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EXTREMAL PROPERTIES OF DISTANCE-BASED GRAPH INVARIANTS FOR k-TREES

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Abstract. Sharp bounds on some distance-based graph invariants of n-vertex k-trees are established in a unified approach, which may be viewed as the weighted Wiener index or weighted Harary index. The main techniques used in this paper are graph transformations and mathematical induction. Our results demonstrate that among k-trees with n vertices the extremal graphs with the maximal and the second maximal reciprocal sum-degree distance are coincident with graphs having the maximal and the second maximal reciprocal product-degree distance (and similarly, the extremal graphs with the minimal and the second minimal degree distance are coincident with graphs having the minimal and the second minimal eccentricity distance sum).

Keywords: distance-based graph invariant; k-tree; simplicial vertex; sharp bound

MSC 2010: 34B16, 34C25

1. Introduction and definitions

In this paper, we consider simple and finite graphs only and assume that all graphs are connected, and refer to Bondy and Murty [7] for notation and terminologies used but not defined here.

Let $G=(V_G,E_G)$ be a graph with vertex set V_G and edge set E_G. Let $d_G(v)$ denote the degree of a vertex v in G and $N_G(v)$ be the set of vertices adjacent to v in G. We denote by $N_G[v]$ the set $N_G(v)\cup\{v\}$ and by $|U|$ the cardinality of a set U. Let $G-v$, and $G-uv$ denote the graph obtained from G by deleting the vertex

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$v \in V_G$, and the edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding the edge $uv \notin E_G$. The *distance* $d_G(u, v)$ between two vertices u, v of G is the length of the shortest u-v path in G. The *eccentricity* $\varepsilon_G(v)$ of the vertex v is the distance between v and the furthest vertex from v. The *diameter* of G, $\mathrm{diam}(G)$, is defined as the maximum of the eccentricities of the vertices of G. For a vertex subset S of V_G we denote by $G[S]$ the subgraph induced by S. Denote by K_n the complete graph with n vertices. The *join* $G_1 \vee G_2$ of two graphs G_1 and G_2 is obtained by adding an edge from each vertex of G_1 to each vertex in G_2.

The study of distances between vertices of a tree was probably started from the classic *Wiener index* (see [39]), one of the most well-used chemical indices that correlate a chemical compounds structure (the "molecular graph") with the compounds physico-chemical properties. The Wiener index $W(G)$, introduced in 1947, is defined as the sum of distances between all pairs of vertices, i.e.,

$$W(G) = \sum_{\{u,v\} \subseteq V_G} d_G(u, v).$$

For more results on Wiener index one may be referred to those in [10], [15], [16] and the references cited therein.

A natural sibling concept, the *Harary index* $H(G)$, was defined as the sum of the reciprocal distances between all pairs of vertices, i.e.,

$$H(G) = \sum_{\{u,v\} \subseteq V_G} \frac{1}{d_G(u, v)}.$$

This graph invariant was introduced, independently, by Ivanciuc et al. [21] and by Plavšić et al. [34] in 1993. For more results on Harary index one may be referred to [5], [19], [24] and the references cited therein.

The motivation for studying the quantity that we intend to call *weighted Wiener index* and *weighted Harary index* of a graph comes from the following observation. A weighted graph (G, w) is a graph $G = (V_G, E_G)$ together with the weight function $w\colon V_G \to \mathbb{N}^+$. Let $\oplus$ denote one of the four operations $+, -, \times, /$. The weighted Wiener index $W(G, w)$ and the weighted Harary index $H(G, w)$ of (G, w) are defined, respectively, as

$$W(G, w) = \sum_{\{u,v\} \subseteq V_G} (w(u) \oplus w(v)) d_G(u, v) \tag{1.1}$$

and

$$H(G, w) = \sum_{\{u,v\} \subseteq V_G} \frac{w(u) \oplus w(v)}{d_G(u, v)}. \tag{1.2}$$

Clearly, if $w \equiv 1$ and $\oplus$ denotes operation $\times$, then $W(G, w) = W(G)$ and $H(G, w) = H(G)$.

If $\oplus$ denotes operation $\times$, then (1.1) is equivalent to

$$W(G, w) = \sum_{\{u,v\} \subseteq V_G} (w(u)w(v))d_G(u, v),$$

which is just the *Wiener number of vertex-weighted graphs*; see [22], [23].

If $\oplus$ denotes operation $+$ and $w(\cdot) \equiv d_G(\cdot)$, then (1.1) is equivalent to

$$DD(G) = \sum_{\{u,v\} \subseteq V_G} (d_G(u) + d_G(v))d_G(u, v) = \sum_{v \in V_G} d_G(v)D_G(v),$$

which is just the *degree distance* or *Schultz molecular topological index*, and where $D_G(v) = \sum\limits_{u \in V_G} d_G(u, v)$. It was proposed by Dobrynin and Kochetova [11] and Gutman [15], independently. For more information on this graph invariant one may be referred to [1], [8], [32], [37] and their references.

If $\oplus$ denotes operation $+$ and $w(\cdot) \equiv \varepsilon_G(\cdot)$, then (1.1) is equivalent to

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V_G} (\varepsilon_G(u) + \varepsilon_G(v))d_G(u, v) = \sum_{v \in V_G} \varepsilon_G(v)D_G(v),$$

which is just the *eccentricity distance sum* (EDS). This novel graph invariant was introduced by Gupta, Singh and Madan in [14]. Recently, more and more researchers focused on this novel invariant; see [4], [13], [18], [27], [28], [30], [31].

Similarly, if $\oplus$ denotes operation $+$ and $\times$ and $w(\cdot) \equiv d_G(\cdot)$, then (1.2) is equivalent to

$$H_A(G) = \sum_{\{u,v\} \subseteq V_G} (d_G(u) + d_G(v))\frac{1}{d_G(u, v)}$$

and

$$H_M(G) = \sum_{\{u,v\} \subseteq V_G} (d_G(u)d_G(v))\frac{1}{d_G(u, v)},$$

which is just the *reciprocal sum-degree distance* and *reciprocal product-degree distance*, respectively. For the research development on $H_A(G)$ and $H_M(G)$, one may be referred to [2], [9], [20], [25], [36].

The notion of the n-vertex k-tree T_n^k for $k \geqslant 1$ was first introduced by Beineke and Pippert [6] in 1969 (its definition is given in the following). The k-tree has been considered fully in mathematical literature, one may be referred to [3], [29], [33], [35], [42] and their references. In particular, Estes and Wei [12] determined sharp bounds on the sum of squares of the vertex degrees and the sum of the products of degrees of pairs of adjacent vertices of n vertex k-trees. To our best knowledge, the weighted Wiener index and the weighted Harary index of k-trees have not been, so far, considered in the mathematical literature.

In this paper, we consider the extremal graphs among k-trees with respect to $W(G)$, $H(G)$, $DD(G)$, $\xi^d(G)$, $H_A(G)$, and $H_M(G)$. It is surprising to see that the corresponding extremal graphs are coincident according to the distance-based graph invariants such as $DD(G)$, $\xi^d(G)$, $H_A(G)$, and $H_M(G)$.

The notion of the k-tree T_n^k for $k \geqslant 1$ was first introduced by Beineke and Pippert [6] in 1969, and is defined recursively as (see also in [12]):

(i) The smallest k-tree is the k-clique K_k.

(ii) If G is a k-tree with n vertices and a new vertex v of degree k is added and joined to the vertices of a k-clique in G, then the larger graph is a k-tree with $n+1$ vertices.

For convenience, let T_n^k denote a k-tree on n vertices, and let $\mathscr{T}_n^k$ be the set of all k-trees on n vertices in the whole context. In particular, we consider several particular classes of k-trees.

Definition 1.1 ([12]). The n-vertex k-path P_n^k is a graph with the vertex set $\{v_1, v_2, \ldots, v_n\}$, where $G[\{v_1, v_2, \ldots, v_k\}] \cong K_k$. For $k+1 \leqslant i \leqslant n$, the vertex v_i is adjacent to vertices $\{v_{i-1}, v_{i-2}, \ldots, v_{i-k}\}$.

It is known [12] that a chordal graph G on at least two vertices contains a *simplicial vertex* u, a vertex whose neighborhood induces a clique. Let $G = G_0$, $G_i = G_{i-1} - u_i$ for $i \geqslant 1$. If each u_i is a simplicial vertex of G_{i-1}, then $\{u_1, u_2, \ldots, u_n\}$ is called a *simplicial elimination ordering* of the n-vertex graph G. In particular, if G is a k-tree, then let $S_1(G)$ denote the set of all simplicial vertices of G.

Definition 1.2 ([12]). The n-vertex k-star $S_{k,n-k}$ (see Fig. 1) is a graph with the vertex set $\{v_1, v_2, \ldots, v_n\}$, where $G[\{v_1, v_2, \ldots, v_k\}] \cong K_k$ and $N(v_i) = \{v_1, v_2, \ldots, v_k\}$ for $k+1 \leqslant i \leqslant n$. Hence, $v_i \in S_1(T_n^k)$ for $k+1 \leqslant i \leqslant n$.

Moreover, let $G[\{v_1, v_2, \ldots, v_k\}]$ denote the initial k-clique, then just by the definition of k-tree we have $|E_{T_n^k}| = |E_{K_k}| + k(n-k) = \frac{1}{2}k(2n-k-1)$ and $d_{T_n^k}(v) \geqslant k$ for any $v \in V_{T_n^k}$. Similarly, we can easily get the following facts.

Fact 1.3. *Let T_n^k be a k-tree on $n \geqslant k+2$ vertices and $S_1(T_n^k)$ be the set of all k-simplicial vertices of T_n^k. Then $d_{T_n^k}(v) = k$ for any $v \in S_1(T_n^k)$ and $T_n^k - v$ is also a k-tree.*

Fact 1.4. *For the k-star on n vertices the degree of a vertex v_i can be characterized as: $d(v_i) = n-1$ for $1 \leqslant i \leqslant k$; $d(v_i) = k$ for $k+1 \leqslant i \leqslant n$.*

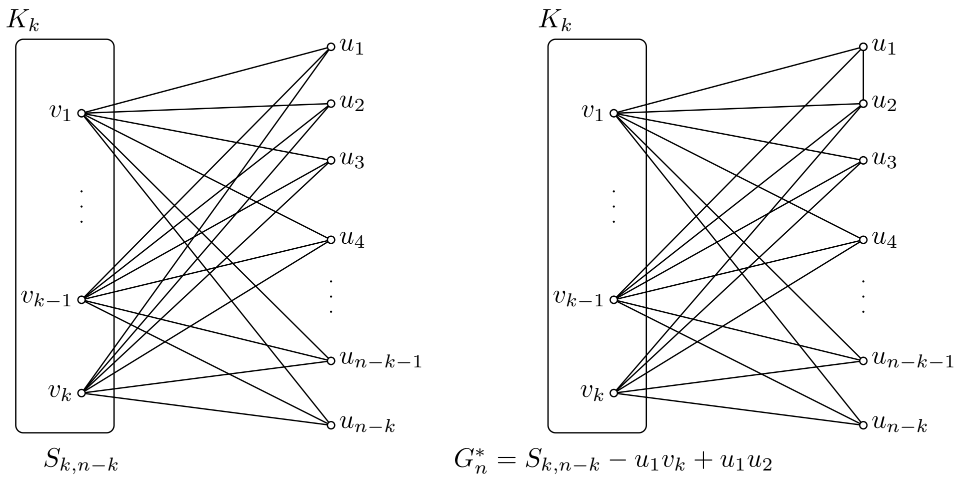

Figure 1. Graphs $S_{k,n-k}$ and G_n^*.

Fact 1.5. *For the k-path on n vertices the degree of a vertex v_i can be characterized as:*

(i) *If $k+2 \leqslant n \leqslant 2k$, then $d(v_i) = k+i-1$ for $1 \leqslant i \leqslant n-k-1$; $d(v_i) = n-1$ for $n-k \leqslant i \leqslant k+1$; $d(v_i) = k+n-i$ for $k+2 \leqslant i \leqslant n$.*

(ii) *If $n \geqslant 2k+1$, then $d(v_i) = k+i-1$ for $1 \leqslant i \leqslant k$; $d(v_i) = 2k$ for $k+1 \leqslant i \leqslant n-k$; $d(v_i) = k+n-i$ for $n-k+1 \leqslant i \leqslant n$.*

For the n-vertex k-tree T_n^k, if $k = 1$, then it is just a tree and the extremal properties of $W(G)$, $H(G)$, $DD(G)$, $\xi^d(G)$, $H_A(G)$, and $H_M(G)$ of n-vertex tree can be referred to in [2], [9], [10], [12], [26], [40], [41]. On the other hand, $T_n^k \cong K_n$ for $k \leqslant n \leqslant k+1$ and $T_n^k \cong P_n^k \cong S_{k,n-k}$ for $n = k+2$. So we consider T_n^k with $n \geqslant k+3$ and $k \geqslant 2$ in the whole context.

Lemma 1.6 ([38]). *Let T_n^k be a k-tree on $n \geqslant k+1$ vertices. Then there exist at least two vertices of degree k in $V_{T_n^k}$.*

Lemma 1.7. *Let T_n^k be a k-tree on n vertices and $S_1(T_n^k)$ be the set of all k-simplicial vertices of T_n^k.*

(i) *If $n \geqslant k+2$, then $|S_1(T_n^k)| \geqslant 2$ and $uv \notin E_{T_n^k}$ for any vertex pair $u, v \in S_1(T_n^k)$.*

(ii) *If there exist two vertices $u, v \in S_1(T_n^k)$ such that $uv \in E_{T_n^k}$, then $n = k+1$ and $T_n^k \cong K_{k+1}$.*

P r o o f. (i) By Lemma 1.6, if $n \geqslant k+2$, then there exist at least two vertices, say v_i and v_j, in $V_{T_n^k}$ such that $d_{T_n^k}(v_i) = d_{T_n^k}(v_j) = k$. By the definition of k-trees, it is routine to check that $v_i, v_j \in S_1(T_n^k)$. So $|S_1(T_n^k)| \geqslant 2$ holds. Now we suppose

$u, v \in S_1(T_n^k)$ and $uv \in E_{T_n^k}$. Then $d_{T_n^k}(u) = d_{T_n^k}(v) = k$ by the definition of $S_1(T_n^k)$. Note that $uv \in E_{T_n^k}$. Hence, we can easily get $d_{T_n^k - v}(u) = k - 1$, a contradiction to the fact that $T_n^k - v$ is also a k-tree. So $uv \notin E_{T_n^k}$ for any vertex pair $u, v \in S_1(T_n^k)$, and (i) holds.

(ii) Follows directly from (i). $\square$

2. The lower bound on the Wiener index and the upper bound on the Harary index of k-trees

In this section, we determine the sharp lower and sharp upper bound on the Wiener index and Harary index, respectively, among k-trees with n vertices.

For any connected graph G on n vertices let $\sigma_i(G)$ be the number of vertex pairs (u, v) in G with $d_G(u, v) = i$, $1 \leqslant i \leqslant \operatorname{diam}(G) \leqslant n - 1$.

Theorem 2.1. *Let T_n^k be a k-tree on $n \geqslant k + 3$ vertices. Then*

$$W(T_n^k) \geqslant n^2 - (k+1)n + \frac{k^2}{2} + \frac{k}{2}.$$

The equality holds if and only if $\operatorname{diam}(T_n^k) = 2$.

P r o o f. By the definition of the Wiener index, we have

$$\begin{aligned} W(T_n^k) &= \sum_{\{u,v\} \subseteq V_{T_n^k}} d_{T_n^k}(u, v) = \sum_{i=1}^{\operatorname{diam}(T_n^k)} i\sigma_i(T_n^k) \\ &\geqslant \sigma_1(T_n^k) + 2 \sum_{i=2}^{\operatorname{diam}(T_n^k)} \sigma_i(T_n^k) \qquad (2.1) \\ &= |E_{T_n^k}| + 2\Big(\frac{n(n-1)}{2} - |E_{T_n^k}|\Big) = n(n-1) - |E_{T_n^k}| \\ &= n^2 - (k+1)n + \frac{k^2}{2} + \frac{k}{2}. \end{aligned}$$

Obviously, the equality in (2.1) holds if and only if $\operatorname{diam}(T_n^k) = 2$. This completes the proof. $\square$

Theorem 2.2. *Let T_n^k be a k-tree on $n \geqslant k + 3$ vertices. Then*

$$H(T_n^k) \leqslant \frac{n^2}{4} + \Big(\frac{k}{2} - \frac{1}{4}\Big)n - \frac{k^2}{4} - \frac{k}{4}$$

with equality if and only if $\operatorname{diam}(T_n^k) = 2$.

P r o o f. By the definition of the Harary index, we have

$$
\begin{aligned}
H(T_n^k) &= \sum_{\{u,v\}\subseteq V_{T_n^k}} \frac{1}{d_{T_n^k}(u,v)} = \sum_{i=1}^{\operatorname{diam}(T_n^k)} \frac{1}{i}\sigma_i(T_n^k) \\
&\leqslant \sigma_1(T_n^k) + \frac{1}{2}\sum_{i=2}^{\operatorname{diam}(T_n^k)} \sigma_i(T_n^k) \qquad (2.2)\\
&= |E_{T_n^k}| + \frac{1}{2}\Big(\frac{n(n-1)}{2} - |E_{T_n^k}|\Big) = \frac{1}{4}n(n-1) + \frac{1}{2}|E_{T_n^k}| \\
&= \frac{n^2}{4} + \Big(\frac{k}{2} - \frac{1}{4}\Big)n - \frac{k^2}{4} - \frac{k}{4}.
\end{aligned}
$$

Obviously, the equality in (2.2) holds if and only if $\operatorname{diam}(T_n^k) = 2$. This completes the proof. $\square$

3. The maximal and the second maximal H_A and H_M of k-trees

In this section, the maximal and the second maximal values of the reciprocal sum-degree distance and the reciprocal product-degree distance of k-trees are determined. The corresponding extremal k-trees are also identified.

The first Zagreb index of a graph G was introduced in 1972 in the report of Gutman and Trinajstić (see [17]) on the topological basis of the π-electron energy, and was denoted by

$$M_1(G) = \sum_{u\in V_G} d_G^2(u) = \sum_{uv\in E_G} (d_G(u) + d_G(v)). \tag{3.1}$$

Comparing with the reciprocal sum-degree distance of a graph G, we define the following invariant, the *reciprocal sum-degree codistance*, for G as

$$\overline{H}_A(G) = \sum_{uv\notin E_G} (d_G(u) + d_G(v))\frac{1}{d_G(u,v)}. \tag{3.2}$$

Let $G_1 = G$ be an n-vertex k-tree. Recall that $S_1(G_1)$ is the set of all simplicial vertices of G_1. Then for $i \geqslant 2$ let $G_i = G_{i-1} - S_1(G_{i-1})$ and $S_i(G)$ denote the set of all simplicial vertices of G_i. Obviously, $|S_1(S_{k,n-k})| = n - k$ and $S_2(T_n^k) = \emptyset$ if and only if $T_n^k \cong S_{k,n-k}$.

Lemma 3.1. *Let T_n^k be in $\mathscr{T}_n^k \setminus \{S_{k,n-k}\}$ with $n \geqslant k+3$ vertices. Let $u \in S_2(T_n^k)$ with $N_{T_n^k}(u) \cap S_1(T_n^k) = \{v_1, v_2, \ldots, v_s\}$ where $s \geqslant 1$. Then there exists a vertex $v \in N_{T_n^k}(u) \setminus \{v_1, v_2, \ldots, v_s\}$ of degree at least k in $T_n^k - \{v_1, v_2, \ldots, v_s\}$ such that $vv_i \notin E_{T_n^k}$ for any $v_i \in \{v_1, v_2, \ldots, v_s\}$.*

P r o o f. Let $G' = T_n^k - \{v_1, v_2, \ldots, v_s\}$ and $X = N_{T_n^k}(u) \setminus \{v_1, v_2, \ldots, v_s\}$. Then we obtain that $d_{G'}(u) = |X| = k$ and $T_n^k[X]$ is a k-clique by $u \in S_2(T_n^k)$. By Fact 1.3, Lemma 1.7 and the definition of k-trees, $d_{G'}(v) \geqslant k$ for all $v \in X$ and $N_{T_n^k}(v_i)$ induces a k-clique in T_n^k. Combining this with $v_i \in N_{T_n^k}(u) \cap S_1(T_n^k)$, we have $N_{T_n^k}(v_i) \subseteq X \cup \{u\}$ for any $v_i \in \{v_1, v_2, \ldots, v_s\}$. Note that $\{v_1, v_2, \ldots, v_s\} \subseteq S_1(T_n^k)$. Hence, by Lemma 1.7, $v_i v_j \notin E_{T_n^k}$ for $1 \leqslant i < j \leqslant n$. In view of the fact that $|N_{T_n^k}(v_i)| = k$, $|X \cup \{u\}| = k + 1$, there exists a vertex $v \in X$ such that $vv_i \notin E_{T_n^k}$ for any vertex $v_i \in \{v_1, v_2, \ldots, v_s\}$.

This completes the proof. $\square$

Lemma 3.2. *Let T_n^k be a k-tree on $n \geqslant k + 3$ vertices and choose a vertex $v \in S_1(T_n^k)$ with $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$ such that $\sum_{i=1}^{k} d_{T_n^k}(u_i)$ is as large as possible. Then*

(i) $\sum_{i=1}^{k} d_{T_n^k}(u_i) \leqslant k(n-1)$ *with equality if and only if* $T_n^k \cong S_{k,n-k}$;

(ii) $\sum_{i=1}^{k} d_{T_n^k}(u_i) \leqslant kn - k - 1$ *if* $T_n^k \ncong S_{k,n-k}$, *and the equality holds if and only if* $T_n^k \cong G_n^*$ *as depicted in Fig.* 1.

P r o o f. (i) Note that $d_{T_n^k}(u) \leqslant n - 1$ for any vertex $u \in V_{T_n^k}$. Hence, (i) follows immediately.

(ii) As $T_n^k \ncong S_{k,n-k}$, clearly there exists a vertex, say u_1, in $\{u_1, u_2, \ldots, u_k\}$ and a vertex $v_0 \in V_{T_n^k} \setminus N_{T_n^k}[v]$ such that $u_1 v_0 \notin E_{T_n^k}$. Hence, $d_{T_n^k}(u_1) \leqslant n - 2$ and $d_{T_n^k}(u_i) \leqslant n - 1$ for $2 \leqslant i \leqslant k$. Then

$$\begin{aligned}\sum_{i=1}^{k} d_{T_n^k}(u_i) &= d_{T_n^k}(u_1) + \sum_{i=2}^{k} d_{T_n^k}(u_i) \\ &\leqslant n - 2 + (k-1)(n-1) \\ &= kn - k - 1.\end{aligned} \tag{3.3}$$

The equality in (3.3) holds if and only if there is just one vertex u_i in $\{u_1, u_2, \ldots, u_k\}$ and one vertex $v_0 \in V_{T_n^k} \setminus N_{T_n^k}[v]$ such that $u_i v_0 \notin E_{T_n^k}$, i.e., $G \cong G_n^*$. Therefore (ii) holds. $\square$

Theorem 3.3. *Let T_n^k be a k-tree on $n \geqslant k + 3$ vertices. Then*

$$H_A(T_n^k) \leqslant \frac{3}{2}kn^2 - \frac{5}{2}kn - \frac{k^3}{2} + \frac{k^2}{2} + k$$

and the equality holds if and only if $T_n^k \cong S_{k,n-k}$.

P r o o f. We prove our result by induction on n. If $n = k+3$, then $\mathscr{T}_n^k = \{P_{k+3}^k, S_{k,3}\}$. By simple calculations we have

$$H_A(P_{k+3}^k) = k^3 + 7k^2 + 7k - 1 \quad \text{and} \quad H_A(S_{k,3}) = k^3 + 7k^2 + 7k.$$

Hence, our result holds for $n = k+3$.

Suppose our result is true for T_m^k with $k+3 \leqslant m < n$, and consider T_n^k. Choose a vertex $v \in S_1(T_n^k)$ with $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$ such that $\sum\limits_{i=1}^{k} d_{T_n^k}(u_i)$ is as large as possible. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. By the definition of k-trees and $v \in S_1(G)$, we get that $G[\{v, u_1, u_2, \ldots, u_k\}] \cong K_{k+1}$ and G' is also a k-tree. It is routine to check that

$$\begin{aligned} H_A(G) &= \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v)) \frac{1}{d_G(u,v)} \\ &= \sum_{uv\in E_G} (d_G(u) + d_G(v)) + \sum_{uv\notin E_G} (d_G(u) + d_G(v)) \frac{1}{d_G(u,v)} = M_1(G) + \overline{H}_A(G), \end{aligned}$$

where $M_1(G)$ and $\overline{H}_A(G)$ are defined in (3.1) and (3.2), respectively.

Note that

$$\begin{aligned} M_1(G) &= M_1(G') + \sum_{i=1}^{k} (d_G(v) + d_G(u_i)) + \sum_{i=1}^{k} (d_G(u_i) - 1) \\ &= M_1(G') + k^2 - k + 2\sum_{i=1}^{k} d_G(u_i) \end{aligned}$$

and

$$\begin{aligned} \overline{H}_A(G) = \overline{H}_A(G') &+ \sum_{u\in V_G\setminus N[v]} \frac{d_G(u) + k}{d_G(u,v)} \\ &+ \sum_{u\in V_G\setminus N[u_1]} \frac{1}{d_G(u,u_1)} + \ldots + \sum_{u\in V_G\setminus N[u_k]} \frac{1}{d_G(u,u_k)}. \end{aligned}$$

Hence, combining this with the fact that $d_G(u,v) \geqslant 2$ for any $u \in V_G \setminus N[v]$ and $d_G(u,u_i) \geqslant 2$ for any $u \in V_G \setminus N[u_i]$ yields

$$\begin{aligned} H_A(G) - H_A(G') &= (M_1(G) + \overline{H}_A(G)) - (M_1(G') + \overline{H}_A(G')) \\ &= k^2 - k + 2\sum_{i=1}^{k} d_G(u_i) + \sum_{u\in V_G\setminus N[v]} \frac{d_G(u) + k}{d_G(u,v)} \\ &\quad + \sum_{u\in V_G\setminus N[u_1]} \frac{1}{d_G(u,u_1)} + \ldots + \sum_{u\in V_G\setminus N[u_k]} \frac{1}{d_G(u,u_k)} \end{aligned}$$

$$
\begin{aligned}
(3.4)\qquad &\leqslant k^2-k+2\sum_{i=1}^{k} d_G(u_i)+\frac12\sum_{u\in V_G\setminus N[v]} d_G(u)\\
&\quad+\frac{k}{2}(n-k-1)+\frac{k}{2}(n-1)-\frac12\sum_{i=1}^{k} d_G(u_i)\\
&=\frac{k}{2}(2n+k-4)+\sum_{i=1}^{k} d_G(u_i)+\frac12\Big(\sum_{i=1}^{k} d_G(u_i)+\sum_{u\in V_G\setminus N[v]} d_G(u)\Big)\\
&=\frac{k}{2}(2n+k-4)+\sum_{i=1}^{k} d_G(u_i)+\frac12(2|E_G|-k)=k(2n-3)+\sum_{i=1}^{k} d_G(u_i)\\
(3.5)\qquad &\leqslant\ k(2n-3)+k(n-1)\\
&=k(3n-4).
\end{aligned}
$$

The equality in (3.4) holds if and only if $d_G(u,v)=2$ for any $u\in V_G\setminus N[v]$ and $d_G(u,u_i)=2$ for any $u\in V_G\setminus N[u_i]$, whereas the equality in (3.5) holds if and only if $T_n^k\cong S_{k,n-k}$ by Lemma 3.2 (i). Based on the definition of k-trees we have $G\cong S_{k,n-k}$. Therefore

$$
\begin{aligned}
(3.6)\qquad & H_A(G)\leqslant H_A(G')+k(3n-4)\\
(3.7)\qquad &\qquad\leqslant k\Big(\frac32(n-1)^2-\frac52(n-1)-\frac{k^2}{2}+\frac{k}{2}+1\Big)+k(3n-4)\\
&\qquad= k\Big(\frac32 n^2-\frac52 n-\frac{k^2}{2}+\frac{k}{2}+1\Big).
\end{aligned}
$$

The equality in (3.6) holds if and only if equalities in (3.4) and (3.5) hold, i.e., $G\cong S_{k,n-k}$. The inequality in (3.7) holds by induction and the equality in (3.7) holds if and only if $G'\cong S_{k,n-k-1}$. By the definition of k-trees, we have $G'\cong S_{k,n-k-1}$ when $G\cong S_{k,n-k}$ holds. Hence, our result holds.

This completes the proof. $\square$

Theorem 3.4. *Let T_n^k be in $\mathscr{T}_n^k\setminus\{S_{k,n-k}\}$ with $n\geqslant k+3$. Then*

$$
H_A(T_n^k)\leqslant\frac32kn^2-\frac52kn-n-\frac{k^3}{2}+\frac{k^2}{2}+2k+2
$$

and the equality holds if and only if $T_n^k\cong G_n^*$, where G_n^* is depicted in Fig. 1.

P r o o f. Choose a vertex $v\in S_1(T_n^k)$ with $N_{T_n^k}(v)=\{u_1,u_2,\dots,u_k\}$ such that $\sum\limits_{i=1}^{k} d_{T_n^k}(u_i)$ is as large as possible. Then T_n^k-v is also a k-tree by Fact 1.3. If $T_n^k-v\cong S_{k,n-k-1}$, combining this with $T_n^k\ncong S_{k,n-k}$, we can easily get $T_n^k\cong G_n^*$ by the definition of T_n^k, our theorem holds. Otherwise, we consider $T_n^k - v \ncong S_{k,n-k-1}$. We will show our result by induction on n.

If $n = k+3$, then $\mathscr{T}_n^k = \{P_{k+3}^k\} = \{G_{k+3}^*\}$ since $T_n^k \ncong S_{k,n-k}$. By simple calculations, $H_A(P_{k+3}^k) = k^3 + 7k^2 + 7k - 1$, our result holds for $n = k+3$.

Suppose that our result is true for T_m^k for $k+3 \leqslant m < n$, and consider T_n^k. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. Combining this with Lemma 3.2 (ii) and the proof of Theorem 3.3, we have

$$\begin{aligned}
&H_A(G) - H_A(G') \leqslant k(2n-3) + \sum_{i=1}^{k} d_G(u_i) && (3.8)\\
&\leqslant k(2n-3) + kn - k - 1 && (3.9)\\
&= 3kn - 4k - 1.
\end{aligned}$$

The equality in (3.8) holds if and only if $d_G(u,v) = 2$ for any vertex $u \in V_G \setminus N[v]$ and $d_G(u,u_i) = 2$ for any vertex $u \in V_G \setminus N[u_i]$, whereas the equality in (3.9) holds if and only if $G \cong G_n^*$ by Lemma 3.2 (ii). Therefore

$$\begin{aligned}
H_A(G) &\leqslant H_A(G') + 3kn - 4k - 1 && (3.10)\\
&\leqslant H_A(G_{n-1}^*) + 3kn - 4k - 1 && (3.11)\\
&= \frac{3}{2}k(n-1)^2 - \frac{5}{2}k(n-1) - (n-1) - \frac{k^3}{2} + \frac{k^2}{2}\\
&\quad + 2k + 2 + 3kn - 4k - 1\\
&= \frac{3}{2}kn^2 - \frac{5}{2}kn - n - \frac{k^3}{2} + \frac{k^2}{2} + 2k + 2.
\end{aligned}$$

The equality in (3.10) holds if and only if the equalities in (3.8) and (3.9) hold, whereas the equality in (3.11) holds if and only if $G' \cong G_{n-1}^*$. Hence, $G \cong G_n^*$, our result holds.

This completes the proof. $\square$

Theorem 3.5. *Let T_n^k be a k-tree on $n \geqslant k+3$ vertices. Then*

$$H_M(T_n^k) \leqslant \Big(\frac{7k^2}{4} - \frac{k}{2}\Big)n^2 - \Big(\frac{3k^3}{2} + \frac{9k^2}{4} - k\Big)n + \frac{k^4}{4} + \frac{5k^3}{4} + \frac{k^2}{2} - \frac{k}{2}$$

and the equality holds if and only if $T_n^k \cong S_{k,n-k}$.

Proof. By direct computation, we get

$$H_M(S_{k,n-k}) = \Big(\frac{7k^2}{4} - \frac{k}{2}\Big)n^2 - \Big(\frac{3k^3}{2} + \frac{9k^2}{4} - k\Big)n + \frac{k^4}{4} + \frac{5k^3}{4} + \frac{k^2}{2} - \frac{k}{2}.$$

In order to complete the proof, it suffices to show that for any $T_n^k \in \mathscr{T}_n^k \setminus \{S_{k,n-k}\}$ there exists an n-vertex k-tree, say G^*, such that $H_M(T_n^k) < H_M(G^*)$.

For simplicity, we denote $G = T_n^k$ in $\mathscr{T}_n^k \setminus \{S_{k,n-k}\}$. Let $u \in S_2(G)$ and $N_G(u) \cap S_1 = \{v_1, v_2, \dots, v_s\}$ with $s \geqslant 1$. Let $G' = G - \{v_1, v_2, \dots, v_s\}$ and $X = N_G(u) - \{v_1, v_2, \dots, v_s\}$. Based on Lemma 3.1, we may choose a vertex, say v_1, in $N_G(u) \cap S_1 = \{v_1, v_2, \dots, v_s\}$ such that there exists a vertex $v \in X$ satisfying $d_{G'}(v) \geqslant k$ and $vv_1 \notin E_G$. We consider the following two possible cases.

Case 1. $d_{G'}(v) = k$. In this case, $v \in S_2(G)$. Combining this with $uv \in E(G')$, we obtain that G' is just a $(k+1)$-clique by Lemma 1.7. We consider the following two possible subcases.

Subcase 1.1. $k = 2$. In this subcase, $d_{G'}(v) = d_{G'}(u) = 2$. Set $N_{G'}(u) \setminus \{v\} = \{x\}$. Note that $G \ncong S_{k,n-k}$. Hence, assume without loss of generality that $xv_i \in E_G$, $vv_i \notin E_G$ for $1 \leqslant i \leqslant t < s$ and $xv_i \notin E_G$, $vv_i \in E_G$ for $t+1 \leqslant i \leqslant s$. Construct a new graph $G^* = (V_{G^*}, E_{G^*})$ with

$$V_{G^*} = V_G, \quad E_{G^*} = E_G - \{xv_1, xv_2, \dots, xv_t\} + \{vv_1, vv_2, \dots, vv_t\}.$$

Then $d_{G^*}(x) = d_G(x) - t$, $d_{G^*}(v) = d_G(v) + t$ and $d_{G^*}(y) = d_G(y)$ for any vertex $y \in V_G \setminus \{x, v\}$. On the other hand, $d_G(v_i, x) = d_{G^*}(v_i, v) = 1$, $d_G(v_i, v) = d_{G^*}(v_i, x) = 2$ for $1 \leqslant i \leqslant t$ and $d_G(z, w) = d_{G^*}(z, w)$ for any other vertex pair. Obviously, G^* is also an n-vertex k-tree and combining this with the fact that $v_i \in S_1(G)$, $d_G(v_i) = 2$ for $1 \leqslant i \leqslant s$, we have

$$\begin{aligned}
&H_M(G^*) - H_M(G)\\
&\quad = \sum_{i=1}^{t}\Big(\frac{d_{G^*}(v_i)d_{G^*}(x)}{d_{G^*}(v_i,x)} - \frac{d_G(v_i)d_G(x)}{d_G(v_i,x)} + \frac{d_{G^*}(v_i)d_{G^*}(v)}{d_{G^*}(v_i,v)} - \frac{d_G(v_i)d_G(v)}{d_G(v_i,v)}\Big)\\
&\qquad + \sum_{i=t+1}^{s}\Big(\frac{d_{G^*}(v_i)d_{G^*}(x)}{d_{G^*}(v_i,x)} - \frac{d_G(v_i)d_G(x)}{d_G(v_i,x)} + \frac{d_{G^*}(v_i)d_{G^*}(v)}{d_{G^*}(v_i,v)} - \frac{d_G(v_i)d_G(v)}{d_G(v_i,v)}\Big)\\
&\qquad + \frac{d_{G^*}(u)d_{G^*}(x)}{d_{G^*}(u,x)} + \frac{d_{G^*}(u)d_{G^*}(v)}{d_{G^*}(u,v)} + \frac{d_{G^*}(x)d_{G^*}(v)}{d_{G^*}(x,v)}\\
&\qquad - \frac{d_G(u)d_G(x)}{d_G(u,x)} - \frac{d_G(u)d_G(v)}{d_G(u,v)} - \frac{d_G(x)d_G(v)}{d_G(x,v)}\\
&\quad = (td_G(x) - td_G(v) - t^2) + \sum_{i=1}^{t}\frac{d_G(v_i)}{2}(-d_G(x) + d_G(v) + t) + \sum_{i=t+1}^{s}\frac{t}{2}d_G(v_i)\\
&\quad = t(d_G(x) - d_G(v) - t) - \sum_{i=1}^{t}(d_G(x) - d_G(v) - t) + \sum_{i=t+1}^{s} t = t(s-t).
\end{aligned}$$

Note that $1 \leqslant t < s$. Hence, $H_M(G^*) - H_M(G) > 0$. That is to say, we have found the k-tree G^* satisfying $H_M(G^*) > H_M(G)$ in this subcase, as desired.

Subcase 1.2. $k \geqslant 3$. Let $x \in X$ be a vertex such that $d_G(x) = \min_{v \in X} d_G(v)$. If $v_i x \notin E_G$ for any $i = 1, 2, \ldots, s$, then $N_G(v_i) = N_G(x) = (X \setminus \{x\}) \cup \{u\}$. So $G \cong S_{k,k+1}$, which is a contradiction. Now, let v_t be a vertex such that $v_t x \in E_G$, $v_t y \notin E_G$ for some $t = 1, 2, \ldots, s$ and $y \in X$. Note that $d_G(x) = \min_{v \in X} d_G(v)$, we get $d_G(x) - 1 < d_G(y)$. Construct a new graph $G^* = (V_{G^*}, E_{G^*})$, where

$$V_{G^*} = V_G, \quad E_{G^*} = E_G - v_t x + v_t y.$$

It is routine to check that G^* is a k-tree on n vertices and that

$$\begin{aligned}
H_M(G^*) - H_M(G) = & \sum_{u \in V \setminus \{x,y,v_t\}} \Big(\frac{d_{G^*}(x) d_{G^*}(u)}{d_{G^*}(x,u)} + \frac{d_{G^*}(y) d_{G^*}(u)}{d_{G^*}(y,u)} \Big) \\
& + \frac{d_{G^*}(x) d_{G^*}(y)}{d_{G^*}(x,y)} + \frac{d_{G^*}(x) d_{G^*}(v_t)}{d_{G^*}(x,v_t)} + \frac{d_{G^*}(y) d_{G^*}(v_t)}{d_{G^*}(y,v_t)} \\
& - \sum_{u \in V \setminus \{x,y,v_t\}} \Big(\frac{d_G(x) d_G(u)}{d_G(x,u)} + \frac{d_G(y) d_G(u)}{d_G(y,u)} \Big) \\
& - \frac{d_G(x) d_G(y)}{d_G(x,y)} - \frac{d_G(x) d_G(v_t)}{d_G(x,v_t)} - \frac{d_G(y) d_G(v_t)}{d_G(y,v_t)} \\
= & \sum_{u \in V \setminus \{x,y,v_t\}} \Big(\frac{(d_G(x) - 1) d_G(u)}{d_G(x,u)} + \frac{(d_G(y) + 1) d_G(u)}{d_G(y,u)} \Big) \\
& + \frac{(d_G(x) - 1)(d_G(y) + 1)}{d_G(x,y)} + \frac{(d_G(x) - 1) d_G(v_t)}{2} \\
& + (d_G(y) + 1) d_G(v_t) - \sum_{u \in V \setminus \{x,y,v_t\}} \Big(\frac{d_G(x) d_G(u)}{d_G(x,u)} + \frac{d_G(y) d_G(u)}{d_G(y,u)} \Big) \\
& - \frac{d_G(x) d_G(y)}{d_G(x,y)} - d_G(x) d_G(v_t) - \frac{d_G(y) d_G(v_t)}{2} \\
= & - \frac{k^2}{2} (d_G(x) - d_G(y) - 1) - \frac{1}{2} (d_G(v_t) - 2)(d_G(x) - d_G(y) - 1).
\end{aligned}$$

Note that $d_G(x) - 1 < d_G(y)$ and $d_G(v_t) = k \geqslant 3$. Hence, we obtain $H_M(G^*) - H_M(G) > 0$. Therefore we find the k-tree G^* satisfies $H_M(G^*) > H_M(G)$ in this subcase, as desired.

Case 2. $d_{G'}(v) \geqslant k + 1$. In this case, reorder the subscripts of $\{v_1, v_2, \ldots, v_s\}$ so that $vv_i \notin E_G$, $i \in [1, s_1]$ with $1 \leqslant s_1 \leqslant s$. By the fact that $G[X]$ is a k-clique, we have $d_G(u) = k + s$ and $d_G(v) \geqslant k + 1 + s - s_1$, that is $d_G(v) \geqslant d_G(u) - s_1 + 1$. Construct a new graph $G^* = (V_{G^*}, E_{G^*})$, where

$$V_{G^*} = V_G, \quad E_{G^*} = E_G - \{uv_1, uv_2, \ldots, uv_{s_1}\} + \{vv_1, vv_2, \ldots, vv_{s_1}\}.$$

It is easy to check that $d_{G^*}(u) = d_G(u) - s_1$, $d_{G^*}(v) = d_G(v) + s_1$ and $d_{G^*}(x) = d_G(x)$ for any vertex $x \in V_G \setminus \{u, v\}$. Note that $G[X \cup \{u\}]$ is a $(k+1)$-clique, and $N_G(v_i) \subseteq N_{G'}(u) \cup \{u\}$ for any i. Hence G^* is also a k-tree. For convenience, let $N_{G'}(u) = \{u_1, u_2, \ldots, u_k\}$ and $V_0 = V_G \setminus N_G[u]$. Obviously, $d_G(v_i, u) = d_{G^*}(v_i, v) = 1$, $d_G(v_i, v) = d_{G^*}(v_i, u) = 2$, $d_{G^*}(v_i, x) \leqslant d_G(v_i, x)$ for any $1 \leqslant i \leqslant s_1$, $x \in V_0$ and $d_{G^*}(y, z) = d_G(y, z)$ for any other vertex pairs. Then

$$
\begin{aligned}
&H_M(G^*) - H_M(G)\\
&= \sum_{i=1}^{s_1}\Big(\frac{d_{G^*}(v_i)d_{G^*}(u)}{d_{G^*}(v_i,u)} - \frac{d_G(v_i)d_G(u)}{d_G(v_i,u)} + \frac{d_{G^*}(v_i)d_{G^*}(v)}{d_{G^*}(v_i,v)} - \frac{d_G(v_i)d_G(v)}{d_G(v_i,v)}\Big)\\
&\quad + \sum_{i=s_1+1}^{s}\Big(\frac{d_{G^*}(v_i)d_{G^*}(u)}{d_{G^*}(v_i,u)} - \frac{d_G(v_i)d_G(u)}{d_G(v_i,u)} + \frac{d_{G^*}(v_i)d_{G^*}(v)}{d_{G^*}(v_i,v)} - \frac{d_G(v_i)d_G(v)}{d_G(v_i,v)}\Big)\\
&\quad + \sum_{1\leqslant i\leqslant k, u_i\neq v}\Big(\frac{d_{G^*}(u_i)d_{G^*}(u)}{d_{G^*}(u_i,u)} - \frac{d_G(u_i)d_G(u)}{d_G(u_i,u)} + \frac{d_{G^*}(u_i)d_{G^*}(v)}{d_{G^*}(u_i,v)} - \frac{d_G(u_i)d_G(v)}{d_G(u_i,v)}\Big)\\
&\quad + \sum_{x\in V_0}\Big(\frac{d_{G^*}(u)d_{G^*}(x)}{d_{G^*}(u,x)} - \frac{d_G(u)d_G(x)}{d_G(u,x)} + \frac{d_{G^*}(v)d_{G^*}(x)}{d_{G^*}(v,x)} - \frac{d_G(v)d_G(x)}{d_G(v,x)}\Big)\\
&\quad + \sum_{1\leqslant i\leqslant s_1, x\in V_0}\Big(\frac{d_{G^*}(v_i)d_{G^*}(x)}{d_{G^*}(v_i,x)} - \frac{d_G(v_i)d_G(x)}{d_G(v_i,x)}\Big) + \frac{d_{G^*}(v)d_{G^*}(u)}{d_{G^*}(v,u)} - \frac{d_G(v)d_G(u)}{d_G(v,u)}\\
&= \sum_{i=1}^{s_1}\Big(\frac{k}{2}(d_G(u)-s_1) - kd_G(u) + k(d_G(v)+s_1) - \frac{k}{2}d_G(v)\Big)\\
&\quad + \sum_{i=s_1+1}^{s}(k(d_G(u)-s_1) - kd_G(u) + k(d_G(v)+s_1) - kd_G(v))\\
&\quad + \sum_{1\leqslant i\leqslant k, u_i\neq v}(-s_1d_G(u_i) + s_1d_G(u_i)) + \sum_{x\in V_0}\Big(\frac{s_1d_G(x)}{d_G(v,x)} - \frac{s_1d_G(x)}{d_G(u,x)}\Big)\\
&\quad + \sum_{1\leqslant i\leqslant s_1, x\in V_0}\Big(\frac{kd_G(x)}{d_{G^*}(v_i,x)} - \frac{kd_G(x)}{d_G(v_i,x)}\Big)\\
&= \frac{s_1}{2}(k-2)(d_G(v) - d_G(u) + s_1) + s_1\sum_{x\in V_0} d_G(x)\Big(\frac{1}{d_G(v,x)} - \frac{1}{d_G(u,x)}\Big)\\
&\quad + k\sum_{1\leqslant i\leqslant s_1, x\in V_0} d_G(x)\Big(\frac{1}{d_{G^*}(v_i,x)} - \frac{1}{d_G(v_i,x)}\Big).
\end{aligned}
$$

Note that $d_{G'}(v) \geqslant k+1$. Hence, we have $1/d_G(v,x) \geqslant 1/d_G(u,x)$ for any vertex $x \in V_0$ and there exists a vertex $x \in V_0$ such that $1/d_G(v,x) > 1/d_G(u,x)$. Combining this with the fact that $d_G(v) - d_G(u) + s_1 > 0$, $k \geqslant 2$ and $1/d_{G^*}(v_i,x) \geqslant$

$1/d_G(v_i,x)$ for any vertex $x \in V_0$, $1 \leqslant i \leqslant s_1$, we get $H_M(G^*) - H_M(G) > 0$. Hence, we find that the k-tree G^* satisfies $H_M(G^*) > H_M(G)$ in this case, as desired.

By Cases 1 and 2, our result holds. $\square$

Theorem 3.6. *Let T_n^k be in $\mathscr{T}_n^k \setminus \{S_{k,n-k}\}$ with $n \geqslant k+3$. Then*

$$H_M(T_n^k) \leqslant \Big(\frac{7k^2}{4} - \frac{k}{2}\Big)n^2 - \Big(\frac{3k^3}{2} + \frac{9k^2}{4} - 1\Big)n + \frac{k^4}{4} + \frac{5k^3}{4} + \frac{3k^2}{2} + \frac{k}{2} - 2,$$

and the equality holds if and only if $T_n^k \cong G_n^*$ as depicted in Fig. 1.

Proof. Choose a vertex $v \in S_1(T_n^k)$ with $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$ such that $\sum\limits_{i=1}^{k} d_{T_n^k}(u_i)$ is as large as possible. Then $T_n^k - v$ is also a k-tree by Fact 1.3. If $T_n^k - v \cong S_{k,n-k-1}$, combining this with $T_n^k \ncong S_{k,n-k}$, we can easily get $T_n^k \cong G_n^*$ by the definition of T_n^k, our theorem holds. Otherwise, we consider $T_n^k - v \ncong S_{k,n-k-1}$. We will show our result by induction on n.

If $n = k+3$, then $\mathscr{T}_n^k = \{P_{k+3}^k\} = \{G_{k+3}^*\}$ since $T_n^k \ncong S_{k,n-k}$. By simple calculations, $H_M(P_{k+3}^k) = \frac{1}{2}k^4 + \frac{9}{2}k^3 + \frac{15}{2}k^2 - 3k + 1$, our result holds for $n = k+3$.

Suppose that our result is true for T_m^k for $k+3 \leqslant m < n$, and consider T_n^k. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. Combining this with the fact that $d_G(v,u_i) = 1$, $d_G(u_i,u_j) = 1$ for any vertex $u_i, u_j \in \{u_1, u_2, \ldots, u_k\}$ and $d_G(v,u) \geqslant 2$ for any vertex $u \in V_G \setminus N[v]$, we have

$$\begin{aligned}
&H_M(G) - H_M(G')\\
&\quad= \sum_{\{u,v\}\subseteq V_G} (d_G(u)d_G(v))\frac{1}{d_G(u,v)} - \sum_{\{u,v\}\subseteq V_G} (d_{G'}(u)d_{G'}(v))\frac{1}{d_{G'}(u,v)}\\
&\quad= \sum_{i=1}^{k} \frac{d_G(v)d_G(u_i)}{d_G(v,u_i)} + \sum_{u\in V_G\setminus N[v]} \frac{d_G(v)d_G(u)}{d_G(v,u)}\\
&\qquad+ \sum_{1\leqslant i<j\leqslant k} \Big(\frac{d_G(u_i)d_G(u_j)}{d_G(u_i,u_j)} - \frac{d_{G'}(u_i)d_{G'}(u_j)}{d_{G'}(u_i,u_j)}\Big)\\
&\qquad+ \sum_{u\in V_G\setminus N[v]} \Big(\frac{d_G(u_1)d_G(u)}{d_G(u_1,u)} + \ldots + \frac{d_G(u_k)d_G(u)}{d_G(u_k,u)}\\
&\qquad- \frac{d_{G'}(u_1)d_{G'}(u)}{d_{G'}(u_1,u)} - \ldots - \frac{d_{G'}(u_k)d_{G'}(u)}{d_{G'}(u_k,u)}\Big)
\end{aligned}$$

$$
\begin{aligned}
&= k\sum_{i=1}^{k} d_G(u_i) + \sum_{u\in V_G\setminus N[v]} \frac{k d_G(u)}{d_G(u,v)} \\
&\quad + \sum_{1\leqslant i<j\leqslant k} (d_G(u_i)d_G(u_j) - (d_G(u_i)-1)(d_G(u_j)-1)) \\
&\quad + \sum_{u\in V_G\setminus N[v]} \Big(\frac{d_G(u_1)d_G(u)}{d_G(u_1,u)} + \ldots + \frac{d_G(u_k)d_G(u)}{d_G(u_k,u)} \\
&\quad - \frac{(d_G(u_1)-1)d_G(u)}{d_G(u_1,u)} - \ldots - \frac{(d_G(u_k)-1)d_G(u)}{d_G(u_k,u)}\Big) \\
&\leqslant k\sum_{i=1}^{k} d_G(u_i) + \frac{k}{2}\sum_{u\in V_G\setminus N[v]} d_G(u) + \sum_{1\leqslant i<j\leqslant k} (d_G(u_i)+d_G(u_j)) \qquad (3.12) \\
&\quad - \frac{k}{2}(k-1) + \sum_{u\in V_G\setminus N[v]} d_G(u)\Big(\frac{1}{d_G(u_1,u)} + \ldots + \frac{1}{d_G(u_k,u)}\Big) \\
&= k\sum_{i=1}^{k} d_G(u_i) + \frac{k}{2}\Big(2|E_G| - k - \sum_{i=1}^{k} d_G(u_i)\Big) + (k-1)\sum_{i=1}^{k} d_G(u_i) \\
&\quad - \frac{k}{2}(k-1) + \sum_{u\in V_G\setminus N[v]} d_G(u)\Big(\frac{1}{d_G(u_1,u)} + \ldots + \frac{1}{d_G(u_k,u)}\Big) \\
&= \Big(\frac{3k}{2} - 1\Big)\sum_{i=1}^{k} d_G(u_i) + \sum_{u\in V_G\setminus N[v]} d_G(u)\Big(\frac{1}{d_G(u_1,u)} + \ldots + \frac{1}{d_G(u_k,u)}\Big) \\
&\quad + k^2 n - \frac{k^3}{2} - \frac{3k^2}{2} + \frac{k}{2}.
\end{aligned}
$$

Equality in (3.12) holds if and only if $d_G(u,v) = 2$ for any vertex $u \in V_G \setminus N[v]$.

Note that $G \ncong S_{k,n-k}$. By Lemma 3.2 (ii), we can easily get

$$\sum_{i=1}^{k} d_G(u_i) \leqslant kn - k - 1$$

with equality if and only if $G \cong G_n^*$.

Since $n \geqslant k+3$, we get $|S_1(G)| \geqslant 2$ by Lemma 1.7. Choose $v' \in S_1(G)\setminus\{v\}$ such that $d_G(v') = k$ and $|N(v') \cap N_G(v)|$ is as small as possible. Then $|N(v') \cap N_G(v)| \leqslant k-1$ since $G \ncong S_{k,n-k}$. So there exists a vertex $u_i \in N_G(v)$ such that $v'u_i \notin E_G$, i.e., $d_G(v', u_i) \geqslant 2$. Then we can easily get

$$d_G(v')\Big(\frac{1}{d_G(v',u_1)} + \ldots + \frac{1}{d_G(v',u_k)}\Big) \leqslant k\Big(k - 1 + \frac{1}{2}\Big) = k^2 - \frac{k}{2}$$

and
$$\frac{1}{d_G(u,u_1)}+\ldots+\frac{1}{d_G(u,u_k)}\leqslant k$$
for any $u\in V_G\setminus\{N_G[v]\cup\{v'\}\}$.

Furthermore, we have

$$\begin{aligned}
&\sum_{u\in V_G\setminus N[v]} d_G(u)\Big(\frac{1}{d_G(u_1,u)}+\ldots+\frac{1}{d_G(u_k,u)}\Big)\\
&\qquad= d_G(v')\Big(\frac{1}{d_G(v',u_1)}+\ldots+\frac{1}{d_G(v',u_k)}\Big)\\
&\qquad\quad+\sum_{u\in V_G\setminus\{N_G[v]\cup\{v'\}\}} d_G(u)\Big(\frac{1}{d_G(u_1,u)}+\ldots+\frac{1}{d_G(u_k,u)}\Big)\\
&\qquad\leqslant k^2-\frac{k}{2}+k\sum_{u\in V_G\setminus\{N_G[v]\cup\{v'\}\}} d_G(u) \qquad (3.13)\\
&\qquad= k^2-\frac{k}{2}+k\Big(2|E_G|-2k-\sum_{i=1}^{k} d_G(u_i)\Big)\\
&\qquad= 2k^2n-k^3-2k^2-\frac{k}{2}-k\sum_{i=1}^{k} d_G(u_i),
\end{aligned}$$

where the equality in (3.13) holds if and only if there exists only one vertex $u_i\in\{u_1,u_2,\ldots,u_k\}$ and one vertex $v'\in V_G\setminus N_G[v]$ such that $u_iv'\notin E_G$, i.e., $G\cong G_n^*$.

Then combining this with induction,

$$\begin{aligned}
H_M(G)&\leqslant H_M(G')+\Big(\frac{3k}{2}-1\Big)\sum_{i=1}^{k} d_G(u_i) \qquad (3.14)\\
&\quad+\sum_{u\in V_G\setminus N[v]} d_G(u)\Big(\frac{1}{d_G(u_1,u)}+\ldots+\frac{1}{d_G(u_k,u)}\Big)\\
&\quad+k^2n-\frac{k^3}{2}-\frac{3k^2}{2}+\frac{k}{2}\\
&\leqslant H_M(G')+\Big(\frac{3k}{2}-1\Big)\sum_{i=1}^{k} d_G(u_i)+2k^2n-k^3-2k^2-\frac{k}{2} \qquad (3.15)\\
&\quad-k\sum_{i=1}^{k} d_G(u_i)+k^2n-\frac{k^3}{2}-\frac{3k^2}{2}+\frac{k}{2}\\
&= H_M(G')+\Big(\frac{k}{2}-1\Big)\sum_{i=1}^{k} d_G(u_i)+3k^2n-\frac{3k^3}{2}-\frac{7k^2}{2}\\
&\leqslant H_M(G_{n-1}^*)+\Big(\frac{k}{2}-1\Big)(kn-k-1)+3k^2n-\frac{3k^3}{2}-\frac{7k^2}{2} \qquad (3.16)
\end{aligned}$$

$$= \Big(\Big(\frac{7k^2}{4} - \frac{k}{2}\Big)(n-1)^2 - \Big(\frac{3k^3}{2} + \frac{9k^2}{4} - 1\Big)(n-1) + \frac{k^4}{4} + \frac{5k^3}{4} + \frac{3k^2}{2} + \frac{k}{2} - 2\Big) + \Big(\frac{7}{2}k^2n - kn - \frac{3k^3}{2} - 4k^2 + \frac{k}{2} + 1\Big)$$
$$= \Big(\frac{7k^2}{4} - \frac{k}{2}\Big)n^2 - \Big(\frac{3k^3}{2} + \frac{9k^2}{4} - 1\Big)n + \frac{k^4}{4} + \frac{5k^3}{4} + \frac{3k^2}{2} + \frac{k}{2} - 2.$$

The equality in (3.14) holds if and only if the equality in (3.12) holds, i.e., $G \cong G_n^*$; the equality in (3.15) and (3.16) holds if and only if $G \cong G_n^*$ and $G' \cong G_{n-1}^*$, respectively. By the definition of k-trees and the fact that $G' \ncong S_{k,n-k-1}$, we have $G' \cong G_{n-1}^*$ when $G \cong G_n^*$ holds. Hence, our result holds.

This completes the proof. □

4. The minimal and the second minimal DD and ξ^d of k-trees

In this section, the minimal and the second minimal values on DD and ξ^d of n-vertex k-trees are determined. The corresponding extremal graphs are characterized.

Theorem 4.1. *Let T_n^k be a k-tree on $n \geqslant k+3$ vertices. Then*

$$DD(T_n^k) \geqslant 3kn^2 - 3k^2n - 4kn + k^3 + 2k^2 + k$$

and the equality holds if and only if $T_n^k \cong S_{k,n-k}$.

Proof. We show our result by induction on n. If $n = k+3$, then $\mathscr{T}_n^k = \{P_{k+3}^k, S_{k,3}\}$. By simple calculations, $DD(P_{k+3}^k) = k^3+7k^2+16k+2$ and $DD(S_{k,3}) = k^3 + 7k^2 + 16k$. Our result follows immediately in this case.

Suppose our result is true for T_m^k with $k+3 \leqslant m < n$, and consider T_n^k. Choose a vertex $v \in S_1(T_n^k)$, then $d_{T_n^k}(v) = k$ and let $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. By the definition of the k-tree and $v \in S_1(G)$, we can easily get $G[\{v, u_1, u_2, \ldots, u_k\}] \cong K_{k+1}$ and G' is also a k-tree. Furthermore, we have

$$\begin{aligned} DD(G) - DD(G') &= \sum_{v\in V_G} d_G(v)D_G(v) - \sum_{v\in V_{G'}} d_{G'}(v)D_{G'}(v) \\ &= d_G(v)D_G(v) + \sum_{i=1}^{k}(d_G(u_i)D_G(u_i) - d_{G'}(u_i)D_{G'}(u_i)) \\ &\quad + \sum_{u\in V_G\setminus N[v]} (d_G(u)D_G(u) - d_{G'}(u)D_{G'}(u)) \end{aligned}$$

$$
\begin{aligned}
&= k\Bigl(k + \sum_{u\in V_G\setminus N[v]} d_G(u,v)\Bigr) \\
&\quad + \sum_{i=1}^{k}(d_G(u_i)D_G(u_i) - (d_G(u_i)-1)(D_G(u_i)-1)) \\
&\quad + \sum_{u\in V_G\setminus N[v]} d_G(u)d_G(u,v) \\
&= k^2 + \sum_{u\in V_G\setminus N[v]} (d_G(u)+k)d_G(u,v) + \sum_{i=1}^{k}(d_G(u_i)+D_G(u_i)) - k \\
&= k^2 - k + \sum_{u\in V_G\setminus N[v]} (d_G(u)+k)d_G(u,v) \\
&\quad + \Bigl(2|E_G| - k - \sum_{u\in V_G\setminus N[v]} d_G(u)\Bigr) + \sum_{i=1}^{k}\Bigl(k + \sum_{u\in V_G\setminus N[v]} d_G(u,u_i)\Bigr) \\
&= k^2 + 2kn - 3k + \sum_{u\in V_G\setminus N[v]} (d_G(u)(d_G(u,v)-1) + kd_G(u,v) \\
&\quad + d_G(u,u_1) + \ldots + d_G(u,u_k)) \\
&\geqslant k^2 + 2kn - 3k + (n-k-1)(k+2k+k) \qquad (4.1) \\
&= 6kn - 3k^2 - 7k.
\end{aligned}
$$

The equality in (4.1) holds if and only if $d_G(u) = k$, $d_G(u,v) = 2$ and $d_G(u,u_1) = d_G(u,u_2) = \ldots = d_G(u,u_k) = 1$ for any vertex $u \in V_G \setminus N[v]$. Hence, by induction we have

$$
\begin{aligned}
DD(G) &\geqslant DD(S_{k,n-k-1}) + 6kn - 3k^2 - 7k \qquad (4.2) \\
&= 3k(n-1)^2 - 3k^2(n-1) - 4k(n-1) \\
&\quad + k^3 + 2k^2 + k + 6kn - 3k^2 - 7k \\
&= 3kn^2 - 3k^2n - 4kn + k^3 + 2k^2 + k.
\end{aligned}
$$

The equality in (4.2) holds if and only if $G' \cong S_{k,n-k-1}$ and the equality in (4.1) holds. Hence, $G \cong S_{k,n-k}$.

This completes the proof. □

Theorem 4.2. *Let T_n^k be in $\mathscr{T}_n^k \setminus \{S_{k,n-k}\}$ with $n \geqslant k+3$. Then*

$$DD(T_n^k) \geqslant 3kn^2 - 3k^2n - 4kn + 2n + k^3 + 2k^2 - k - 4,$$

and the equality holds if and only if $T_n^k \cong G_n^*$ as depicted in Fig. 1.

P r o o f. Choose a vertex $v \in S_1(T_n^k)$ with $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$ such that $\sum\limits_{i=1}^{k} d_{T_n^k}(u_i)$ is as large as possible. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. Note that $v \in S_1(G)$ and by the definition of the k-tree, we can easily get $G[\{v, u_1, u_2, \ldots, u_k\}] \cong K_{k+1}$ and G' is also a k-tree. If $G' \cong S_{k,n-k-1}$, then combining it with $T_n^k \ncong S_{k,n-k}$, we can easily get $T_n^k \cong G_n^*$ by the definition of T_n^k, our result holds in this case. Otherwise we consider $G' \ncong S_{k,n-k-1}$ and we proceed by induction on n.

If $n = k + 3$, then $\mathscr{T}_n^k = \{P_{k+3}^k\} = \{G_{k+3}^*\}$ since $T_n^k \ncong S_{k,n-k}$. By simple calculations, $DD(P_{k+3}^k) = k^3 + 7k^2 + 16k + 2$, our result holds in this subcase.

Suppose our result is true for T_m^k with $k + 3 \leqslant m < n$, and consider T_n^k. Since $G \ncong S_{k,n-k}$, by Lemma 3.2 (ii) we can easily get

$$\sum_{i=1}^{k} d_G(u_i) \leqslant kn - k - 1$$

with equality if and only if $G \cong G_n^*$.

Notice that $n \geqslant k+3$. Hence, by Lemma 1.7, $|S_1(G)| \geqslant 2$. Choose $v' \in S_1(G)\setminus\{v\}$ such that $|N(v') \cap N_G(v)|$ is as small as possible. As $G \ncong S_{k,n-k}$, we have $|N(v') \cap N_G(v)| \leqslant k - 1$. So there exists a vertex $u_i \in N_G(v)$ such that $v'u_i \notin E_{T_n^k}$. Then we can easily get

$$d_G(v', u_1) + d_G(v', u_2) + \ldots + d_G(v', u_k) \geqslant k + 1$$

and

$$d_G(u, u_1) + d_G(u, u_2) + \ldots + d_G(u, u_k) \geqslant k$$

for any $u \in V_G \setminus (N_G[v] \cup \{v'\})$. Hence,

$$\sum_{u \in V_G \setminus N_G[v]} (d_G(u, u_1)+d_G(u, u_2)+\ldots+d_G(u, u_k)) \geqslant k+1+k(n-k-2) = kn-k^2-k+1$$

with equality if and only if there is only one vertex $u_i \in \{u_1, u_2, \ldots, u_k\}$ and one vertex $v' \in V_G \setminus N_G[v]$ such that $u_i v' \notin E_G$ and $v' \in S_1(G)$, i.e., $G \cong G_n^*$.

Furthermore, based on the proof of Theorem 4.1, we have

$$\begin{aligned} DD(G) - DD(G') = k^2 + 2kn - 3k + \sum_{u \in V_G \setminus N[v]} &(d_G(u)(d_G(u, v) - 1) \\ &+ k d_G(u, v) + d_G(u, u_1) + \ldots + d_G(u, u_k)) \end{aligned}$$

$$
\begin{aligned}
(4.3) \qquad & \geqslant k^2 + 2kn - 3k + \sum_{u \in V_G \setminus N[v]} (d_G(u) + 2k) \\
& \quad + \sum_{u \in V_G \setminus N[v]} (d_G(u, u_1) + d_G(u, u_2) + \ldots + d_G(u, u_k)) \\
& = k^2 + 2kn - 3k + 2k(n-k-1) + \left(2|E_G| - k - \sum_{i=1}^{k} d_G(u_i)\right) \\
& \quad + \sum_{u \in V_G \setminus N[v]} (d_G(u, u_1) + d_G(u, u_2) + \ldots + d_G(u, u_k)) \\
(4.4) \qquad & \geqslant 6kn - 2k^2 - 7k - (kn - k - 1) + kn - k^2 - k + 1 \\
& = 6kn - 3k^2 - 7k + 2.
\end{aligned}
$$

The equality in (4.3) holds if and only if $d_G(u, v) = 2$ for any vertex $u \in V_G \setminus N[v]$, whereas the equality in (4.4) holds if and only if $\sum\limits_{i=1}^{k} d_G(u_i) = kn - k - 1$ and $\sum\limits_{u \in V_G \setminus N[v]} (d_G(u, u_1) + d_G(u, u_2) + \ldots + d_G(u, u_k)) = kn - k^2 - k + 1$. Hence, $G \cong G_n^*$.

Combining this with induction,

$$
\begin{aligned}
(4.5) \qquad DD(G) & \geqslant DD(G_{n-1}^*) + 6kn - 3k^2 - 7k + 2 \\
& = 3k(n-1)^2 - 3k^2(n-1) - 4k(n-1) + 2(n-1) \\
& \quad + k^3 + 2k^2 - k - 4 + 6kn - 3k^2 - 7k + 2 \\
& = 3kn^2 - 3k^2 n - 4kn + 2n + k^3 + 2k^2 - k - 4.
\end{aligned}
$$

The equality in (4.5) holds if and only if $G' \cong G_{n-1}^*$ and the equality in (4.3) and (4.4) holds. Hence, $G \cong G_n^*$.

This completes the proof. $\square$

Theorem 4.3. *Let T_n^k be a k-tree on $n \geqslant k+3$ vertices. Then*

$$
\xi^d(T_n^k) \geqslant 4n^2 - 5kn - 4n + 2k^2 + 3k
$$

and the equality holds if and only if $T_n^k \cong S_{k,n-k}$.

Proof. We proceed by induction on n. If $n = k+3$, then $\mathscr{T}_{k+3}^k = \{P_{k+3}^k, S_{k,3}\}$. By simple calculations, we have

$$
\xi^d(P_{k+3}^k) = k^2 + 9k + 26, \qquad \xi^d(S_{k,3}) = k^2 + 8k + 24.
$$

Our result holds immediately in this case.

Suppose our result is true for T_m^k with $k+3 \leqslant m < n$, and next consider T_n^k. Choose a vertex $v \in S_1(T_n^k)$, then $d_{T_n^k}(v) = k$ and let $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. By the definition of k-tree and $v \in S_1(G)$, it is routine to check that $G[\{v, u_1, u_2, \ldots, u_k\}] \cong K_{k+1}$ and G' is also a k-tree. Furthermore, we have

$$\begin{aligned}
\xi^d(G) = & \sum_{u \in V_G} \varepsilon_G(u) D_G(u) = \varepsilon_G(v) D_G(v) + \sum_{i=1}^{k} \varepsilon_G(u_i) D_G(u_i) \\
& + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) D_G(u) = \varepsilon_G(v) D_G(v) + \sum_{i=1}^{k} \varepsilon_{G'}(u_i)(D_{G'}(u_i) + 1) \\
& + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u)(D_{G'}(u) + d_G(u, v)) \\
= & \sum_{i=1}^{k} \varepsilon_{G'}(u_i) D_{G'}(u_i) + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) D_{G'}(u) + \varepsilon_G(v) D_G(v) \\
& + \sum_{i=1}^{k} \varepsilon_{G'}(u_i) + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) d_G(u, v).
\end{aligned}$$

Obviously, $\varepsilon_G(v) \geqslant 2$, $D(v) \geqslant k + 2(n-1-k) = 2n-k-2$, $\varepsilon_{G'}(u_i) \geqslant 1$ for $1 \leqslant i \leqslant k$ and $\varepsilon_G(u) \geqslant 2$, $d_G(u, v) \geqslant 2$ for any $u \in V_G \setminus N[v]$. Combining this with the fact that $\varepsilon_G(u) \geqslant \varepsilon'_G(u)$ for $u \in V_G \setminus N[v]$ and by induction, we have

$$\xi^d(G) \geqslant \xi^d(G') + \varepsilon_G(v) D_G(v) + \sum_{i=1}^{k} \varepsilon_{G'}(u_i) + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) d_G(u, v) \tag{4.6}$$

$$\geqslant \xi^d(S_{k,n-k-1}) + 2(2n-k-2) + k + 2 \cdot 2(n-k-1) \tag{4.7}$$

$$= 4n^2 - 5kn - 4n + 2k^2 + 3k.$$

The equality in (4.6) holds if and only if $\varepsilon_G(u) = \varepsilon'_G(u)$ for any vertex $u \in V_G \setminus N[v]$, whereas the equality in (4.7) holds if and only if $\varepsilon_{G'}(u_i) = 1$ for $1 \leqslant i \leqslant k$, $\varepsilon_G(v) = \varepsilon_G(u) = 2$ for any $u \in V_G \setminus N[v]$ and $G' \cong S_{k,n-k-1}$, which implies $G \cong S_{k,n-k}$.

This completes the proof. □

Theorem 4.4. *Let T_n^k be in $\mathscr{T}_n^k \setminus \{S_{k,n-k}\}$ with $n \geqslant k+3$. Then*

$$\xi^d(T_n^k) \geqslant 4n^2 - 5kn - 3n + 2k^2 + 3k - 1$$

with equality if and only if $T_n^k \cong G_n^*$, where G_n^* is depicted in Fig. 1.

P r o o f. Choose a vertex $v \in S_1(T_n^k)$, then $d_{T_n^k}(v) = k$ and let $N_{T_n^k}(v) = \{u_1, u_2, \ldots, u_k\}$. For simplicity, let $G = T_n^k$ and $G' = T_n^k - v$. As $v \in S_1(G)$, by the definition of the k-tree, it is routine to check that $G[\{v, u_1, u_2, \ldots, u_k\}] \cong K_{k+1}$ and G' is also a k-tree. If $G' \cong S_{k,n-k-1}$, combining it with $G \not\cong S_{k,n-k}$, then we can easily get $G \cong G_n^*$ by the definition of k-trees, our result holds in this case. Otherwise we consider $G' \not\cong S_{k,n-k-1}$ and complete our proof by induction on n.

If $n = k+3$, as $T_n^k \not\cong S_{k,n-k}$, we have $\mathscr{T}_n^k = \{P_{k+3}^k\} = \{G_{k+3}^*\}$. By simple calculations, $\xi^d(P_{k+3}^k) = k^2 + 9k + 26$, our result holds in this case. Suppose this is true for T_m^k with $k+3 \leqslant m < n$, and consider T_n^k. According to the proof of Theorem 4.3, we have

$$\begin{aligned}\xi^d(G) = \sum_{i=1}^{k} \varepsilon_{G'}(u_i) D_{G'}(u_i) &+ \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) D_{G'}(u) + \varepsilon_G(v) D_G(v) \\ &+ \sum_{i=1}^{k} \varepsilon_{G'}(u_i) + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) d_G(u,v).\end{aligned}$$

Note that $G \not\cong S_{k,n-k}$, there exists a vertex $u_i \in N_G(v)$ and a vertex $x \in V_G \setminus N[v]$ such that $xu_i \notin E_G$. It is routine to check that $\varepsilon_{G'}(u_i) \geqslant 2$. Hence, $\sum\limits_{i=1}^{k} \varepsilon_{G'}(u_i) \geqslant k+1$. Obviously, $\varepsilon_G(v) \geqslant 2$, $D_G(v) \geqslant k + 2(n-1-k) = 2n-k-2$ and $\varepsilon_G(u) \geqslant \varepsilon_{G'}(u)$, $\varepsilon_G(u) \geqslant 2$, $d_G(u,v) \geqslant 2$ for any $u \in V_G \setminus N[v]$. According to the proof of Theorem 4.3 and by induction, we get

$$\xi^d(G) \geqslant \xi^d(G') + \varepsilon_G(v) D_G(v) + \sum_{i=1}^{k} \varepsilon_{G'}(u_i) + \sum_{u \in V_G \setminus N[v]} \varepsilon_G(u) d_G(u,v) \tag{4.8}$$

$$\geqslant \xi^d(G_{n-1}^*) + 2(2n-k-2) + k + 1 + 2 \cdot 2(n-k-1) \tag{4.9}$$

$$= 4n^2 - 5kn - 3n + 2k^2 + 3k - 1.$$

The equality in (4.8) holds if and only if $\varepsilon_G(u) = \varepsilon'_G(u)$ for $u \in V_G \setminus N[v]$, while the equality in (4.9) holds if and only if $\varepsilon_G(v) = \varepsilon_G(u) = 2$ for any $u \in V_G \setminus N[v]$, $\sum\limits_{i=1}^{k} \varepsilon_{G'}(u_i) = k+1$ and $G' \cong G_{n-1}^*$, which implies that $G \cong G_n^*$. Hence, our result holds.

This completes the proof. $\square$

5. Conclusion remark

In this paper we determine the sharp upper and sharp lower bound on Wiener index and Harary index, respectively, of k-trees; The k-tree with the maximal and the second maximal H_A and H_M are characterized. Furthermore, the k-tree with the minimal and the second minimal DD and ξ^d are also identified. It may be interesting to determine the sharp lower and sharp upper bound on Wiener index and Harary index, respectively, of k-trees; to characterize the k-tree with the minimal and the second mimimal H_A and H_M. Furthermore, it would be also interesting to identify the k-tree with the maximal and the second maximal DD and ξ^d.

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