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Research article

Extremal degree-based topological indices for trees with given segment number

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Abstract: A degree-based topological index of a tree T is termed as

$$TI_f(T) = \sum_{v_1v_2 \in E(T)} f(d(v_1), d(v_2)),$$

in which $f(x, y) = f(y, x)$ denotes a real-valued function with $x, y \geq 1$. This paper mainly focuses on the extremal topological index problems for trees with a given segment number. We respectfully present the sufficient conditions for achieving the smallest and largest values of TI_f, as well as depict the associated extremal graphs. As an application, it is verified that there are eight types of degree-based indices that meet these sufficient conditions, including the recently proposed Euler Sombor index and diminished Sombor index.

Keywords: extremal values; topological indices; trees; segment number
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1. Introduction

In mathematical chemistry, a molecular graph serves as a graph-theoretic depiction of a molecular structure. In this representation, vertices stand for atoms and edges represent chemical bonds, ignoring details such as atomic size and bond length while retaining only the topological connectivity features. The graph-theoretic invariant derived from molecular graphs are called topological indices, whose primary role is to establish the structure-property correlation. Specifically, its applications include: In physical chemistry, it enables the prediction of properties like a compound's boiling point and solubility through QSPR (Quantitative Structure-Property Relationship) models [1, 2]; In drug discovery, it supports the virtual screening of candidate molecules for bioactivity and toxicity via

QSAR (Quantitative Structure-Activity Relationship) models [3,4]; in the field of materials science, it guides the structural design and performance optimization of polymers and catalysts [5]. Nowadays, as a core feature input into machine learning models, topological indices are driving chemical research toward a more data-driven and precise paradigm [6,7].

According to the calculation method, topological indices can be classified into degree-based types (ABS index [8], Lanzhou index [9]), distance-based types (Wiener index [2], Mostar index [10]), and so on. They are capable of converting invisible molecular structures into specific, comparable numerical values. Currently, degree-based topological indices occupy a dominant position in the field of chemical graph theory. A degree-based topological index of G is designated as

$$TI_f = TI_f(G) = \sum_{v_1 v_2 \in E(G)} f(d(v_1), d(v_2)),$$

in which $d(v_i)$ is used to stand for the degree of v_i, while $f(x, y) = f(y, x)$ is a real-valued function. Specifically, let $m_{x,y}$ represent the number of edges with $(d(v_1), d(v_2)) = (x, y)$, and Δ stands for the maximum degree of the vertices in G. Then, TI_f can be expressed alternatively as

$$TI_f = \sum_{1 \le x \le y \le \Delta} m_{x,y} f(x, y).$$

In 2021, Gutman [11] introduced the Sombor index, which originates from geometric distance. It is denoted as

$$SO(G) = \sum_{v_1 v_2 \in E(G)} \sqrt{d(v_1)^2 + d(v_2)^2}.$$

Subsequently, various forms of the Sombor index have been proposed successively, including the Euler Sombor index [12, 13], the elliptic Sombor index [14], the hyperbolic Sombor index [15], and the diminished Sombor index [16]. It is worth noting that all these derived Sombor indices belong to degree-based topological indices. Through relevant studies, they have been proven to exhibit wide applications in the research of physicochemical properties and biological activities, providing reliable quantitative tools for exploring the structure-property/activity relationships of chemical molecules.

As trees are crucial components in the molecular structures of compounds, research on various indices of trees, especially the problem of extremal trees with given parameters, has been extensively conducted. In 2022, Chen et al. [17] established the minimum and maximum Sombor index for trees with specified parameters and depicted the relevant extremal graphs. These parameters include the number of pendant vertices, segment number, branching number, etc. In 2024, Li and Ye [18] found the greatest values of ABS_σ (with $\sigma \ge 0$) among graphs having certain predefined parameters (e.g., matching number, chromatic number). In 2025, Ahmad et al. [19] further extended this research by identifying the smallest and largest values of the elliptic Sombor index for trees with specific parameters, such as maximum degree, branching vertices, and segment number.

The exploration of a universal method to study some topological indices problems has long been a focus of researchers, as it can significantly improve the efficiency of solving extremal problems for different indices and avoid repetitive analyses for individual indices. As early as 2005, Li and Zheng [20] introduced two transformations to investigate the maximum and minimum values of several topological indices for trees. In 2022, Li and Peng [21] further summarized the research progress on extremal problems and spectral problems oriented to finding unified methods. In 2025, Gao [22] obtained the trees corresponding to the maximum and minimum values of several topological indices by proposing sufficient conditions. For more results in this field, please refer to References [23] and [24].

Inspired by the aforementioned studies, we attempt to solve the extremal problems of degree-based indices in trees using a general approach. Let $\mathcal{J}_{n,s}$ denote the collection of trees having n vertices and s segments. This present paper is structured as follows: In Section 2, the preliminary knowledge is presented. In Section 3 and Section 4, the sufficient conditions for the smallest and largest topological indices of $TI_f(T)$ (where $T \in \mathcal{J}_{n,s}$) are provided, respectively, and the associated extremal graphs are described. In an application of the aforementioned sufficient conditions, in Section 5, it is verified that eight types of degree-based indices satisfy these conditions for achieving minimum and maximum values.

2. Preliminaries

First, we introduce some definitions and terminology involved in this paper. Every graph considered within this study is simple and connected. A connected acyclic graph is called a tree, denoted by T. Let the vertex set and edge set of tree T be denoted as $V(T)$ and $E(T)$, respectively. If the total number of vertices satisfies $|V(T)| = n$, then $|E(T)| = n - 1$. For $u \in V(T)$, $N_T(u)$ (abbreviated as $N(u)$) is referred to as the collection of all vertices adjacent to u. The degree of u, designated by $d_T(u)$ (abbreviated as $d(u)$), is given by $d(u) = |N(u)|$. In particular, if $|N(u)| \leq 4$ for all $u \in V(T)$, then T is called a chemical tree, denoted by CT. A path and a star that have n vertices are represented by P_n and S_n, respectively. Vertex u is referred to as a pendant vertex (or leaf) if $d(u) = 1$, and a branching vertex if $d(u) \geq 3$. If $P_l = u_1u_2 \cdots u_l$ is an induced sub-path of T satisfying $d(u_1) \geq 3$, $d(u_2) = d(u_3) = \cdots = d(u_{l-1}) = 2$, and $d(u_l) = 1$, then P_l is termed a pendant path. For $E' \in E(T)$, $T - E'$ denotes the graph gained by removing the edge set E' from T. Likewise, $T + F$ represents the graph acquired through the addition of the edge set F to T, where $F \cap E(T) = \emptyset$. Other undefined concepts and terminology follow those in the graph theory Reference [25].

Let $\pi(T) = (d(u_1), d(u_2), \cdots, d(u_n))$ denote the degree sequence of T, in which $d(u_i)$ is the degree of $u_i \in V(T)$. Clearly, $d(u_1) \geq d(u_2) \geq \cdots \geq d(u_n)$ represents a non-increasing sequence made up of non-negative integers. In a tree T, let Δ denote the maximum degree of its vertices. Let $m_{i,j}$ represent the total count of edges with $(d(u), d(v)) = (i, j)$ (where $uv \in E(T)$), while n_i stands for the total count of vertices with degree i. Thus, the following equations hold.

Proposition 2.1. *For any tree T, the following equations hold:*

$$\begin{cases} \sum_{i=1}^{\Delta} n_i = n, \\ \sum_{j=1,\neq i}^{\Delta} m_{i,j} + 2m_{i,i} = i \cdot n_i, \ \textit{where}\ 1 \leq i \leq \Delta, \\ \sum_{i=1}^{\Delta} i \cdot n_i = 2n - 2. \end{cases} \tag{1}$$

A segment in tree T, denoted as $P = v_1v_2 \cdots v_k$, is a sub-path where all internal vertices v_i $(2 \leq i \leq k - 1)$ have degree 2, and the two end vertices (v_1, v_k) are either pendant vertices or branching vertices. A starlike tree refers to a tree with exactly one vertex whose degree is greater than 2. For convenience, let $\mathcal{J}_{n,s}$ denote the collection of trees having n vertices and s segments. It is easy to observe that $\mathcal{J}_{n,1} = \{P_n\}$, $\mathcal{J}_{n,2} = \emptyset$, and $\mathcal{J}_{n,n-1} = \{S_n\}$. Thus, this paper mainly considers the case where $3 \leq s \leq n-2$. In references [19, 26], it is shown that by squeezing the 2-degree vertices in each segment of T, the number of segments remains unchanged. Therefore, we have the following property.

Proposition 2.2. *Let $T \in \mathcal{J}_{n,s}$, then $s = n - n_2 - 1$.*

3. The minimum TI_f trees in $\mathcal{J}_{n,s}$

Before presenting the main results, we first need to define the following sets, and then provide two useful lemmas. Let $\Omega_1 = \{(1, x) \in (\mathbb{N}, \mathbb{N}) : 2 \leq x \leq n-1\}$, $\Omega_2 = \{(x, y) \in (\mathbb{N}, \mathbb{N}) : 2 \leq x \leq y \leq n-1 \textit{ and } x + y \leq n\} - \{(2, 2), (2, 3), (3, 3)\}$, and $\Omega = \Omega_1 \cup \Omega_2 \cup \{(2, 2), (2, 3), (3, 3)\}$. Let

$$\varphi(x, y) = f(x, y) + f(3, 3) - 2f(2, 3) + 6\frac{x + y - xy}{xy}(f(3, 3) - f(2, 3)). \tag{2}$$

Clearly, $\varphi(2, 3) = \varphi(3, 3) = 0$.

Lemma 3.1. *(Su and Deng [24]) Let T denote a tree of order n. Then*

$$TI_f(T) = (2n + 4)f(2, 3) - (n + 5)f(3, 3) + \varphi(2, 2)m_{2,2} + \sum_{(x,y)\in\Omega_1\cup\Omega_2} \varphi(x, y)m_{x,y}, \tag{3}$$

where $\varphi(x, y)$ is defined in (2).

Lemma 3.2. *(i) A tree $T \in \mathcal{J}_{n,s}$ exists such that $n_i(T) = 0$ for all $i \geq 4$. Then $n_1 = n_3 + 2$ and s is odd. Furthermore, $n_1 = \frac{s+3}{2}$, $n_2 = n - s - 1$, and $n_3 = \frac{s-1}{2}$.*

(ii) A tree $T \in \mathcal{J}_{n,s}$ exists such that $n_i(T) = 0$ for all $i \geq 5$, with $n_4(T) = 1$. Then $n_1 = n_3 + 4$ and s is even. Furthermore, $n_1 = \frac{s}{2} + 2$, $n_2 = n - s - 1$, and $n_3 = \frac{s}{2} - 2$.

Proof. Firstly, we establish (i). Since $n_i = 0$ holds for all $i \geq 4$, it follows from Eq (1) that

$$n_1 + 2n_2 + 3n_3 = 2n - 2, \quad n_1 + n_2 + n_3 = n.$$

Thus, we have $n_1 = n_3 + 2$. Additionally, by Proposition 2.2 (where $s = n - n_2 - 1$), we deduce

$$s = n_1 + n_2 + n_3 - n_2 - 1 = n_1 + n_3 - 1 = 2n_1 - 3.$$

Clearly, $s = 2n_1 - 3$ is odd. Combining the above results, it is straightforward to derive that

$$n_1 = \frac{s + 3}{2}, \; n_3 = \frac{s - 1}{2}, \; n_2 = n - s - 1.$$

Therefore, the conclusion of Lemma 3.2(i) holds.

Next, we prove (ii). Since $n_i = 0$ for all $i \geq 5$, it follows from Eq (1) that

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - 2, \quad n_1 + n_2 + n_3 + n_4 = n.$$

This, together with $n_4 = 1$, implies that $n_1 = n_3 + 4$. Moreover, as given by $s = n - n_2 - 1$, we deduce

$$s = n_1 + n_2 + n_3 + n_4 - n_2 - 1 = n_1 + n_3 + 1 - 1 = 2n_1 - 4.$$

Clearly, $s = 2n_1 - 4$ is even. Combining the above results, we get

$$n_1 = \frac{s}{2} + 2,\ n_2 = n - s - 1,\ n_3 = \frac{s}{2} - 2,\ n_4 = 1.$$

Thus, the conclusion of Lemma 3.2(ii) holds. □

Lemma 3.3. *Let $T \in \mathcal{J}_{n,s}$, as shown in Figure 1. Suppose edges u_1u_2, u_2u_3, and $v_1v_2 \in E(T)$, where $d(u_1) = d(u_2) = 2$, $d(u_3) = 3$, $d(v_1) = 1$, and $d(v_2) = 3$ or 4. If the inequality $f(2, x) - f(1, x) < f(2, 2) - f(1, 2)$ holds for $x = 3$ and 4, then there exists a tree $T' \in \mathcal{J}_{n,s}$, such that $TI_f(T') < TI_f(T)$.*

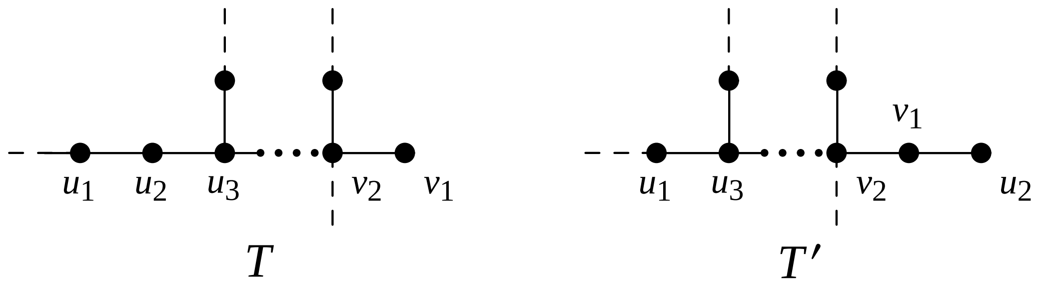

Figure 1. Trees of T and T' in Transformation 1.

Proof. We perform the following transformation on T.
Transformation 1: $T' = T - u_1u_2 - u_2u_3 + u_1u_3 + v_1u_2$.

Then, $d_{T'}(v_1) = d_T(v_1) + 1 = 2$, $d_{T'}(u_2) = d_T(u_2) - 1 = 1$, and the degrees of all other vertices remain unchanged. Therefore, we have

$$\begin{aligned} TI_f(T') - TI_f(T) &= f(d_{T'}(v_1), d_{T'}(v_2)) - f(d_T(v_1), d_T(v_2)) \\ &\quad + f(d_{T'}(u_2), d_{T'}(v_1)) - f(d_T(u_2), d_T(u_1)) \\ &= f(2, d_T(v_2)) - f(1, d_T(v_2)) + f(1, 2) - f(2, 2). \end{aligned}$$

For $d_T(v_2) = 3$ or 4, by the conditions of the lemma, we immediately deduce that

$$TI_f(T') - TI_f(T) < 0.$$

The lemma is thus proved. □

Let the degree sequences of T be

$$\pi_1(T) = (\underbrace{3, \cdots, 3}_{\frac{s-1}{2}}, \underbrace{2, \cdots, 2}_{n-s-1}, \underbrace{1, \cdots, 1}_{\frac{s+3}{2}}),\ \pi_2(T) = (4, \underbrace{3, \cdots, 3}_{\frac{s}{2}-2}, \underbrace{2, \cdots, 2}_{n-s-1}, \underbrace{1, \cdots, 1}_{\frac{s}{2}+2}).$$

Before presenting Theorem 3.1, we first define several sets of graphs. Let

$A^1_{n,s} = \{T \in \mathcal{J}_{n,s} : D(T) = \pi_1(T),\ m_{1,2} = m_{2,3} = \frac{s+3}{2},\ m_{3,3} = \frac{s-3}{2},\ m_{2,2} = \frac{2n-3s-5}{2},\ where\ 3 \le s \le \frac{2n-5}{3}\ and\ s\ is\ odd\}$;

$A^2_{n,s} = \{T \in \mathcal{J}_{n,s} : D(T) = \pi_1(T), m_{1,2} = m_{2,3} = n-s-1, m_{1,3} = \frac{3s-2n+5}{2}, m_{3,3} = \frac{s-3}{2},\ where\ \frac{2n-5}{3} \le s \le n-2\ and\ s\ is\ odd\}$;

$A^3_{n,s} = \{T \in \mathcal{J}_{n,s} : D(T) = \pi_2(T), m_{1,2} = \frac{s}{2}+2, m_{2,3} = s-4, m_{2,4} = 6-\frac{s}{2}, m_{3,4} = \frac{s}{2}-2, and m_{2,2} = n-\frac{3s}{2}-3,\ where\ 4 \le s \le 10\ and\ s\ is\ even\}$;

$A^4_{n,s} = \{T \in \mathcal{J}_{n,s} : D(T) = \pi_2(T), m_{1,2} = m_{2,3} = \frac{s}{2}+2, m_{3,3} = \frac{s}{2}-6, m_{3,4} = 4, m_{2,2} = n-\frac{3s}{2}-3,\ where\ 12 \le s \le \frac{2n-6}{3}\ and\ s\ is\ even\}$;

$A^5_{n,s} = \{T \in \mathcal{J}_{n,s} : D(T) = \pi_2(T), m_{1,2} = m_{2,3} = n-s-1, m_{1,3} = \frac{3s}{2}-n+3, m_{3,3} = \frac{s}{2}-6, m_{3,4} = 4,\ where\ \frac{2n-6}{3} \le s \le n-2\ and\ s\ is\ even\}$.

Clearly, $A^i_{n,s} \in \mathcal{J}_{n,s}$ for $1 \le i \le 5$.

Theorem 3.1. *Let $T \in \mathcal{J}_{n,s}$. If the following conditions hold:*

(i) $\varphi(2,2) < 0$, and $\varphi(x,y) > 0$ for any pair $(x,y) \in \Omega_1 \cup \Omega_2$;

(ii) $\varphi(1,2) < \varphi(1,3) < \varphi(1,y)$ for all $y \ge 4$;

(iii) $\varphi(3,4) < \varphi(2,4) < \varphi(x,4)$ for all $x \ne 2,3$;

(iv) The expression $f(x,y) - f(x-1,y)$ is strictly decreasing with $y \ge 1$.

Then, the following conclusion holds:

(I) s is odd, then

$$TI_f(T) \ge \begin{cases} \frac{s+3}{2}(f(1,2)+f(2,3)) + \frac{s-3}{2}f(3,3) + \frac{2n-3s-5}{2}f(2,2), & for\ 3 \le s \le \frac{2n-5}{3}, \\ (n-s-1)f(1,2) + \frac{3s-2n+5}{2}f(1,3) + (n-s-1)f(2,3) + \frac{s-3}{2}f(3,3), & for\ \frac{2n-5}{3} \le s \le n-2, \end{cases}$$

the equality occurs iff $T \in A^1_{n,s}$ for $3 \le s \le \frac{2n-5}{3}$ and $T \in A^2_{n,s}$ for $\frac{2n-5}{3} \le s \le n-2$.

(II) s is even, then

$$TI_f(T) \ge \begin{cases} (\frac{s}{2}+2)f(1,2) + (s-4)f(2,3) + (6-s)f(2,4) + (\frac{s}{2}-2)f(3,4) + (n-\frac{3s}{2}-3)f(2,2), & for\ 4 \le s \le 10, \\ (\frac{s}{2}+2)(f(1,2)+f(2,3)) + (\frac{s}{2}-6)f(3,3) + 4f(3,4) + (n-\frac{3s}{2}-3)f(2,2), & for\ 12 \le s \le \frac{2n-6}{3}, \\ (n-s-1)(f(1,2)+f(2,3)) + (\frac{3s}{2}-n+3)f(1,3) + (\frac{s}{2}-6)f(3,3) + 4f(3,4), & for\ \frac{2n-6}{3} \le s \le n-2, \end{cases}$$

the equality occurs iff $T \in A^3_{n,s}$ for $4 \le s \le 10$, $T \in A^4_{n,s}$ for $12 \le s \le \frac{2n-6}{3}$, and $T \in A^5_{n,s}$ for $\frac{2n-6}{3} < s \le n-2$.

Proof. Let $T \in \mathcal{J}^{min}_{n,s}$. Given $\varphi(2,3) = \varphi(3,3) = 0$, along with the conditions $\varphi(2,2) < 0$ and $\varphi(x,y) >$

0 for any $(x, y) \in \Omega_1 \cup \Omega_2$, to minimize $TI_f(T)$, we should take as many $m_{2,2}$ and as few $m_{x,y}$ as possible (where $(x, y) \in \Omega_1 \cup \Omega_2$) in accordance with Eq (3) of Lemma 3.1. According to the parity of s, we take into account the following two cases.

Case 1. For s is odd.

Case 1.1. For $3 \le s \le \frac{2n-5}{3}$. Since T is a tree, it must contain elements of type $m_{1,i}$. By the condition that $\varphi(1,2) < \varphi(1,3) < \varphi(1,y)$ for all $y \ge 4$, we take $\Sigma m_{1,i} = m_{1,2} = n_1$. Moreover, by Lemma 3.2(i), $m_{1,2} = n_1 = \frac{s+3}{2}$. Thus, by virtue of the minimality of T, we only take $(1,2) \in \Omega_1$ and let $m_{2,2} = x$. According to Eq. (3) of Lemma 3.1, we have

$$\begin{aligned} TI_f(T) &\ge (2n+4)f(2,3) - (n+5)f(3,3) + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &\quad + \frac{s+3}{2}(f(1,2) + 4f(3,3) - 5f(2,3)) \\ &= \frac{s+3}{2}f(1,2) + (2n - \frac{5s+7}{2} - 2x)f(2,3) + (2s - n + x + 1)f(3,3) + xf(2,2). \end{aligned}$$

Since, in a tree containing only edges of types $m_{1,2}$, $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$, edges of type $m_{1,2}$ must be either directly adjacent to edges of type $m_{2,3}$ or connected to them via edges of type $m_{2,2}$, it follows that $m_{1,2} \le m_{2,3}$. Furthermore, given $\varphi(2,2) = f(2,2) + f(3,3) - 2f(2,3) < 0$, the smaller $m_{2,3}$ is, the larger $x = m_{2,2}$ becomes. Thus, we take $m_{1,2} = m_{2,3}$, i.e., $\frac{s+3}{2} = 2n - \frac{5s+7}{2} - 2x$, which yields $x = n - \frac{3s+5}{2}$. Consequently, we have

$$TI_f(T) \ge \frac{s+3}{2}f(1,2) + \frac{s+3}{2}f(2,3) + \frac{s-3}{2}f(3,3) + \frac{2n-3s-5}{2}f(2,2).$$

The equality occurs precisely when $m_{1,2} = m_{2,3} = \frac{s+3}{2}$, $m_{3,3} = \frac{s-3}{2}$, and $m_{2,2} = \frac{2n-3s-5}{2}$.

In particular, the fact that s is odd follows from Lemma 3.2(i), while the upper bound and lower bound of $3 \le s \le \frac{2n-5}{3}$ are derived from $m_{3,3} = \frac{s-3}{2} \ge 0$ and $m_{2,2} = \frac{2n-3s-5}{2} \ge 0$, respectively.

Case 1.2. For $\frac{2n-5}{3} < s \le n-2$. First, we state the following claim.

Claim 1: $m_{1,2} < \frac{s+3}{2}$.

Proof of Claim 1. Otherwise, it follows from Lemma 3.2(i) that $m_{1,2} = \frac{s+3}{2} = n_1$. This, together with $m_{2,3} \ge m_{1,2}$ and Eq (1), we deduce

$$m_{1,2} + m_{2,3} \le m_{1,2} + m_{2,3} + 2m_{2,2} = 2n_2.$$

Moreover, Lemma 3.2(i) gives $n_2 = n - s - 1$. Thus, we have

$$\frac{s+3}{2} + \frac{s+3}{2} \le 2n_2 = 2(n-s-1).$$

That is, $s \le \frac{2n-5}{3}$, which contradicts the given condition that $s > \frac{2n-5}{3}$, thereby proving the claim.

Thus, it follows from Claim 1 and Lemma 3.2(i) that there exist edges $m_{1,i}$ other than $m_{1,2}$. Since $\varphi(1,2) < \varphi(1,3) < \varphi(1,x)$ for all $x \ge 4$, by virtue of the minimality of T, we take the pendant edges as

$m_{1,2}$ and $m_{1,3}$. Let $m_{1,2} = x$, then $m_{1,3} = \frac{s+3}{2} - x$. And let $m_{2,2} = y$. Thus, by Eq (3), we have

$$\begin{aligned} TI_f(T) &\geq (2n+4)f(2,3) - (n+5)f(3,3) + x(f(1,2) + 4f(3,3) - 5f(2,3)) \\ &+ (\frac{s+3}{2} - x)(f(1,3) + 3f(3,3) - 4f(2,3)) + y(f(2,2) + f(3,3) - 2f(2,3)) \\ &= xf(1,2) + (\frac{s+3}{2} - x)f(1,3) + yf(2,2) + (2n - 2s - x - 2y - 2)f(2,3) \\ &+ (\frac{3s-1}{2} - n + x + y)f(3,3). \end{aligned}$$

Claim 2: $m_{2,2} = 0$.

Proof of Claim 2. Otherwise, $m_{2,2} = y \geq 1$. Clearly, Condition (iv) implies that $f(2,x) - f(1,x) < f(2,2) - f(1,2)$ holds for $x = 3, 4$. In this case, tree T satisfies the conditions of Lemma 3.3. Thus, there exists a tree T' such that $TI_f(T') < TI_f(T)$. This contradicts the fact that $T \in \mathcal{J}_{n,s}^{min}$, and Claim 2 is thus proven. □

Now returning to the proof of the theorem. By Claim 2, $m_{2,2} = y = 0$. Thus, the edges incident to 2-degree vertices in T are $m_{1,2}$ and $m_{2,3}$, which implies $m_{1,2} = m_{2,3}$, i.e., $x = 2n - 2s - x - 2$. Further simplification yields $x = n - s - 1$. Consequently, we have

$$\begin{aligned} TI_f(T) &\geq xf(1,2) + (\frac{s+3}{2} - x)f(1,3) + (2n - 2s - x - 2)f(2,3) + (\frac{3s-1}{2} - n + x)f(3,3) \\ &= (n-s-1)f(1,2) + \frac{3s-2n+5}{2}f(1,3) + (n-s-1)f(2,3) + \frac{s-3}{2}f(3,3). \end{aligned}$$

The equality occurs precisely when $m_{1,2} = m_{2,3} = n - s - 1$, $m_{1,3} = \frac{3s-2n+5}{2}$, and $m_{3,3} = \frac{s-3}{2}$.

In particular, the upper bound and lower bound of $\frac{2n-5}{3} < s \leq n-2$ are derived from the fact that $m_{1,2} = n - s - 1 \geq 1$ and $m_{1,3} = \frac{3s-2n+5}{2} > 0$, respectively.

Case 2. For s is even.

By Lemma 3.2(ii), we have $n_4 \geq 1$. Since $\varphi(3,4) < \varphi(2,4) < \varphi(x,4)$ for all $x \neq 2, 3$, we take $n_4 = 1$ and $n_i = 0$ for all $i \geq 5$. Among edges incident to 4-degree vertices, we only take $m_{3,4} > 0$ and $m_{2,4} \geq 0$ (If $m_{2,4} = 0$, then $m_{3,4} = 4n_4 = 4$). Similarly, by the condition that $\varphi(1,2) < \varphi(1,3) < \varphi(1,y)$ for all $y \geq 4$, among edges incident to pendant vertices, we take $m_{1,2} > 0$ and $m_{1,3} \geq 0$ (If $m_{1,3} = 0$, then $m_{3,4} = n_1$). By Lemma 3.2(ii) and Eq (1), we have the following relations:

$$\begin{cases} m_{1,2} + m_{1,3} = \frac{s}{2} + 2, \\ m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2(n-s-1), \\ m_{2,3} + 2m_{3,3} + m_{3,4} = 3(\frac{s}{2} - 2), \\ m_{2,4} + m_{3,4} = 4. \end{cases} \tag{4}$$

Case 2.1. For $4 \leq s \leq 10$. Since $\varphi(1,2) < \varphi(1,y)$ for all $y \geq 3$, we take $m_{1,2} = n_1$ and $m_{1,3} = 0$. Without loss of generality, let $m_{3,4} = x$, then $m_{2,4} = 4 - x$. And let $m_{2,2} = y$. Thus, by Eq (3) of Lemma 3.1, we have

$$TI_f(T) \geq (2n+4)f(2,3)-(n+5)f(3,3)+(\frac{s}{2}+2)(f(1,2)+4f(3,3)-5f(2,3))$$
$$+x(f(3,4)-\frac{3}{2}f(3,3)+\frac{1}{2}f(2,3))+(4-x)(f(2,4)-\frac{1}{2}f(3,3)-\frac{1}{2}f(2,3))$$
$$+y(f(2,2)+f(3,3)-2f(2,3))$$
$$=(\frac{s}{2}+2)f(1,2)+(2n-\frac{5s}{2}+x-2y-8)f(2,3)+(4-x)f(2,4)$$
$$+(2s-n-x+y+1)f(3,3)+xf(3,4)+yf(2,2). \quad (5)$$

Thus, in a tree containing only edges of types $m_{1,2}$, $m_{2,2}$, $m_{2,3}$, and edges incident to 4-degree vertices of type $m_{2,4}$ (with $m_{2,4} \geq 1$), we always have $m_{1,2} \leq m_{2,3} + m_{2,4}$. Therefore, by Eq (5), we obtain

$$\frac{s}{2}+2 \leq 2n-\frac{5s}{2}+x-2y-8+4-x,$$

that is, $y \leq n - \frac{3}{2}s - 3$. From the preceding analysis, the larger value of $y = m_{2,2}$, yields the smaller value of TI_f. Thus, we deduce $y = n - \frac{3}{2}s - 3$ in T. Eq (5) can be transformed into

$$TI_f(T) \geq (\frac{s}{2}+2)f(1,2)+(\frac{s}{2}+x-2)f(2,3)+(4-x)f(2,4)+(\frac{s}{2}-x-2)f(3,3)$$
$$+xf(3,4)+(n-\frac{3}{2}s-3)f(2,2). \quad (6)$$

Clearly, in Eq (6), when x takes its maximum value, i.e., $x = max\{x : \frac{s}{2}+x-2 \geq 0,\ n-\frac{3}{2}s-3 \geq 0\} = \frac{s}{2}-2$, we deduce

$$TI_f(T) \geq (\frac{s}{2}+2)f(1,2)+(s-4)f(2,3)+(6-\frac{s}{2})f(2,4)$$
$$+(\frac{s}{2}-2)f(3,4)+(n-\frac{3}{2}s-3)f(2,2),$$

the equality occurs precisely when $m_{1,2} = \frac{s}{2}+2$, $m_{2,3} = s-4$, $m_{2,4} = 6-\frac{s}{2}$, $m_{3,4} = \frac{s}{2}-2$, and $m_{2,2} = n - \frac{3s}{2} - 3$.

It is specifically noted that the fact that s is even follows from Lemma 3.2(ii), while the upper bound and lower bound of $4 \leq s \leq 10$ are derived from $m_{2,4} = 6 - \frac{s}{2} \geq 1$ and $m_{2,3} = s - 4 \geq 0$, respectively.

Case 2.2. For $12 \leq s \leq \frac{2n-6}{3}$. Since $\varphi(1,2) < \varphi(1,y)$ for all $y \geq 3$, we take $m_{1,2} = n_1$ and $m_{1,3} = 0$. Moreover, let $m_{3,4} = x$ and $m_{2,2} = y$. Analogously to Case 2.1, we derive (5). In this case, by the condition $\varphi(3,4) < \varphi(2,4)$, we take as many $m_{3,4}$ as possible and as few $m_{2,4}$ as possible. Thus, when $m_{2,4} = 0$, we have $m_{3,4} = x = 4$, Eq (5) can then be transformed into

$$TI_f(T) \geq (\frac{s}{2}+2)f(1,2)+(2n-\frac{5s}{2}-2y-4)f(2,3)$$
$$+(2s-n+y-3)f(3,3)+4f(3,4)+yf(2,2).$$

Furthermore, by $m_{1,2} \leq m_{2,3}$, i.e., $\frac{s}{2}+2 \leq 2n-\frac{5s}{2}-2y-4$, we obtain $y \leq n-\frac{3s}{2}-3$. Thus, when $y = n - \frac{3s}{2} - 3$, we obtain

$$TI_f(T) \geq (\frac{s}{2}+2)f(1,2)+(\frac{s}{2}+2)f(2,3)$$
$$+(\frac{s}{2}-6)f(3,3)+4f(3,4)+(n-\frac{3s}{2}-3)f(2,2).$$

The equality occurs precisely when $m_{1,2} = m_{2,3} = \frac{s}{2} + 2$, $m_{3,3} = \frac{s}{2} - 6$, $m_{3,4} = 4$, and $m_{2,2} = n - \frac{3s}{2} - 3$.

Notably, the upper bound and lower bound of $12 \le s \le \frac{2n-6}{3}$ are derived from $m_{2,2} = n - \frac{3s}{2} - 3 \ge 0$ and $m_{3,3} = \frac{s}{2} - 6 \ge 0$, respectively.

Case 2.3. For $\frac{2n-6}{3} < s \le n-2$. Similar to the proofs of Claims 1 and 2 in the previous part, we state the following claim, and its proof are omitted herein.

Claim 3: $m_{1,2} < \frac{s}{2} + 2$ and $m_{2,2} = 0$.

Thus, it follows from Claim 3 and Lemma 3.2(ii) that, in addition to $m_{1,2}$, there exist other pendant edges of type $m_{1,i}$. Since $\varphi(1,2) < \varphi(1,3) < \varphi(1,y)$ for all $y \ge 4$, by virtue of the minimality of T, let $m_{1,2} = x$ and $m_{1,3} = \frac{s}{2} + 2 - x$. And in this case, $m_{2,2} = 0$. Therefore, by Eq (3) of Lemma 3.1, we have

$$\begin{aligned} TI_f(T) \ge\ & (2n+4)f(2,3) - (n+5)f(3,3) + x(f(1,2) + 4f(3,3) - 5f(2,3)) \\ & + (\frac{s}{2} + 2 - x)(f(1,3) + 3f(3,3) - 4f(2,3)) + 4(f(3,4) - \frac{3}{2}f(3,3) + \frac{1}{2}f(2,3)) \\ =\ & xf(1,2) + (\frac{s}{2} + 2 - x)f(1,3) + (2n - 2s - x - 2)f(2,3) \\ & + (\frac{3s}{2} - n + x - 5)f(3,3) + 4f(3,4). \end{aligned}$$

Furthermore, by $m_{1,2} = m_{2,3}$, i.e., $x = 2n - 2s - x - 2$, which implies $x = n - s - 1$. Consequently, we have

$$TI_f(T) \ge (n-s-1)f(1,2) + (\frac{3s}{2} - n + 3)f(1,3) + (n-s-1)f(2,3) + (\frac{s}{2} - 6)f(3,3) + 4f(3,4),$$

the equality occurs precisely when $m_{1,2} = m_{2,3} = n - s - 1$, $m_{1,3} = \frac{3s}{2} - n + 3$, $m_{3,3} = \frac{s}{2} - 6$, and $m_{3,4} = 4$.

Notably, the upper bound and lower bound of $\frac{2n-6}{3} < s \le n-2$ are derived from $m_{1,2} = n - s - 1 \ge 1$ and $m_{1,3} = \frac{3s}{2} - n + 3 > 0$, respectively.

Thus, the proof of the theorem is completed. □

4. The maximum TI_f trees in $\mathcal{T}_{n,s}$

In this section, we present two sufficient conditions for achieving the maximum TI_f, and we first provide the following lemma.

Lemma 4.1. *Let $P_l = u_1u_2\cdots, u_l$ be an induced sub-path of tree T, where $d_T(u_1) \ge 2$, $d_T(u_l) \ge 2$, and $d_T(u_i) = 2$ for all $2 \le i \le l-1$. We construct a transformation as shown in Figure 2.*

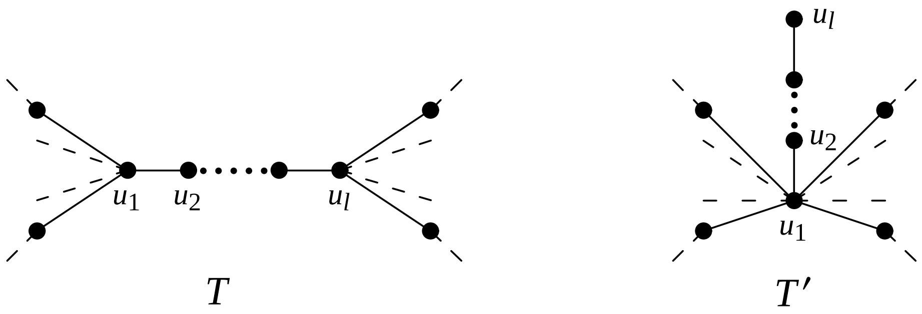

Figure 2. Trees of T and T' in Transformation 2.

Transformation 2: $T' = T - \sum_{v\in N_T(u_l)\backslash u_{l-1}} u_l v + \sum_{v\in N_T(u_l)\backslash u_{l-1}} u_1 v$.

The process of deriving T' from T is referred to as the path lifting transformation; see Figure 2. In the case that $f(x, y)$ meets the following conditions:

(i) $f(x, y)$ is strictly increasing in terms of x;

(ii) $f(x, y) < f(x + y - 1, 1)$ holds for all $x, y \geq 2$;

(iii) $g(x) = f(2, x)$ is strictly convex downward with respect to x.

Then $TI_f(T) < TI_f(T')$.

Proof. Let $d_T(u_1) = x \geq 2$ and $d_T(u_l) = y \geq 2$. Next, we analyze two cases depending on whether l is equal to 2 or not.

Case 1. $l = 2$. Then $u_1u_l = u_1u_2 \in E(T)$. By virtue of the path lifting transformation, we have

$$\begin{aligned}
&TI_f(T) - TI_f(T') \\
&= f(d_T(u_1), d_T(u_2)) - f(d_{T'}(u_1), d_{T'}(u_2)) + \sum_{v \in N_T(u_1)\backslash u_2} f(d_T(u_1), d_T(v)) \\
&+ \sum_{w \in N_T(u_2)\backslash u_1} f(d_T(u_2), d_T(w)) - \sum_{v \in N_T(u_1) \cup N_T(u_2)\backslash \{u_1,u_2\}} f(d_T(u_1) + d_T(u_2) - 1, d_T(v)) \\
&= \sum_{v \in N_T(u_1)\backslash u_2} \Big(f(x, d_T(v)) - f(x+y-1, d_T(v))\Big) \\
&+ \sum_{w \in N_T(u_2)\backslash u_1} \Big(f(y, d_T(w)) - f(x+y-1, d_T(w))\Big) + f(x,y) - f(x+y-1, 1).
\end{aligned}$$

Since $f(x, y)$ is strictly increasing regarding x, we deduce

$$\sum_{v \in N_T(u_1)\backslash u_2} \Big(f(x, d_T(v)) - f(x+y-1, d_T(v))\Big) + \sum_{w \in N_T(u_2)\backslash u_1} \Big(f(y, d_T(w)) - f(x+y-1, d_T(w))\Big) < 0.$$

Consequently, by condition (ii), we derive

$$TI_f(T) - TI_(T') < f(x,y) - f(x+y-1, 1) < 0.$$

That is, $TI_f(T) < TI_f(T')$.

Case 2. $l > 2$. Then $u_1u_l \notin E(T)$. According to the path lifting transformation, we derive

$$\begin{aligned}
&TI_f(T) - TI_f(T') \\
&= f(d_T(u_1), d_T(u_2)) - f(d_{T'}(u_1), d_{T'}(u_2)) + f(d_T(u_{l-1}), d_T(u_l)) - f(d_{T'}(u_{l-1}), d_{T'}(u_l)) \\
&+ \sum_{v \in N_T(u_1)\backslash u_2} f(d_T(u_1), d_T(v)) + \sum_{w \in N_T(u_l)\backslash u_{l-1}} f(d_T(u_l), d_T(w)) \\
&- \sum_{v \in N_T(u_1) \cup N_T(u_l)\backslash \{u_2,u_{l-1}\}} f(d_T(u_1) + d_T(u_l) - 1, d_T(v)) \\
&= f(2,x) - f(2, x+y-1) + f(2,y) - f(2,1) + \sum_{v \in N_T(u_1)\backslash u_2} \Big(f(x, d_T(v)) - f(x+y-1, d_T(v))\Big) \\
&+ \sum_{w \in N_T(u_2)\backslash u_1} \Big(f(y, d_T(w)) - f(x+y-1, d_T(w))\Big)
\end{aligned}$$

Since $g(x) = f(2, x)$ is strictly convex downward regarding x, then $g(x) + g(y) < g(x+y-1) + g(1)$, which amounts to

$$f(2,x) + f(2,y) < f(2, x+y-1) + f(2,1).$$

Moreover, as $f(x, y)$ is strictly increasing with respect to x, we have

$$\sum_{v \in N_T(u_1)\backslash u_2} \Big(f(x, d_T(v)) - f(x+y-1, d_T(v))\Big) + \sum_{w \in N_T(u_2)\backslash u_1} \Big(f(y, d_T(w)) - f(x+y-1, d_T(w))\Big) < 0.$$

Thus, based on the two preceding inequalities, we deduce that $TI_f(T) - TI_f(T') < 0$.

Combining the two cases above, the lemma follows. □

Lemma 4.2. *Let $T \in \mathcal{J}_{n,s}^{max}$, and T be a starlike tree.*

(i) If $f(x, y) - f(x-1, y)$ is strictly decreasing with $y \geq 1$, then T contains exactly one segment of length at least 2.

(ii) If $f(x, y) - f(x-1, y)$ is strictly increasing with $y \geq 1$, then all segments in T are of length at least 2 or at most 2.

Proof. (i) Suppose to the contrary that there exist two segments (pendant paths) of length at least 2 in the starlike tree T, denoted without loss of generality as $P_1 = wu_1u_2 \cdots u_r$ and $P_2 = wv_1v_2 \cdots v_t$, where $d(w) = s \geq 3$ and $r \geq t \geq 2$. We then derive a contradiction by constructing a transformation (see Figure 3).

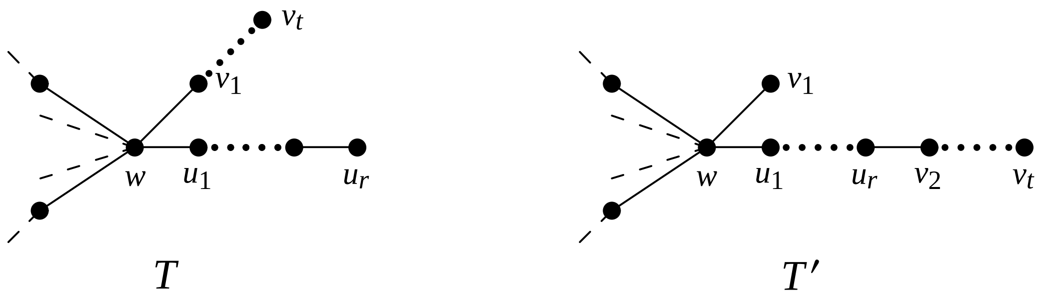

Figure 3. Trees of T and T' in Transformation 3.

Transformation 3: $T' = T - v_1v_2 + v_2u_r$.

By condition (i), $f(x, y) - f(x-1, y)$ is strictly decreasing with respect to y; it follows that $f(2, 2) - f(1, 2) > f(2, s) - f(1, s)$. Combining with Transformation 3, we have

$$\begin{aligned} TI_f(T') - TI_f(T) &= f(d_{T'}(v_1), d_{T'}(w)) + f(d_{T'}(u_{r-1}), d_{T'}(u_r)) \\ &\quad - f(d_T(v_1), d_T(w)) - f(d_T(u_{r-1}), d_T(u_r)) \\ &= f(1, s) + f(2, 2) + f(2, s) - f(2, 1) > 0, \end{aligned}$$

which implies that $TI_f(T') > TI_f(T)$. This contradicts that $T \in \mathcal{J}_{n,s}^{max}$. Therefore, the assumption is false, and the conclusion (i) is proven.

(ii) Assume to the contrary that there exist two pendant paths in the starlike tree T: one of length 1, and the other of length $l \geq 3$. Denoted without loss of generality as $P_3 = wv_1$ and $P_4 = wu_1u_2 \cdots u_l$, where $d(w) = s \geq 3$. We construct the following transformation as shown in Figure 4.

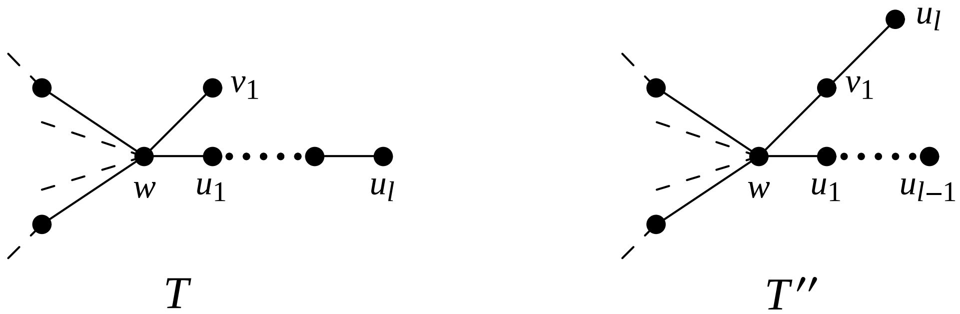

Figure 4. Trees of T and T'' in Transformation 4.

Transformation 4: $T'' = T - u_{l-1}u_l + u_l v_1$.

By condition (ii), $f(x, y) - f(x-1, y)$ is strictly increasing with respect to y, it follows that $f(2, s) - f(1, s) > f(2, 2) - f(1, 2)$. This, together with Transformation 4, we deduce

$$\begin{aligned} TI_f(T'') - TI_f(T) &= f(d_{T''}(v_1), d_{T''}(w)) + f(d_{T''}(u_{l-1}), d_{T''}(u_{l-2})) \\ &\quad - f(d_T(v_1), d_T(w)) - f(d_T(u_{l-1}), d_{T''}(u_{l-2})) \\ &= f(2, s) + f(2, 1) + f(1, s) - f(2, 2) > 0. \end{aligned}$$

That is, $TI_f(T'') > TI_f(T)$, this contradicts with $T \in \mathcal{J}_{n,s}^{max}$. Therefore, the assumption is not true, and the theorem is proven. □

Before presenting the following two theorems, we first define several sets of graphs. Let $B_{n,s}$ be the graph gained by identifying an end-vertex of the path P_{n-s+1} with the central vertex of the star S_s; $C_{n,s}^1$ stands for the graph acquired through the identification of one end-vertex of each of $n-s-1$ paths P_3 with the central vertex of the star S_{2s-n+2}; $C_{n,s}^2$ is defined as the graph formed by identifying an end-vertex of each of s paths P_3 together; $C_{n,s}^3$ denotes the graph formed by identifying an end-vertex of each of $s-1$ paths (each of length at least 2) and one end-vertex of one path (length at least 3) together.

Clearly, $B_{n,s}, C_{n,s}^1, C_{n,s}^2, C_{n,s}^3 \in \mathcal{J}_{n,s}$.

Theorem 4.1. *Let $T \in \mathcal{J}_{n,s}$ with $3 \leq s \leq n-2$. If the following conditions hold:*
(i) $f(x, y)$ is strictly increasing with $x \geq 1$;
(ii) $f(x, y) < f(x+y-1, 1)$ holds for all $x, y \geq 2$;
(iii) $g(x) = f(2, x)$ is strictly convex downward with regard to x;
(iv) The expression $f(x, y) - f(x-1, y)$ is strictly decreasing with $y \geq 1$.
Then,

$$TI_f(T) \leq f(1, 2) + (s-1)f(1, s) + (n-s-2)f(2, 2) + f(2, s),$$

the equality occurs precisely when $m_{1,2} = m_{2,s} = 1$, $m_{1,s} = s-1$, and $m_{2,2} = n-s-2$. That is, $T \cong B_{n,s}$.

Proof. Let $T^* \in \mathcal{J}_{n,s}^{max}$. We can claim that T^* is a starlike tree. Otherwise, there exists a segment composed of non-pendant edges; that is, there exists an induced sub-path $P_l = u_1u_2\cdots u_l$, where $d_{T^*}(u_1) \geq 2$ and $d_{T^*}(u_l) \geq 2$. Using the path lifting transformation from Lemma 4.1, we derive that $TI_f(T^*) < TI_f(T')$, which contradicts the fact that $T^* \in \mathcal{J}_{n,s}^{max}$.

Thus, T^* is a starlike tree. By condition (iv) of the theorem and Lemma 4.2(i), there is precisely one pendant path with length no less than 2 in T^*. Therefore, we have $T^* \cong B_{n,s}$, and consequently,

$$TI_f(T) \leq TI_f(T^*) = f(1, 2) + (s-1)f(1, s) + (n-s-2)f(2, 2) + f(2, s),$$

the equality occurs precisely when $m_{1,2} = m_{2,s} = 1$, $m_{1,s} = s-1$, and $m_{2,2} = n-s-2$. This completes the proof of the theorem. □

Theorem 4.2. *Let $T \in \mathcal{J}_{n,s}$ with $3 \leq s \leq n-2$. If the following conditions hold:*
(i) $f(x, y)$ is strictly increasing with $x \geq 1$;
(ii) $f(x, y) < f(x+y-1, 1)$ holds for all $x, y \geq 2$;
(iii) $g(x) = f(2, x)$ is strictly convex downward with regard to x;

(iv) The expression $f(x, y) - f(x-1, y)$ is strictly increasing with $y \geq 1$.
Then,

$$TI_f(T) \leq \begin{cases} (n-s-1)(f(1,2)+f(2,s)) + (2s-n+1)f(1,s), & \text{when } n \leq 2s, \\ s(f(1,2)+f(2,s)), & \text{when } n = 2s+1, \\ s(f(1,2)+f(2,s)) + (n-2s-1)f(2,2), & \text{when } n \geq 2s+2. \end{cases}$$

the equality occurs precisely when $T \cong C^1_{n,s}$ for $n \leq 2s$, $T \cong C^2_{n,s}$ for $n = 2s+1$, and $T \cong C^3_{n,s}$ for $n \geq 2s+2$.

Proof. Let $T^* \in \mathcal{J}^{max}_{n,s}$. Analogously to Theorem 4.1, on the one hand, it follows from conditions (i)–(iii) and Lemma 4.1 that T^* is a starlike tree. On the other hand, by condition (iv) of the theorem and Lemma 4.2(ii), all pendant paths in T^* are of length at least 2 or at most 2. Therefore, we have

$$T^* \cong \begin{cases} C^1_{n,s}, & if\ n \leq 2s, \\ C^2_{n,s}, & if\ n = 2s+1, \\ C^3_{n,s}, & if\ n \geq 2s+2. \end{cases}$$

Consequently,

$$TI_f(T) \leq \begin{cases} (n-s-1)(f(1,2)+f(2,s)) + (2s-n+1)f(1,s), & \text{when } n \leq 2s, \\ s(f(1,2)+f(2,s)), & \text{when } n = 2s+1, \\ s(f(1,2)+f(2,s)) + (n-2s-1)f(2,2), & \text{when } n \geq 2s+2. \end{cases}$$

This completes the proof of the theorem. □

5. Applications

In this section, we verify the degree-based indices that satisfy the sufficient conditions for the minimum and maximum values established in the previous two sections. First, we verify the indices corresponding to the sufficient conditions for the minimum value. Through direct computation, we obtain the following conclusion, and the detailed computation process is omitted herein.

Proposition 5.1. *The degree-based indices from No.1 to No.7 in Table 1 satisfy the conditions:*
(i) $\varphi(2,2) < 0$, and $\varphi(x,y) > 0$ for any pair $(x,y) \in \Omega_1 \cup \Omega_2$;
(ii) $\varphi(1,2) < \varphi(1,3) < \varphi(1,y)$ for all $y \geq 4$;
(ii) $\varphi(3,4) < \varphi(2,4) < \varphi(x,4)$ for all $x \neq 2, 3$;
(iv) The expression $f(x,y) - f(x-1,y)$ is strictly decreasing with $y \geq 1$.

Table 1. Some degree-based indices with determined extremal values of TI_f.

No.	$f(x,y)$	Indices	Min	Max	Ref.
1	$\sqrt{x+y}$	Reciprocal sum-connectivity index	$A_{n,s}$		
2	$\sqrt{x^2+y^2}$	Sombor index	$A_{n,s}$	$B_{n,s}$	[17]
3	$\sqrt{(x-1)^2+(y-1)^2}$	Reduced Sombor index	$A_{n,s}$	$B_{n,s}$	
4	$\sqrt{x^2+y^2+xy}$	Euler Sombor index	$A_{n,s}$	$B_{n,s}$	
5	$\sqrt{2}\pi\frac{x^2+y^2}{x+y}$	Third Sombor index	$A_{n,s}$		
6	$\frac{\pi}{2}(\frac{x^2+y^2}{x+y})^2$	Fourth Sombor index	$A_{n,s}$		
7	$\frac{\sqrt{x^2+y^2}}{x+y}$	Diminished Sombor index	$A_{n,s}$		
8	$(x+y)\sqrt{x^2+y^2}$	Elliptic Sombor index		$C_{n,s}$	[19]

From Theorem 3.1 and Proposition 5.1, we can immediately deduce the following theorem. We note that, since all vertices of the extremal tree have degree less than 4, this theorem is also applicable to chemical trees.

Theorem 5.1. *Let $T \in \mathcal{J}_{n,s}$ ($T \in C\mathcal{J}_{n,s}$) with $3 \le s \le n-2$. For degree-based indices from No.1 to No.7 in Table 1, the following conclusions hold.*

(i) s is odd, then

$$TI_f(T) \ge \begin{cases} \frac{s+3}{2}(f(1,2)+f(2,3)) + \frac{s-3}{2}f(3,3) + \frac{2n-3s-5}{2}f(2,2), \\ \qquad\qquad for\ 3 \le s \le \frac{2n-5}{3}, \\ (n-s-1)f(1,2) + \frac{3s-2n+5}{2}f(1,3) + (n-s-1)f(2,3) + \frac{s-3}{2}f(3,3), \\ \qquad\qquad for\ \frac{2n-5}{3} \le s \le n-2, \end{cases}$$

the equality occurs iff $T \in A^1_{n,s}$ for $3 \le s \le \frac{2n-5}{3}$ and $T \in A^2_{n,s}$ for $\frac{2n-5}{3} \le s \le n-2$.

(ii) s is even, then

$$TI_f(T) \ge \begin{cases} (\frac{s}{2}+2)f(1,2) + (s-4)f(2,3) + (6-s)f(2,4) + (\frac{s}{2}-2)f(3,4) + (n-\frac{3s}{2}-3)f(2,2), \\ \qquad\qquad for\ 4 \le s \le 10, \\ (\frac{s}{2}+2)(f(1,2)+f(2,3)) + (\frac{s}{2}-6)f(3,3) + 4f(3,4) + (n-\frac{3s}{2}-3)f(2,2), \\ \qquad\qquad for\ 12 \le s \le \frac{2n-6}{3}, \\ (n-s-1)(f(1,2)+f(2,3)) + (\frac{3s}{2}-n+3)f(1,3) + (\frac{s}{2}-6)f(3,3) + 4f(3,4), \\ \qquad\qquad for\ \frac{2n-6}{3} \le s \le n-2, \end{cases}$$

the equality occurs iff $T \in A^3_{n,s}$ for $4 \le s \le 10$, $T \in A^4_{n,s}$ for $12 \le s \le \frac{2n-6}{3}$, and $T \in A^5_{n,s}$ for $\frac{2n-6}{3} \le s \le n-2$.

Now, we verify the degree-based indices that satisfy the sufficient conditions for the maximum value. Through direct computation, we deduce the following conclusions, and the detailed computation process is omitted herein.

Proposition 5.2. *The degree-based indices from No.2 to No.4 in Table 1 satisfy the conditions:*
(i) $f(x, y)$ *is strictly increasing with* $x \geq 1$*;*
(ii) $f(x, y) < f(x + y - 1, 1)$ *holds for all* $x, y \geq 2$*;*
(iii) $g(x) = f(2, x)$ *is strictly convex downward with regard to x;*
(iv) The expression $f(x, y) - f(x - 1, y)$ *is strictly decreasing with* $y \geq 1$.

Proposition 5.3. *The degree-based index of No.8 in Table 1 satisfies the conditions:*
(i) $f(x, y)$ *is strictly increasing with* $x \geq 1$*;*
(ii) $f(x, y) < f(x + y - 1, 1)$ *holds for all* $x, y \geq 2$*;*
(iii) $g(x) = f(2, x)$ *is strictly convex downward with regard to x;*
(iv) The expression $f(x, y) - f(x - 1, y)$ *is strictly increasing with* $y \geq 1$.

Thus, from Theorem 4.1 and Proposition 5.2, we can deduce the following Theorem 5.2. Similarly, from Theorem 4.2 and Proposition 5.3, Theorem 5.3 holds.

Theorem 5.2. *Let* $T \in \mathcal{J}_{n,s}$ *with* $3 \leq s \leq n - 2$. *For degree-based indices from No.2 to No.4 in Table 1, then*

$$TI_f(T) \leq f(1, 2) + (s - 1)f(1, s) + (n - s - 2)f(2, 2) + f(2, s),$$

the equality occurs precisely when $T \cong B_{n,s}$.

Theorem 5.3. *Let* $T \in \mathcal{J}_{n,s}$ *with* $3 \leq s \leq n - 2$. *For degree-based index of No.8 in Table 1, then*

$$TI_f(T) \leq \begin{cases} (n - s - 1)(f(1, 2) + f(2, s)) + (2s - n + 1)f(1, s), & \text{when } n \leq 2s, \\ s(f(1, 2) + f(2, s)), & \text{when } n = 2s + 1, \\ s(f(1, 2) + f(2, s)) + (n - 2s - 1)f(2, 2), & \text{when } n \geq 2s + 2. \end{cases}$$

the equality occurs precisely when $T \cong C^1_{n,s}$ *for* $n \leq 2s$*,* $T \cong C^2_{n,s}$ *for* $n = 2s + 1$*, and* $T \cong C^3_{n,s}$ *for* $n \geq 2s + 2$.

6. Concluding remarks

The main work of this paper is to determine the minimum and maximum TI_f values of several degree-based topological indices for trees with a given segment number by providing sufficient conditions, and to characterize the corresponding extremal trees. Among these indices, those whose maximum values are first determined in this paper include the reciprocal sum-connectivity index, the reduced Sombor index, the Euler Sombor index, the third Sombor index, the fourth Sombor index, and the diminished Sombor index. Meanwhile, the reduced Sombor index and the Euler Sombor index are the ones whose minimum values are first determined herein. Additionally, we derived the already established minimum and maximum values of the Sombor index, as well as the maximum value of the elliptic Sombor index. Possible future work is to further investigate the extremal problems of connected graphs with different given parameters, such as girth, maximum degree, chromatic number, etc. Based on this, we propose a relevant and noteworthy problem.

Problem 1. Determining the extremal unicyclic and bicyclic graphs for degree-based topological indices with a given maximum degree.

Use of Generative-AI tools declaration

The author declares he has not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The author declares no conflicts of interest.

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