

On the Sum of Topological Index and Its Reciprocal Index of Trees with Fixed Matching Number

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Abstract

The sum of the degree-based topological index and its reciprocal index of a graph G is defined as

$$TI_f(G) + RTI_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)) + \sum_{uv \in E(G)} \frac{1}{f(d(u), d(v))},$$

where $f(x, y) = f(y, x)$ is a symmetric real-valued function. In this paper, for the first Zagreb index ($f(x, y) = x + y$), the forgotten index ($f(x, y) = x^2 + y^2$), and the Sombor index $f(x, y) = \sqrt{x^2 + y^2}$, we establish the sharp upper bounds of $TI_f(G) + RTI_f(G)$ for trees with fixed order n and matching number m , and characterize the corresponding extremal graphs. These results extend the results on trees obtained by Gao [W. Gao, MATCH Commun. Math. Comput. Chem. 93 (2025) 535–547].

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1 Introduction

All graphs we considered are simple, undirected, and connected, denoted by $G = (V(G), E(G))$, where $V(G)$ represents the vertex set and $E(G)$ the edge set of G . For a vertex $u \in V(G)$, $d_G(u)$ (or simply $d(u)$ for brevity) denotes the degree of u , i.e., the number of vertices adjacent to u . $N_G(u)$ denotes the set of all vertices adjacent to u . A vertex u is called a pendant vertex if $d(u) = 1$. An edge uv is called a pendant edge or leaf if $d(u) = 1$ or $d(v) = 1$. For convenience, $G - u$ denotes the graph obtained by removing all edges incident to u from G .

A subset $M \subseteq E(G)$ is called a matching of G if no two edges in M are adjacent. A matching M is maximum if there exists no matching M' such that $|M'| > |M|$. A vertex $v \in V(G)$ is said to be M -saturated if it is incident to an edge in M . In particular, if every vertex in G is M -saturated, then M is called a perfect matching. The number of edges in a maximum matching is referred to as the matching number of G . A connected acyclic graph is called a tree, denoted by T . Let $\mathcal{J}_{n,m}$ denote the set of all trees with n vertices and matching number m . Other undefined concepts and terminologies follow those in standard graph theory references [6].

Chemical graph theory is an important branch of mathematical chemistry, which models molecular structures and presents chemical information in a mathematical manner. In this field, atoms are represented by vertices and chemical bonds by edges between vertices, resulting in a molecular graph. Graph-theoretic invariants of molecular graphs are called topological indices, which assist chemists in analyzing and predicting the physical and chemical properties of compounds. Topological indices have been widely applied in drug screening, new chemical development, and related fields [12, 17, 19].

As an important class of topological indices, the degree-based topological index of a graph G is defined as

$$TI_f = TI_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where $f(x, y) = f(y, x)$ is a real-valued symmetric function. The reciprocal

index is defined as

$$RTI_f = RTI_f(G) = \sum_{uv \in E(G)} \frac{1}{f(d(u), d(v))}.$$

For a long time, research in the literature has focused on individual topological indices TI_f , such as the ABS index [1, 2], Sombor index [9, 10], and forgotten index [8]. In particular, researchers have introduced numerous graph-theoretic parameters to investigate various topological indices, including the matching number, domination number, girth, and so on [15, 21, 23, 24].

In addition, attention has shifted to the study of relationships between different indices, such as the difference indices of distinct topological indices [5, 20], and the product of an index and its reciprocal index [4, 11, 16, 22]. Notably, in 2025, Gao [13] first studied the sum of a topological index and its reciprocal index ($TI_f + RTI_f$), and determined the trees that achieve the maximum and minimum values of this sum for the First Zagreb index, second Zagreb index, and forgotten index. In the same year, Albalahi et al. [3] obtained the extremal unicyclic graphs for the sum of several topological indices and their reciprocal indices. In 2026, Gao [14] investigated the maximum and minimum values of the sum of the Randić index and its reciprocal index for uniform hypergraphs. Additionally, Li and Zhang [18] derived the extreme values of the sum of the Second Zagreb index and its reciprocal index on bicyclic graphs.

Motivated by the above works, this paper extends Gao's results [13] by studying the maximum value of $TI_f + RTI_f$ for trees with fixed order n and matching number m . We determine the maximum values of the sums of the First Zagreb index, forgotten index, and Sombor index with their respective reciprocal indices, and characterize the corresponding extremal trees.

2 Preliminaries

In this section, we present several useful lemmas, which will be applied in the subsequent sections.

Lemma 1. Let $uv \in T$ be a non-pendant edge, and let T' be the graph obtained from T by performing a lifting transformation on uv : first contract edge uv into a new vertex w , then add an isolated vertex z , and join w and z to form a pendant edge wz , as illustrated in Figure 1. Then, the inequality

$$TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T)$$

holds for $f(x, y) = x + y$, $x^2 + y^2$, and $\sqrt{x^2 + y^2}$.

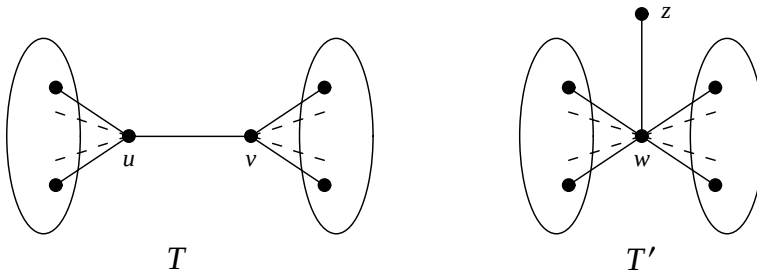


Figure 1. Trees of T and T' in Lemma 1.

Proof. Let $d_T(u) = r \geq 2$, $d_T(v) = s \geq 2$, $N_T(u) = \{v, u_1, u_2, \dots, u_{r-1}\}$, and $N_T(v) = \{u, v_1, v_2, \dots, v_{s-1}\}$. From the lifting transformation,

$$\begin{aligned} & TI_f(T') + RTI_f(T') - TI_f(T) - RTI_f(T) \\ &= f(1, r + s - 1) + \frac{1}{f(1, r + s - 1)} - f(r, s) - \frac{1}{f(r, s)} \\ &+ \sum_{i=1}^{r-1} \left[f(r + s - 1, d(u_i)) + \frac{1}{f(r + s - 1, d(u_i))} - f(r, d(u_i)) - \frac{1}{f(r, d(u_i))} \right] \\ &+ \sum_{i=1}^{s-1} \left[f(r + s - 1, d(v_i)) + \frac{1}{f(r + s - 1, d(v_i))} - f(s, d(v_i)) - \frac{1}{f(s, d(v_i))} \right]. \end{aligned}$$

(i) For $f(x, y) = x + y$, then $f(1, r + s - 1) + \frac{1}{f(1, r + s - 1)} - f(r, s) - \frac{1}{f(r, s)} = 0$, and

$$\begin{aligned} & f(r + s - 1, d(u_i)) + \frac{1}{f(r + s - 1, d(u_i))} - f(r, d(u_i)) - \frac{1}{f(r, d(u_i))} \\ &= s - 1 + \frac{1}{r + s - 1 + d(u_i)} - \frac{1}{r + s + d(u_i)} > 0. \end{aligned}$$

Accordingly, we obtain that $TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T)$.

(ii) For $f(x, y) = x^2 + y^2$, then it follows that $f(1, r+s-1) + \frac{1}{f(1, r+s-1)} - f(r, s) - \frac{1}{f(r, s)} = 2(r-1)(s-1) \left[1 - \frac{1}{((r+s-1)^2+1)(r^2+s^2)} \right] > 0$, and

$$\begin{aligned} & f(r+s-1, d(u_i)) + \frac{1}{f(r+s-1, d(u_i))} - f(r, d(u_i)) - \frac{1}{f(r, d(u_i))} \\ &= (s-1)(2r+s-1) \left[1 - \frac{1}{((r+s-1)^2)(r^2+t^2)} \right] > 0. \end{aligned}$$

Consequently, we have $TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T)$.

(iii) For $f(x, y) = \sqrt{x^2 + y^2}$, then $f(1, r+s-1) + \frac{1}{f(1, r+s-1)} - f(r, s) - \frac{1}{f(r, s)} = \left(\sqrt{(r+s-1)^2+1} - \sqrt{r^2+s^2} \right) \left(1 - \frac{1}{\sqrt{((r+s-1)^2+1)(r^2+s^2)}} \right) > 0$, and

$$\begin{aligned} & f(r+s-1, d(u_i)) + \frac{1}{f(r+s-1, d(u_i))} - f(r, d(u_i)) - \frac{1}{f(r, d(u_i))} \\ &= \left(\sqrt{(r+s-1)^2 + d(u_i)^2} - \sqrt{r^2 + d(u_i)^2} \right) \cdot \\ & \left(1 - \frac{1}{\sqrt{((r+s-1)^2 + d(u_i)^2)(r^2 + d(u_i)^2)}} \right) > 0. \end{aligned}$$

Therefore, we deduce $TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T)$. ■

Lemma 2. Let $f(x, y) = x + y$ or $f(x, y) = x^2 + y^2$, where $a, x \geq 1$ are positive integers. Then,

- (i) $g_1(x) = f(x, a) + \frac{1}{f(x, a)}$ is strictly increasing with respect to x ;
- (ii) $g_2(x) = f(x, a) + \frac{1}{f(x, a)} - f(x, a-1) - \frac{1}{f(x, a-1)}$ is strictly increasing for x ;
- (iii) $g_3(x) = f(x, a) + \frac{1}{f(x, a)} - f(x-1, a) - \frac{1}{f(x-1, a)}$ is strictly increasing with respect to x .

Proof. We first prove (i). If $f(x, y) = x + y$, then $g_1(x) = x + a + \frac{1}{x+a}$ and $g_1'(x) = 1 - \frac{1}{(x+a)^2}$. The conclusion follows immediately. The case $f(x, y) = x^2 + y^2$ can be obtained similarly.

Next we prove (ii). If $f(x, y) = x + y$, then $g_2(x) = 1 - \frac{1}{(x+a)(x+a-1)}$, which is strictly increasing in x . If $f(x, y) = x^2 + y^2$, then $g_2(x) = 2a -$

$1 + \frac{1}{x^2+a^2} - \frac{1}{x^2+(a-1)^2}$, and

$$g'_2(x) = 2x \left[\frac{1}{(x^2 + (a-1)^2)^2} - \frac{1}{(x^2 + a^2)^2} \right] > 0.$$

Hence $g_2(x)$ is strictly increasing in x .

We now prove (iii). If $f(x, y) = x + y$, then $g_3(x) = 1 - \frac{1}{(x+a)(x+a-1)}$, which is strictly increasing in x . If $f(x, y) = x^2 + y^2$, then $g_3(x) = 2x - 1 + \frac{1}{x^2+a^2} - \frac{1}{(x-1)^2+a^2}$, and

$$g'_3(x) = 2 - \frac{2x}{(x^2 + a^2)^2} + \frac{2(x-1)}{((x-1)^2 + a^2)^2} > 0.$$

Thus $g_3(x)$ is strictly increasing in x . This completes the proof of the lemma. ■

Lemma 3. Let $f(x, y) = \sqrt{x^2 + y^2}$, where $a, x \geq 1$ are positive integers.

- (i) $g_1(x) = f(x, a) + \frac{1}{f(x, a)}$ is strictly increasing with respect to x ;
- (ii) $g_2(x) = f(x, a) + \frac{1}{f(x, a)} - f(x, a-1) - \frac{1}{f(x, a-1)}$ is strictly decreasing with respect to x ($a \geq 2$);
- (iii) $g_3(x) = f(x, a) + \frac{1}{f(x, a)} - f(x-1, a) - \frac{1}{f(x-1, a)}$ is strictly increasing for x .

Proof. (i) Since $g_1(x) = \sqrt{x^2 + a^2} + \frac{1}{\sqrt{x^2 + a^2}}$, we have

$$g'_1(x) = \frac{x[(x^2 + a^2) - 1]}{(x^2 + a^2)^{\frac{3}{2}}} > 0.$$

Thus $g_1(x)$ is strictly increasing with respect to x .

(ii) Since $g_2(x) = \left(\sqrt{x^2 + a^2} + \frac{1}{\sqrt{x^2 + a^2}} \right) - \left(\sqrt{x^2 + (a-1)^2} + \frac{1}{\sqrt{x^2 + (a-1)^2}} \right)$, we obtain

$$g'_2(x) = x \left[\frac{x^2 + a^2 - 1}{(x^2 + a^2)^{\frac{3}{2}}} - \frac{x^2 + (a-1)^2 - 1}{(x^2 + (a-1)^2)^{\frac{3}{2}}} \right].$$

Let $\varphi(s) = \frac{s-1}{s^{\frac{3}{2}}}$, where $s > 3$. It is straightforward to verify that $\varphi(s)$ is strictly decreasing, which implies

$$\varphi(x^2 + a^2) < \varphi(x^2 + (a-1)^2).$$

This implies $g'_2(x) < 0$. Therefore, $g_2(x)$ is strictly decreasing for x .

(iii) Since $g_3(x) = \left(\sqrt{x^2 + a^2} + \frac{1}{\sqrt{x^2 + a^2}} \right) - \left(\sqrt{(x-1)^2 + a^2} + \frac{1}{\sqrt{(x-1)^2 + a^2}} \right)$, we have

$$g'_3(x) = \frac{x(x^2 + a^2 - 1)}{(x^2 + a^2)^{\frac{3}{2}}} - \frac{(x-1)[(x-1)^2 + a^2 - 1]}{((x-1)^2 + a^2)^{\frac{3}{2}}} = \phi(x) - \phi(x-1).$$

The function $\phi(x) = \frac{x(x^2 + a^2 - 1)}{(x^2 + a^2)^{\frac{3}{2}}}$ is strictly increasing with respect to x , so $g'_3(x) > 0$. Hence $g_3(x)$ is strictly increasing with respect to x . This completes the proof of the lemma. $\blacksquare$

3 Maximal $TI_f + RTI_f$ of trees with fixed matching number

In this section, we derive the maximum value of $TI_f + RTI_f$ for all n -vertex trees with matching number m , and characterize the corresponding extremal trees. Firstly, we define a special class of trees.

Let T_m^n be the graph obtained by attaching $m-1$ pendant vertices to $m-1$ leaves of the star graph S_{n-m+1} , see Figure 2. Clearly, $2m \leq n$. In particular, if $n = 2m$, then $T_m^n = T_m^{2m}$ and it has an m -perfect matching.

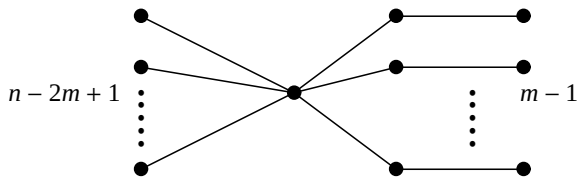


Figure 2. Trees of T_m^n .

Lemma 4. ([7]) Let $T \in \mathcal{J}_{2m,m}$ with $m \geq 2$, Then T contains a pendant vertex of degree two in its neighborhood.

Lemma 5. Let $T \in \mathcal{J}_{n,m}$ be a tree attaining the maximum value of $TI_f(T) + RTI_f(T)$, where $f(x, y) = x + y$, $x^2 + y^2$, and $\sqrt{x^2 + y^2}$. Let M be an m -matching of T . Then

- (i) If $uv \in M$, then uv is a pendant edge;
- (ii) If u is a non-pendant vertex, then u is M -saturated.

Proof. (i) Suppose that uv is not a pendant edge. Since $uv \in M$, let T' be the graph obtained from T by performing the lifting transformation on uv . By Lemma 1, we have

$$TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T),$$

which contradicts the maximality of T .

(ii) If $T \cong S_n$, the conclusion holds. Now consider the case $T \not\cong S_n$. Assume for contradiction that u is not M -saturated. Since u is a non-pendant vertex, there exists a non-pendant vertex v such that $uv \in E(T)$. As u is not M -saturated, we have $uv \notin M$. Perform the lifting transformation on uv to obtain the graph T' . Again by Lemma 1, we obtain

$$TI_f(T') + RTI_f(T') > TI_f(T) + RTI_f(T),$$

which contradicts the maximality of T . Therefore, the assumption is false, and the lemma is proved. ■

Theorem 1. Let $T \in \mathcal{J}_{2m,m}$ with $m \geq 1$. Let TI_f be the first Zagreb index ($f(x, y) = x + y$), the forgotten index ($f(x, y) = x^2 + y^2$), and the Sombor index ($f(x, y) = \sqrt{x^2 + y^2}$). Then

$$\begin{aligned} TI_f(T) + RTI_f(T) &\leq (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right] + (m-1) [f(2, m) \\ &\quad + \frac{1}{f(2, m)}] + f(1, m) + \frac{1}{f(1, m)}. \end{aligned}$$

Equality holds if and only if $T \cong T_m^{2m}$.

Proof. We prove the theorem by mathematical induction on m . When $m = 1, 2$, T is isomorphic to P_2 and P_4 , respectively, and the conclusion follows immediately. Assume that the theorem holds for $m - 1$. Let $T \in \mathcal{J}_{2m,m}$ be a tree attaining the maximum value of $TI_f(T) + RTI_f(T)$. By Lemma 4, there exists a pendant vertex u , and let v be its neighbor with degree two. Let M be a perfect matching of T . Then $uv \in M$. Set $N_T(v) = \{u, w\}$ and $N_T(w) = \{v, w_1, w_2, \dots, w_{r-1}\}$, with $d_T(w) = r$. We first present the following two claims.

Claim 1. There exists some vertex, say w_1 , such that $d(w_1) = 1$, and $d(w_i) \geq 2$ for all $2 \leq i \leq r - 1$.

Proof. Since $uv \in M$, by Lemma 5, there exists a vertex w_i adjacent to w , say w_1 , such that $ww_1 \in M$ and $d(w_1) = 1$. For $2 \leq i \leq r - 1$, since M is a perfect matching, we have $d(w_i) \neq 1$, i.e., $d(w_i) \geq 2$. ■

Claim 2. $r \leq m$, and $r + d_T(w_i) \leq m + 2$ for all $2 \leq i \leq r - 1$.

Proof. On the one hand, by Lemma 5(i), T contains at least m pendant edges and a perfect matching consisting of m edges. Thus there are at least $m - 1$ pendant edges not incident to w . Therefore,

$$r = d(w) \leq 2m - 1 - (m - 1) = m.$$

On the other hand, by Claim 1, we have $uv, ww_1 \in M$. If $r = m$, then for $2 \leq i \leq r - 1$, exactly $m - 2$ edges belong to M . Hence by Lemma 5(i), there exist $m - 2$ pendant edges $w_i z_i \in M$ incident to w , satisfying $d(w_i) = 2$ and $d(z_i) = 1$, which implies $T \cong T_m^{2m}$.

If $r \leq m - 1$, then there are at least $2(m - 1)$ edges not incident to w , among which $m - r$ edges in M are pendant edges. Thus, except for the pendant paths incident to w_i and the vertex w , there are at most $m - r$ edges incident to each w_i . This yields $d(w_i) \leq 2 + m - r = m - r + 2$, and consequently $r + d(w_i) \leq m + 2$. This completes the proof of Claim 2. ■

We now return to the proof of the theorem, and construct the following transformation.

Transformation 1: $T' = T - u - v$.

Since $uv \in M$, we have $T' \in \mathcal{J}_{2(m-1), m-1}$. By Transformation 1, we obtain

$$\begin{aligned} & TI_f(T) + RTI_f(T) \\ &= TI_f(T') + RTI_f(T') + f(1, 2) + \frac{1}{f(1, 2)} + f(2, r) \\ &+ \frac{1}{f(2, r)} + f(1, r) + \frac{1}{f(1, r)} - f(1, r - 1) - \frac{1}{f(1, r - 1)} \end{aligned}$$

$$+ \sum_{i=2}^{r-1} \left[f(r, d(w_i)) + \frac{1}{f(r, d(w_i))} - f(r-1, d(w_i)) - \frac{1}{f(r-1, d(w_i))} \right].$$

(i) If $f(x, y) = x + y$. By Lemma 2(i) and Lemma 2(iii), together with $r \leq m$, we have

$$\begin{aligned} f(2, r) + \frac{1}{f(2, r)} &\leq f(2, m) + \frac{1}{f(2, m)}, \\ f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\ &\leq f(1, m) + \frac{1}{f(1, m)} - f(1, m-1) - \frac{1}{f(1, m-1)}. \end{aligned}$$

Therefore, combining Claim 2 and the inductive hypothesis for $m-1$, we deduce

$$\begin{aligned} &TI_f(T) + RTI_f(T) \\ &\leq (m-2) \left[f(1, 2) + \frac{1}{f(1, 2)} \right] + (m-2) \left[f(2, m-1) + \frac{1}{f(2, m-1)} \right] \\ &+ f(1, m-1) + \frac{1}{f(1, m-1)} + f(1, 2) + \frac{1}{f(1, 2)} + f(2, m) + \frac{1}{f(2, m)} \\ &+ f(1, m) + \frac{1}{f(1, m)} - f(1, m-1) - \frac{1}{f(1, m-1)} \\ &+ \sum_{i=2}^{r-1} \left[f(m, 2) + \frac{1}{f(m, 2)} - f(m-1, 2) - \frac{1}{f(m-1, 2)} \right] \\ &= (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right] + (m-1) \left[f(2, m) + \frac{1}{f(2, m)} \right] \\ &+ f(1, m) + \frac{1}{f(1, m)}. \end{aligned}$$

Equality holds if and only if $T' \cong T_{m-1}^{2m-2}$, $r = m$, $d_T(w_1) = 1$, and $d_T(w_i) = 2$ for all $2 \leq i \leq m-1$, i.e., $T \cong T_m^{2m}$.

(ii) If $f(x, y) = x^2 + y^2$. On the one hand, by Lemma 3(i) and (iii), we have

$$f(2, r) + \frac{1}{f(2, r)} \leq f(2, m) + \frac{1}{f(2, m)},$$

$$\begin{aligned}
& f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\
& \leq f(1, m) + \frac{1}{f(1, m)} - f(1, m-1) - \frac{1}{f(1, m-1)}.
\end{aligned}$$

On the other hand, note that

$$\begin{aligned}
g(x, y) &= f(x, y) + \frac{1}{f(x, y)} - f(x-1, y) - \frac{1}{f(x-1, y)} \\
&= 2x-1 + \frac{1}{x^2+y^2} - \frac{1}{(x-1)^2+y^2}.
\end{aligned}$$

It is clear that $2x-1 > \frac{1}{(x-1)^2+y^2} - \frac{1}{x^2+y^2}$, so $g(x, y)$ increases faster with respect to x than with respect to y . Thus, by $r + d(w_i) \leq m+2$, $r \leq m$ and $d(w_i) \geq 2$, we obtain

$$\begin{aligned}
& f(r, d(w_i)) + \frac{1}{f(r, d(w_i))} - f(r-1, d(w_i)) - \frac{1}{f(r-1, d(w_i))} \\
& \leq f(m, 2) + \frac{1}{f(m, 2)} - f(m-1, 2) - \frac{1}{f(m-1, 2)}.
\end{aligned}$$

Therefore, combining the inductive hypothesis for $m-1$, similarly to case (i), we derive

$$\begin{aligned}
TI_f(T) + RTI_f(T) &\leq (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right] \\
&\quad + (m-1) \left[f(2, m) + \frac{1}{f(2, m)} \right] + f(1, m) + \frac{1}{f(1, m)}.
\end{aligned}$$

Equality holds if and only if $T' \cong T_{m-1}^{2m-2}$, $r = m$, $d_T(w_1) = 1$, and $d_T(w_i) = 2$ for all $2 \leq i \leq m-1$, i.e., $T \cong T_m^{2m}$.

(iii) If $f(x, y) = \sqrt{x^2 + y^2}$. On the one hand, by Lemma 3(i) and (iii), we have

$$\begin{aligned}
& f(2, r) + \frac{1}{f(2, r)} \leq f(2, m) + \frac{1}{f(2, m)}, \\
& f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\
& \leq f(1, m) + \frac{1}{f(1, m)} - f(1, m-1) - \frac{1}{f(1, m-1)}.
\end{aligned}$$

On the other hand, by Lemma 3(iii) and (ii), we obtain

$$\begin{aligned}
& \sum_{i=2}^{r-1} \left[f(r, d(w_i)) + \frac{1}{f(r, d(u_i))} - f(r-1, d(w_i)) - \frac{1}{f(r-1, d(u_i))} \right] \\
& \leq \sum_{i=2}^{r-1} \left[f(r, 2) + \frac{1}{f(r, 2)} - f(r-1, 2) - \frac{1}{f(r-1, 2)} \right] \\
& \leq (m-2) \left[f(m, 2) + \frac{1}{f(m, 2)} - f(m-1, 2) - \frac{1}{f(m-1, 2)} \right].
\end{aligned}$$

Therefore, combining the inductive hypothesis for $m-1$, similarly to case (i), we conclude

$$\begin{aligned}
TI_f(T) + RTI_f(T) & \leq (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right] \\
& \quad + (m-1) \left[f(2, m) + \frac{1}{f(2, m)} \right] + f(1, m) + \frac{1}{f(1, m)}.
\end{aligned}$$

Equality holds if and only if $T \cong T_m^{2m}$.

Combining the above arguments, we finish the proof of the theorem. ■

Theorem 2. *Let $T \in \mathcal{J}_{n,m}$ with $m \geq 1$ and $n \geq 2$. If $f(x, y) = x + y$, $x^2 + y^2$, or $\sqrt{x^2 + y^2}$, then*

$$\begin{aligned}
TI_f(T) + RTI_f(T) & \leq (n-2m+1) \left[f(1, n-m) + \frac{1}{f(1, n-m)} \right] \\
& \quad + (m-1) \left[f(2, n-m) + \frac{1}{f(2, n-m)} \right] + (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right].
\end{aligned}$$

Equality holds if and only if $T \cong T_m^n$.

Proof. Let $T \in \mathcal{J}_{n,m}$. Then we have $n \geq 2m$. If $n = 2m$, the conclusion follows from Theorem 1. For $n \geq 2m+1$, we prove the theorem by mathematical induction on n .

When $n = 2$ or 3 , T is isomorphic to P_2 and P_3 , respectively. By direct calculation, it is easy to verify that Theorem 2 holds. Assume that the theorem holds for order $n-1$. It suffices to prove that the theorem holds for order n .

Let $T \in \mathcal{J}_{n,m}$ be a tree attaining the maximum value of $TI_f(T) + RTI_f(T)$. Since $n \geq 2m + 1$, by Lemma 5, there exists a maximum matching M and a pendant vertex u such that u is not M -saturated. Let $uv \in E(T)$. Since M is a maximum matching, v is M -saturated. Suppose $d_T(v) = r$ and $N_T(v) = \{u, v_1, v_2, \dots, v_{r-1}\}$. For convenience, let k be the number of vertices $v_i \in N_T(v) \setminus \{u\}$ with $d_T(v_i) = 1$.

If $m = 1$, then $T \cong S_n \cong T_1^n$. Thus

$$TI_f(T) + RTI_f(T) = (n-1) \left[f(1, n-1) + \frac{1}{f(1, n-1)} \right],$$

and the conclusion holds. Now consider the case $m \geq 2$, i.e., $T \not\cong S_n$. We first present two claims.

Claim 1. $k \leq n - 2m$, and the number of vertices satisfying $d_T(v_i) \geq 2$ is $r - k - 1$ (≥ 1).

Proof. Since $m \geq 2$, among the r neighbors of v , there exists at least one vertex v_i such that $d_T(v_i) \geq 2$. The number of pendant vertices adjacent to v satisfies $1 \leq k + 1 \leq r - 1$. Hence there are at least k neighbors of v that are not M -saturated. On the other hand, there are $n - 2m$ vertices in T that are not M -saturated, so $k \leq n - 2m$. Therefore, the number of vertices with $d_T(v_i) \geq 2$ is $r - k - 1$, and $r - k - 1 \geq 1$. ■

Claim 2. $r \leq n - m$, and $r + d_T(v_i) \leq n - m + 2$ for all vertices v_i with $d_T(v_i) \geq 2$.

Proof. On the one hand, by Lemma 5(i), T contains at least m pendant edges and an m -edge matching. Thus there are at least $m - 1$ pendant edges not incident to v . Therefore,

$$r \leq n - 1 - (m - 1) = n - m.$$

On the other hand, if $r = n - m$, then $uv \in M$. By Lemma 5(i), there exist another $m - 1$ pendant edges in M . Since $r = n - m$, there are $m - 1$ vertices v_i with $d_T(v_i) = 2$, and $n - 2m$ pendant vertices v_i (excluding u) adjacent to v . This implies $T \cong T_m^n$.

If $r \leq n - m - 1$, then there are at least $2(m - r)$ edges not incident to v , among which $m - r$ edges in M are pendant edges. Thus, except for the pendant path incident to v_i and the vertex v , there are at most $(n - m - r)$ edges incident to v_i . This yields

$$r + d_T(v_i) \leq r + (n - m - r) + 2 = n - m + 2.$$

This completes the proof of Claim 2. ■

We now return to the proof of the theorem, and construct Transformation 2 as follows.

Transformation 2: $T' = T - u$.

Since u is not M -saturated, we have $T' \in \mathcal{J}_{n-1, m}$. By Transformation 2, we obtain

$$\begin{aligned} & TI_f(T) + RTI_f(T) \\ &= TI_f(T') + RTI_f(T') + f(1, r) + \frac{1}{f(1, r)} \\ &+ k \left[f(1, r) + \frac{1}{f(1, r)} - f(1, r - 1) - \frac{1}{f(1, r - 1)} \right] \\ &+ \sum_{i=k+1}^{r-1} \left[f(r, d(v_i)) + \frac{1}{f(r, d(v_i))} - f(r - 1, d(v_i)) - \frac{1}{f(r - 1, d(v_i))} \right]. \end{aligned}$$

In the above formula, $d(v_i) \geq 2$.

(i) If $f(x, y) = x + y$. By Claim 2, $r + d_T(v_i) \leq n - m + 2$ for all vertices v_i with $d_T(v_i) \geq 2$. Then

$$\begin{aligned} & \sum_{i=k+1}^{r-1} \left[f(r, d(v_i)) + \frac{1}{f(r, d(v_i))} - f(r - 1, d(v_i)) - \frac{1}{f(r - 1, d(v_i))} \right] \\ & \leq (r - 1 - k) \left(1 + \frac{1}{n - m + 2} - \frac{1}{n - m + 1} \right). \end{aligned}$$

Therefore, we deduce that

$$\begin{aligned}
& f(1, r) + \frac{1}{f(1, r)} + k \left[f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \right] \\
& + \sum_{i=k+1}^{r-1} \left[f(r, d(v_i)) + \frac{1}{f(r, d(v_i))} - f(r-1, d(v_i)) - \frac{1}{f(r-1, d(v_i))} \right] \\
& \leq r+1 + \frac{1}{r+1} + (r-1) \left(1 + \frac{1}{n-m+2} - \frac{1}{n-m+1} \right) \\
& + (r-1-k) \left(1 + \frac{1}{r+1} - \frac{1}{r} - \frac{1}{n-m+2} + \frac{1}{n-m+1} \right) \\
& = \left(3r-1 + \frac{r}{r+1} - \frac{r-1}{r} \right) - \left(1 - \frac{1}{r(r+1)} + \frac{1}{(n-m+1)(n-m+2)} \right) k \\
& = g(r, k).
\end{aligned}$$

Clearly, $g(r, k)$ is strictly increasing in r and strictly decreasing in k . The corresponding partial derivatives with respect to r and k read

$$\begin{aligned}
\frac{\partial g}{\partial r} &= 3 - (k+1) \frac{2r+1}{r^2(r+1)^2}, \\
\frac{\partial g}{\partial k} &= - \left(1 - \frac{1}{r(r+1)} + \frac{1}{(n-m+1)(n-m+2)} \right).
\end{aligned}$$

Combined with the constraint $r \geq k+1$, we derive the inequality $\frac{\partial g}{\partial r} > |\frac{\partial g}{\partial k}|$. This implies that the increasing rate of $g(r, k)$ with respect to r dominates the decreasing rate with respect to k . Consequently, the maximum of $g(r, k)$ is attained at $r = n - m$.

On the other hand, when $r = n - m$, since $n > 2m$, we have $n - m > m$. That is, each vertex v_i with $d_T(v_i) \geq 2$ is adjacent to exactly one pendant edge. By Lemma 5(i), the number of vertices v_i with $d_T(v_i) \geq 2$ is $m - 1$. Thus $k = n - 2(m - 1) - 2 = n - 2m$. Combining the inductive hypothesis

that the theorem holds for $n - 1$, we obtain

$$\begin{aligned}
& TI_f(T) + RTI_f(T) \\
& \leq TI_f(T_m^{n-1}) + RTI_f(T_m^{n-1}) + f(1, n-m) + \frac{1}{f(1, n-m)} \\
& + (n-2m) \left[f(1, n-m) + \frac{1}{f(1, n-m)} - f(1, n-m-1) - \frac{1}{f(1, n-m-1)} \right] \\
& + (m-1) \left[f(n-m, 2) + \frac{1}{f(n-m, 2)} - f(n-m-1, 2) - \frac{1}{f(n-m-1, 2)} \right] \\
& = (n-2m+1) \left[f(1, n-m) + \frac{1}{f(1, n-m)} \right] \\
& + (m-1) \left[f(2, n-m) + \frac{1}{f(2, n-m)} \right] + (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right].
\end{aligned}$$

Equality holds if and only if $T' \cong T_m^{n-1}$, $r = n-m$, $d_T(u) = 1$, $k = n-2m$, and the number of vertices v_i with $d_T(v_i) = 2$ equals $m-1$, i.e., $T \cong T_m^n$.

(ii) If $f(x, y) = x^2 + y^2$. Firstly, by Lemma 2(i) and Lemma 2(iii), we have

$$\begin{aligned}
& f(1, r) + \frac{1}{f(1, r)} \leq f(1, n-m) + \frac{1}{f(1, n-m)}, \\
& f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\
& \leq f(1, m) + \frac{1}{f(1, m)} - f(1, m-1) - \frac{1}{f(1, m-1)}.
\end{aligned}$$

Secondly, note that

$$\begin{aligned}
g(x, y) &= f(x, y) + \frac{1}{f(x, y)} - f(x-1, y) - \frac{1}{f(x-1, y)} \\
&= 2x-1 + \frac{1}{x^2+y^2} - \frac{1}{(x-1)^2+y^2}.
\end{aligned}$$

It is clear that $2x-1 > \frac{1}{(x-1)^2+y^2} - \frac{1}{x^2+y^2}$, so $g(x, y)$ increases faster with respect to x than with respect to y . Therefore, by $r \leq n-m$ and $d_T(v_i) \geq 2$, we deduce

$$\begin{aligned}
& f(r, d(v_i)) + \frac{1}{f(r, d(v_i))} - f(r-1, d(v_i)) - \frac{1}{f(r-1, d(v_i))} \\
& \leq f(n-m, 2) + \frac{1}{f(n-m, 2)} - f(n-m-1, 2) - \frac{1}{f(n-m-1, 2)}.
\end{aligned}$$

Thirdly, by Lemma 2(ii),

$$\begin{aligned} & f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\ & < f(d(v_i), r) + \frac{1}{f(d(v_i), r)} - f(d(v_i), r-1) - \frac{1}{f(d(v_i), r-1)}. \end{aligned}$$

Therefore, combining the inductive hypothesis for $m-1$, similarly to case (i), we conclude

$$\begin{aligned} TI_f(T) + RTI_f(T) & \leq (n-2m+1) \left[f(1, n-m) + \frac{1}{f(1, n-m)} \right] \\ & + (m-1) \left[f(2, n-m) + \frac{1}{f(2, n-m)} \right] + (m-1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right]. \end{aligned}$$

Equality holds if and only if $T \cong T_m^n$.

(iii) If $f(x, y) = \sqrt{x^2 + y^2}$. On the one hand, by Lemma 3(i) and (ii), we have

$$\begin{aligned} & f(1, r) + \frac{1}{f(1, r)} \leq f(1, n-m) + \frac{1}{f(1, n-m)}, \\ & f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \\ & > f(d_T(v_i), r) + \frac{1}{f(d(v_i), r)} - f(d(v_i), r-1) - \frac{1}{f(d(v_i), r-1)}. \end{aligned}$$

On the other hand, by Lemma 3(ii), (iii), $k \leq n-2m$ from Claim 1, and $r \leq n-m$ from Claim 2, we obtain

$$\begin{aligned} & k \left[f(1, r) + \frac{1}{f(1, r)} - f(1, r-1) - \frac{1}{f(1, r-1)} \right] \\ & + \sum_{i=k+1}^{r-1} \left[f(d(v_i), r) + \frac{1}{f(d(v_i), r)} - f(d(v_i), r-1) - \frac{1}{f(d(v_i), r-1)} \right] \\ & \leq k \left[f(1, n-m) + \frac{1}{f(1, n-m)} - f(1, n-m-1) - \frac{1}{f(1, n-m-1)} \right] \\ & + (r-1-k) \left[f(2, r) + \frac{1}{f(2, r)} - f(2, r-1) - \frac{1}{f(2, r-1)} \right] \\ & \leq (n-2m) \left[f(1, n-m) + \frac{1}{f(1, n-m)} - f(1, n-m-1) - \frac{1}{f(1, n-m-1)} \right] \\ & + (m-1) \left[f(2, n-m) + \frac{1}{f(2, n-m)} - f(2, n-m-1) - \frac{1}{f(2, n-m-1)} \right]. \end{aligned}$$

Therefore, combining the inductive hypothesis

$$TI_f(T') + RTI_f(T') \leq TI_f(T_m^{n-1}) + RTI_f(T_m^{n-1}).$$

similarly to case (i), we derive

$$\begin{aligned} TI_f(T) + RTI_f(T) &\leq (n - 2m + 1) \left[f(1, n - m) + \frac{1}{f(1, n - m)} \right] \\ &+ (m - 1) \left[f(2, n - m) + \frac{1}{f(2, n - m)} \right] + (m - 1) \left[f(1, 2) + \frac{1}{f(1, 2)} \right]. \end{aligned}$$

Equality holds if and only if $T \cong T_m^n$. ■

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