note that $p_1 \geq p_m + 2$. Then

$$\frac{\partial^3 Z}{\partial p_1^3} \geq \left.\frac{\partial^3 Z}{\partial p_1^3}\right|_{p_1=p_m+2} = 12\left(12p_m^4+130p_m^3+479p_m^2+719p_m+372\right) > 0.$$

Similarly,

$$\frac{\partial^2 Z}{\partial p_1^2} \geq \left.\frac{\partial^2 Z}{\partial p_1^2}\right|_{p_1=p_m+2} = 4\left(12p_m^5+183p_m^4+1036p_m^3+2749p_m^2+3420p_m+1562\right) > 0,$$
$$\frac{\partial Z}{\partial p_1} \geq \left.\frac{\partial Z}{\partial p_1}\right|_{p_1=p_m+2} = 4\left(2p_m^6+42p_m^5+343p_m^4+1414p_m^3+3109p_m^2+3422p_m+1416\right) > 0.$$

Then

$$Z \geq Z\Big|_{p_1=p_m+2} = 8\left(p_m^6+19p_m^5+147p_m^4+581p_m^3+1222p_m^2+1272p_m+486\right) > 0.$$

So, $Y - 2X < 0$ and it is a contradiction. □

Theorem 2.2. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then $p_m \geq 2$, that is, T has no vertices of degree 2.*

Proof. Suppose to the contrary that $p_m = 1$. By Lemma 2.3 and Theorem 2.1, $p_i = 2$ for $i = 1, \ldots, m-1$. Then $\Delta \geq 8$ follows from Table 1 of [5]. Let $T' = T - v_mv_{m,1} + v_1v_{m,1}$, where $v_{m,1} \in N(v_m)$ with $d_T(v_{m,1}) = 1$. Then $T' \in \mathcal{TS}_n$, and

$$\begin{aligned} ISI(T) - ISI(T') =& f(\Delta,3) + 2f(3,1) + f(\Delta,2) + f(2,1) - f(\Delta,4) - 3f(4,1) - f(\Delta,1) \\ =& \frac{3\Delta}{\Delta+3} + \frac{3}{2} + \frac{2\Delta}{\Delta+2} + \frac{2}{3} - \frac{4\Delta}{\Delta+4} - \frac{12}{5} - \frac{\Delta}{\Delta+1} \\ =& \frac{-7\Delta^4 + 50\Delta^3 + 55\Delta^2 - 350\Delta - 168}{30(\Delta+1)(\Delta+2)(\Delta+3)(\Delta+4)} < 0, \end{aligned}$$

that is, $ISI(T) < ISI(T')$. It is a contradiction. □

Theorem 2.3. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then $ISI(T) < 2n - 2 - \Delta - \frac{n-\Delta}{n}$.*

Proof. Let T be an optimal tree over $\mathcal{TS}_n$. By Lemma 2.3 and Theorem 2.1, $p_{m-1} \geq 2$, and $|p_i - p_j| \leq 1$ for $i, j \in \{1, 2, \ldots, m\}$. So, we may assume that $p_i = p$ for $i = 1, \ldots, s$, and $p_i = p - 1$ for $i = s+1, \ldots, m$, where $p \geq 2$ and $1 \leq s \leq m \leq \Delta$. Then $n = 1 + \Delta + sp + (m-s)(p-1) = 1 + \Delta + s + m(p-1)$, and

$$\begin{aligned} ISI(T) =& s\left(f(\Delta, p+1) + pf(p+1, 1)\right) + (m-s)\left(f(\Delta, p) + (p-1)f(p, 1)\right) + (\Delta - m)f(\Delta, 1) \\ =& s\left(\frac{\Delta(p+1)}{\Delta + p + 1} + \frac{p(p+1)}{p+2}\right) + (m-s)\left(\frac{\Delta p}{\Delta + p} + \frac{p(p-1)}{p+1}\right) + \frac{\Delta(\Delta - m)}{\Delta + 1} \\ <& s\left(\frac{\Delta(p+1)}{\Delta + p} + \frac{p(p+1)}{p+1}\right) + (m-s)\left(\frac{\Delta p}{\Delta + p} + \frac{p(p-1)}{p+1}\right) + \Delta - m \\ =& \frac{mp^2(p + 2\Delta - 1) + s\left(2p^2 + 3p\Delta + \Delta\right)}{(p+1)(p+\Delta)} + \Delta - m. \end{aligned}$$

So,

$$\begin{aligned} &(2n - 2 - \Delta - \frac{n-\Delta}{n}) - ISI(T) \\ >& 2\left(\Delta + s + m(p-1)\right) - \Delta - \frac{1 + s + m(p-1)}{1 + \Delta + s + m(p-1)} - \left(\frac{mp^2(p + 2\Delta - 1) + s\left(2p^2 + 3p\Delta + \Delta\right)}{(p+1)(p+\Delta)} + \Delta - m\right) \\ =& \frac{a\Delta^2 + b\Delta + c}{(p+1)(p+\Delta)(1 + \Delta + s + m(p-1))}, \end{aligned}$$

where

$$\begin{aligned} a &= (p-1)(m-s), \\ b &= mp^3 + mp^2(m - s + 1) - p\left(2m^2 - 3ms + s^2 + 1\right) + m^2 - 2ms + s^2 - 1, \\ c &= m^2 p\left(p^3 + p^2 - 3p + 1\right) + mp\left(p^2 s + 4ps + 2p - 3s\right) + p\left(2s^2 + s - ps - p - 1\right). \end{aligned}$$

Note that $p \geq 2$ and $1 \leq s \leq m \leq \Delta$. Then $a \geq 0$, and

$$c \geq c|_{m=s} = p(p+1)(p^2 s^2 + ps^2 + s - 1) > 0.$$

Since

$$\frac{\partial^2 b}{\partial p^2} = 6mp + 2m(m - s + 1) > 0,$$

we have that $\frac{\partial b}{\partial p}$ is increasing in p. Then

$$\frac{\partial b}{\partial p} \geq \left.\frac{\partial b}{\partial p}\right|_{p=2} = 2m^2 - ms - s^2 + 16m - 1 > 0.$$

So,

$$b \geq b|_{p=2} = m^2 - s^2 + 12m - 3 > 0.$$

Thus, $a\Delta^2 + b\Delta + c > 0$; that is, $ISI(T) < 2n - 2 - \Delta - \frac{n-\Delta}{n}$. □

Combining the obtained conclusions, we get the following main theorem:

Theorem 2.4. *Let $n \geq 20$ and $T \in \mathcal{TS}_n$. If T is an optimal tree over $\mathcal{TS}_n$, then*

(i) *$m \geq 2$;*

(ii) *$|p_i - p_j| \leq 1$ for $i, j \in \{1, 2, \ldots, m\}$;*

(iii) *T has no vertices of degree 2 (or equivalently, $p_m \geq 2$); and*

(iv) *$ISI(T) < 2n - 2 - \Delta - \frac{n-\Delta}{n}$.*

3. Conclusion

Characterizing trees with the maximal ISI index (optimal trees) among trees of order n appears to be difficult. In 2021, Chen et al. [5] gave some structural properties and three conjectures regarding an optimal tree (Conjectures 1.1, 1.2, and 1.3). In 2022, Lin et al. [10] investigated Conjectures 1.1 and 1.3. We note that if the second part of Conjecture 1.2 holds, then the optimal tree(s) among trees of order n will belong to $\mathcal{TS}_n$. So, in this article, we investigate the optimal tree(s) over $\mathcal{TS}_n$. Although we have not completely solved the problem of characterizing optimal tree(s) over $\mathcal{TS}_n$ yet, we have found several structural properties associated with an optimal tree. We believe that these properties will contribute greatly to the final solution of the optimal tree over $\mathcal{TS}_n$ and hence to settle Conjecture 1.2. Based on Theorem 2.4, it is not difficult to find that the key to determining the optimal tree(s) over $\mathcal{TS}_n$ is to determine the value of m for a given n. In the author's opinion, this is going to be a very challenging problem.

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