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On Trees with a Given Diameter and the Extremal Number of Distance-k Independent Sets

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Abstract—The set of vertices of a graph is called *distance-k independent* if the distance between any two of its vertices is greater than some integer $k \geq 1$. In this paper, we describe n-vertex trees with a given diameter d that have the maximum and minimum possible number of distance-k independent sets among all such trees. The maximum problem is solvable for the case of $1 < k < d \leq 5$. The minimum problem is much simpler and can be solved for all $1 < k < d < n$.

Keywords: *tree, independent set, distance-k independent set, diameter*

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INTRODUCTION

An *independent set* of a graph is an arbitrary subset of its pairwise nonadjacent vertices. A *Distance-k Independent Set* (abbreviated as k-DIS) of a graph is a subset of its vertices any two of which are at a distance of more than $k \geq 1$ from each other. In particular, a 1-DIS is an ordinary independent set. The *diameter* $\operatorname{diam}(G)$ of a connected graph G is the maximum possible distance between two of its vertices. By $i_k(G)$ we denote the number of different k-DIS's that the graph G contains. An n-vertex tree of diameter d is said to be (i_k, d, n)-*maximal* ((i_k, d, n)-*minimal*) if it contains the maximally (minimum) possible number of k-DIS's among all such trees.

We denote by $S_{d,n}$ the n-vertex tree of diameter d obtained from the path P_d by attaching $n - d$ leaves to one of its ends. Obviously, the star S_n isomorphic to $S_{2,n}$ is the only $(i_1, 2, n)$-maximal tree. It is shown in [1] that for all $2 < d < n$ the only (i_1, d, n)-maximal tree is the graph $S_{d,n}$. On the other hand, (i_1, d, n)-minimal trees are much more complicated, and the problem of describing them in the case of $d \geq 8$ remains open. The paper [2] describes (i_1, d, n)-minimal trees for $d \leq 4$ and an arbitrary n, as well as for $d = 5$ and all sufficiently large n. Some important properties of (i_1, d, n)-minimal trees for $d \geq 6$ are proved and the structure of $(i_1, 6, n)$-minimal trees is partially described in [3]. The recent paper [4] describes $(i_1, 6, n)$-minimal and $(i_1, 7, n)$-minimal trees for $n > 160$ and $n > 400$, respectively.

To date, relatively few results related to k-DIS's in graphs are known. In [5–9], estimates were obtained for the *number of distance-k independence* of a graph (i.e., for the largest cardinality of its k" DIS). The k-DIS's of a simple path P_n are listed under some additional constraints in [10].

In this paper we study (i_k, d, n)-maximal and (i_k, d, n)-minimal trees in the case of $k \geq 2$. It is clear that for $k \geq d$ each n-vertex tree of diameter d contains exactly $n + 1$ k-DIS's (in this case, each k-DIS contains at most one vertex of the tree), so only the nontrivial case of $k < d$ is of interest. For all $1 < k < d \leq 5$ and $n \geq 120$, we find the (i_k, d, n)-maximal tree $\widehat{T}_{k,d,n}$ and prove that it is unique. In addition, for all $1 < k < d < n$, the (i_k, d, n)-minimal tree $T_{k,d,n}$ is found and all triples (k, d, n) for which this tree is unique are indicated.

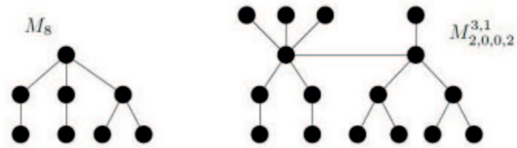

Fig. 1. Trees M_8 and $M^{3,1}_{2,0,0,2}$.

1. SOME DEFINITIONS AND NOTATION

As usual, $N[v]$ denotes the *closed neighborhood* of vertex v, i.e., a set consisting of v and all vertices adjacent to it. For $s \geq 1$ we denote by $N_s[v]$ the set of all vertices located at a distance of at most s from vertex v.

A vertex of a tree T is called *preleaf* if it is adjacent to at least one of its leaves and *central* if it is located at a distance of at most $\lfloor \frac{\operatorname{diam}(T)+1}{2} \rfloor$ from all its leaves. As is well known, trees of even diameter contain exactly one central vertex, and trees of odd diameter, exactly two. The *diametrical path* of a tree T is its simple path containing $\operatorname{diam}(T)+1$ vertices. Let us call a leaf of tree T that is the endpoint of a diametrical path T *diametrical*.

Recall that $i_k(G)$ denotes the number of distinct k-DIS's that the graph G contains. By $i_k^+(G,v)$ ($i_k^-(G,v)$) we denote the number of k-DIS's of the graph G containing (not containing) vertex v. It is easy to see that for all $n \geq 2$ and $k \geq 1$ the strict inequality $i_k^+(T,v) < i_k^-(T,v)$ holds for any n-vertex tree T and any of its vertices v. Indeed, let us denote by u an arbitrary neighbor of v. Then

$$i_k^-(T,v) \geq i_k\big(T \setminus N_1[v]\big) + i_k^+(T,u) > i_k\big(T \setminus N_k[v]\big) = i_k^+(T,v).$$

Let $M^l_{a,b}$ denote a tree of diameter 4 whose central vertex is adjacent to l leaves, a paths P_2, and b central vertices of paths P_3. Let $M^{p,q}_{a,b,c,d'}$ denote the tree of diameter 5 obtained from the forest $M^p_{a,b} \cup M^q_{c,d'}$ by connecting the central vertices of its two subtrees. We will use the notation $M_{a,b}$ for the tree $M^0_{a,b}$ and M_n, for the n-vertex tree $M_{a,b}$, where $a \leq 2$ (see Fig. 1). In addition, by $M'_{a,b,c,d'}$ we denote the tree $M^{1,0}_{a,b,c,d'}$ and by $M_{a,b,c,d'}$, the tree $M^{0,0}_{a,b,c,d'}$.

We will call an (i_k, d, n)-maximal ((i_k, d, n)-minimal) tree simply *maximal* (*minimal*) if the values of the parameters k, d, and n are clear from the context.

2. CASE OF $(i_{2k'}, 2k'+1, n)$-MAXIMAL TREES

Consider a tree T of diameter $2k'+1$ with central vertices u and v. Let us denote by T_u the inclusion-maximal subtree of T containing the vertex u and not containing the vertex v. Let us define a subtree T_v in a similar way. Let us denote by l_u and l_v the number of diametrical leaves of T contained in the subtrees T_u and T_v, respectively.

Theorem 1. *For all $n \geq 2k'+2$ and $k' \geq 1$, each $(i_{2k'}, 2k'+1, n)$-maximal tree is unique and isomorphic to the path $P_{2k'}$ to the ends of which $\lfloor \frac{n-2k'+1}{2} \rfloor$ and $\lfloor \frac{n-2k'}{2} \rfloor$ leaves, respectively, are attached.*

Proof. It is obvious that each $2k'$-DIS of the tree T contains at most one vertex of the subtree T_u and at most one vertex of the subtree T_v. Moreover, if it contains exactly two vertices, then both of them are diametrical leaves of T. Then there exists $(l_u+1)(l_v+1)$ k-DIS's (including the empty set) all elements of which are diametrical leaves. In addition, there exist $(n-l_u-l_v)$ k-DIS's consisting of one vertex that is not a diametrical leaf. Thus,

$$i_{2k'}(T) = (n-l_u-l_v) + (l_u+1)(l_v+1) = n + l_u l_v + 1.$$

It is clear that the quantity $l_u l_v$ will take the greatest value in the case where T contains the minimum possible number of nonleaf vertices and $|l_u - l_v| \leq 1$. This means that T is isomorphic

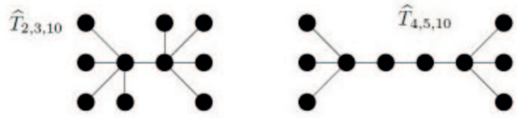

Fig. 2. Trees $\widehat{T}_{2,3,10}$ and $\widehat{T}_{4,5,10}$.

to a simple path $P_{2k'}$ with l_u and l_v leaves attached to its endpoints, respectively. We assume that $l_u \geq l_v$; then $l_u = \lfloor \frac{n-2k'+1}{2} \rfloor$ and $l_v = \lfloor \frac{n-2k'}{2} \rfloor$. The proof of Theorem 1 is complete. □

Thus, this section describes $(i_2, 3, n)$-maximal trees $\widehat{T}_{2,3,n}$ and $(i_4, 5, n)$-maximal trees $\widehat{T}_{4,5,n}$ (see Fig. 2). It is shown that for all admissible values of n such trees are unique up to isomorphism.

3. CASE OF $(i_k, 4, n)$-MAXIMAL TREES

Recall that the graph $S_{4,n}$ is the only $(i_1, 4, n)$-maximal tree up to isomorphism [1]. In this section, we will show that for $k \in \{2, 3\}$ and $n \geq 53$ the graph M_n is the only $(i_k, 4, n)$-maximal tree.

3.1. Variant $d = 4$, $k = 2$

Let the central vertex u of a tree T of diameter 4 be adjacent to l leaves, as well as to $m \geq 2$ preleaf vertices $u_1, \ldots, u_m$. Let us introduce the notation $\mathcal{L} = \prod_{i=1}^{m} \deg(u_i)$.

Lemma 1. *The following relation holds*:

$$i_2(T) = 1 + \sum_{i=1}^{m} \frac{\mathcal{L}}{\deg(u_i)} + (l+1) \cdot \mathcal{L}.$$

Proof. It is easy to see that there exist $\mathcal{L}$ 2-DIS's all of whose elements are diametrical leaves. Then there exist $(l+1) \cdot \mathcal{L}$ 2-DIS's that do not contain any nonleaf vertices of the tree. In addition, for each $1 \leq i \leq m$ there exist $\frac{\mathcal{L}}{\deg(u_i)}$ 2-DIS's containing the vertex u_i, and each of them does not contain other vertices from the neighborhood $N[u]$. Finally, there exists a unique 2-DIS $\{u\}$ containing the central vertex u. The proof of Lemma 1 is complete. □

For trees of the form $M^l_{a,b}$ we have the relation $\mathcal{L} = 2^a \cdot 3^b$, and hence

$$i_2\big(M^l_{a,b}\big) = 1 + a \cdot 2^{a-1} \cdot 3^b + b \cdot 2^a \cdot 3^{b-1} + (l+1) \cdot 2^a \cdot 3^b.$$

Theorem 2. *For all $n \geq 53$ the only $(i_2, 4, n)$-maximal tree is the tree M_n.*

Proof. Consider some $(i_2, 4, n)$-maximal tree T and prove step by step that it coincides with M_n.

STEP 1. Let us show that T has the form $M^l_{a,b}$. Let it not be the case. Then its central vertex u is adjacent to at least one vertex u_0 of degree $q_0 \geq 4$. Let us denote by w_1 and w_2 two arbitrary leaves adjacent to u_0. By T_1 we denote the tree obtained by removing these leaves from T, and by T_2, the tree obtained by removing the vertex u_0 and all leaves adjacent to it from T. In the tree T we replace the edges u_0w_1 and u_0w_2 by uw_1 and w_1w_2 and denote the resulting tree as T'. It is easy to see that

$$i_2(T) = i_2(T_1) + i_2^+(T, w_1) + i_2^+(T, w_2) = i_2(T_1) + 2 \cdot i_2^-(T_2, u),$$
$$i_2(T') = i_2(T_1) + i_2^+(T', w_2) + i_2^+(T', w_1) \geq i_2(T_1) + i_2^-(T_1, u) + 1.$$

Denote by w_3 an arbitrary leaf adjacent to u_0 in T_1. Then

$$i_2^-(T_1, u) \geq (q_0 - 2) \cdot i_2^+(T_1, w_3) \geq (q_0 - 2) \cdot i_2^-(T_2, u),$$

and hence $i_2(T') > i_2(T)$; this contradicts the maximality of T.

STEP 2. Let us show that T has the form $M_{a,b}$. Suppose that this is not the case. Then T has the form $M^l_{a,b}$, where $l > 0$. If $a > 0$, then consider the tree $M^{l-1}_{a-1,b+1}$. We have the relations

$$i_2\big(M^l_{a,b}\big) = 1 + a \cdot 2^{a-1} \cdot 3^b + b \cdot 2^a \cdot 3^{b-1} + (l+1) \cdot 2^a \cdot 3^b,$$
$$i_2\big(M^{l-1}_{a-1,b+1}\big) = 1 + (a-1) \cdot 2^{a-2} \cdot 3^{b+1} + (b+1) \cdot 2^{a-1} \cdot 3^b + l \cdot 2^{a-1} \cdot 3^{b+1}.$$

It is easy to check that for $a, b, l \geq 0$ the inequality

$$i_2\big(M^{l-1}_{a-1,b+1}\big) > i_2\big(M^l_{a,b}\big)$$

is equivalent to the inequality $3a + 2b + 6l > 15$, which holds true for all $n \geq 53$.

If, however, $a = 0$, then T has the form $M^l_{0,b}$ and $i_2\big(M^l_{0,b}\big) = 1 + b \cdot 3^{b-1} + (l+1) \cdot 3^b$. Then for all $b, l \geq 1$ we have

$$i_2\big(M^{l-1}_{2,b-1}\big) = 1 + 4 \cdot 3^{b-1} + 4 \cdot (b-1) \cdot 3^{b-2} + 4 \cdot l \cdot 3^{b-1} > i_2\big(M^l_{0,b}\big).$$

Thus, for $l > 0$ the tree $M^l_{a,b}$ is not maximal.

STEP 3. Let us show that T is isomorphic to M_n. It is sufficient to prove that the inequality $i_2(M_{a,b}) < i_2(M_{a-3,b+2})$ holds true for $n \geq 53$ and $a \geq 3$. We have

$$i_2(M_{a,b}) = 1 + a \cdot 2^{a-1} \cdot 3^b + b \cdot 2^a \cdot 3^{b-1} + 2^a \cdot 3^b,$$
$$i_2(M_{a-3,b+2}) = 1 + (a-3) \cdot 2^{a-4} \cdot 3^{b+2} + (b+2) \cdot 2^{a-3} \cdot 3^{b+1} + 2^{a-3} \cdot 3^{b+2}.$$

Since we have $3a + 2b \geq 40$ for $n \geq 53$ and $a \geq 3$—the required inequality is satisfied.

The proof of Theorem 1 is complete. □

Note that for $n = 52$ the theorem is false, since

$$i_2(M_{3,15}) = i_2(M_{0,17}).$$

3.2. Variant $d = 4$, $k = 3$

The object of our study is still the tree T of diameter 4 with the central vertex u adjacent to leaves, as well as to the preleaf vertices $u_1, \dots, u_m$, with $\mathcal{L} = \prod_{i=1}^m \deg(u_i)$.

Lemma 2. *One has the relation $i_3(T) = 1 + \deg(u) + \mathcal{L}$.*

Proof. It is clear that there exist exactly $1 + \deg(u)$ 3-DIS's containing at least one vertex from the neighborhood $N[u]$. In addition, there exist $\mathcal{L}$ 3-DIS's that do not contain any vertices from $N[u]$; this implies the required relation. The proof of Lemma 2 is complete. □

Theorem 3. *For $n \geq 5$ and $n \neq 7$, the only $(i_3, 4, n)$-maximal tree is the tree M_n. For $n = 7$, the trees M_7 and $M_{3,0}$ are the only $(i_3, 4, n)$-maximal trees.*

Proof. For $5 \leq n \leq 7$, the validity of the conditions in the theorem can be easily verified by searching through all n-vertex trees of diameter 4. Suppose that for $n \geq 8$ there exists an $(i_3, 4, n)$-maximal tree T not isomorphic to M_n. Similar to the previous theorem, we will carry out the proof step by step.

STEP 1. Let us show that T has the form $M^l_{a,b}$. Suppose that this is not the case. Then its central vertex u is adjacent to some vertex u_0 such that $\deg(u_0) = q_0 \geq 4$. We denote by $u_1, \dots, u_m$ the other neighbors of the vertex u and set $\mathcal{L}' = \prod_{i=1}^m \deg(u_i)$. Let us denote by w_1 and w_2 two arbitrary leaves adjacent to u_0. In T we replace the edges u_0w_1 and u_0w_2 with the edges uw_1 and w_1w_2 and denote the resulting tree by T'. Then

$$i_3(T') = 1 + \big(\deg(u) + 1\big) + 2 \cdot (q_0 - 2) \cdot \mathcal{L}' > 1 + \deg(u) + q_0 \cdot \mathcal{L}' = i_3(T);$$

this contradicts the T being maximal.

STEP 2. Let us show that T has the form $M_{a,b}$. Let it not be the case. Then T has the form $M^l_{a,b}$, where $l \geq 1$, i.e., the vertex u is adjacent to at least one leaf w. In this case, $i^+_3(T, w) = 1$, since all vertices of the tree T are located at a distance of at most 3 from w. Consider some diametrical path $w_1u_1uu_2w_2$ in T, replace the edge uw with the edge u_1w, and denote the resulting tree by T'. It is clear that the set $\{w, w_2\}$ is a 3-DIS in T', whence $i^+_3(T', w) \geq 2$. On the other hand, $i^-_3(T, w) = i^-_3(T', w) = i_3(M^{l-1}_{a,b})$, whence $i_3(T) < i_3(T')$; this contradicts the maximality of T.

STEP 3. Let us show that T is isomorphic to M_n. Let it not be so. Then T is isomorphic to the tree $M_{a,b}$, where $a \geq 3$. Let us show that $i_3(M_{a,b}) < i_3(M_{a-3,b+2})$. Since $2^{a-3} \cdot 3^b > 1$ is true for $n \geq 8$ and $a \geq 3$, we have

$$i_3(M_{a,b}) = 1 + (a + b) + 2^a \cdot 3^b < 1 + (a + b - 1) + 2^{a-3} \cdot 3^{b+2} = i_3(M_{a-3,b+2});$$

this is a contradiction with the T being maximal.

The proof of Theorem 3 is complete. □

4. CASE OF $(i_k, 5, n)$-MAXIMAL TREES

4.1. Variant $d = 5$, $k = 2$

Let T'' denote the tree $M^{1,1}_{a,b,c,d'}$ with the central vertices u and v that are adjacent to the leaves u' and v', respectively. Denote by T' the result of removing the leaf v' from T'' and by T the result of removing the leaf u' from T'. Note that the trees T and T' are isomorphic to the trees $M_{a,b,c,d'}$ and $M'_{a,b,c,d'}$, respectively.

Lemma 3. *The following relations hold*:

$$\begin{aligned}
i^-_2(T_u, u) &= 2^a \cdot 3^b + a \cdot 2^{a-1} \cdot 3^b + b \cdot 2^a \cdot 3^{b-1},\\
i^-_2(T_v, v) &= 2^c \cdot 3^{d'} + c \cdot 2^{c-1} \cdot 3^{d'} + d' \cdot 2^c \cdot 3^{d'-1},\\
i_2(T) &= 2^a \cdot 3^b + 2^c \cdot 3^{d'} + i^-_2(T_u, u) \cdot i^-_2(T_v, v),\\
i_2(T') &= i_2(T) + 2^a \cdot 3^b \cdot i^-_2(T_v, v),\\
i_2(T'') &= i_2(T') + 2^c \cdot 3^{d'} \cdot i^-_2(T_u, u) + 2^{a+c} \cdot 3^{b+d'}.
\end{aligned}$$

Proof. The first two equalities follow from Lemma 1. Let us prove the third equality. If some 2-DIS I of the tree T contains its central vertex u (respectively v), then all other vertices I are diametrical leaves of the subtree T_v (T_u). Moreover, for every 2-DIS I_u of the tree T_u and every 2-DIS I_v of the tree T_v not containing the vertices u and v, respectively, the set $I_u \cup I_v$ is a 2-DIS of the tree T. The fourth equality follows from the relations $i^-_2(T', u') = i_2(T)$ and $i^+_2(T', u') = 2^a \cdot 3^b \cdot i^-_2(T_v, v)$. Similarly, the fifth equality follows from the relations $i^-_2(T'', v') = i_2(T')$ and $i^+_2(T'', v') = 2^c \cdot 3^{d'} \cdot i^-_2(T_u, u) + 2^{a+c} \cdot 3^{b+d'}$. The proof of Lemma 3 is complete. □

Lemma 4. *For $n \geq 120$, each $(i_2, 5, n)$-maximal tree has the form $M_{a,b,c,d'}$.*

Proof. Assume that there exists an $(i_2, 5, n)$-maximal tree T for which the lemma is false. Let us consider four cases.

CASE 1. At least one of the central vertices T (we assume that it is the vertex u) is adjacent to the vertex u_0 of degree $q_0 \geq 4$. In this case, we proceed similarly to Step 1 in Theorem 2. Let us denote by w_1 and w_2 two arbitrary leaves adjacent to u_0. Let T_1 denote the tree obtained by removing these leaves from T. Let T_2 denote the tree obtained by removing the vertex u_0 and all leaves adjacent to it from T. In the tree T we replace the edges u_0w_1 and u_0w_2 by uw_1 and w_1w_2 and denote the resulting tree by T'. It's not hard to see that

$$\begin{aligned}
i_2(T) &= i_2(T_1) + i^+_2(T, w_1) + i^+_2(T, w_2) = i_2(T_1) + 2 \cdot i^-_2(T_2, u),\\
i_2(T') &= i_2(T_1) + i^+_2(T', w_2) + i^+_2(T', w_1) \geq i_2(T_1) + (q_0 - 2) \cdot i^-_2(T_2, u) + 1.
\end{aligned}$$

Thus, $i_2(T') > i_2(T)$; this contradicts the maximality of T.

CASE 2. At least one of the central vertices T (we assume that this is the vertex u) is adjacent to two different leaves u' and u''. Let us remove the edge uu'', add the edge $u'u''$, and denote the resulting tree by T'. It is obvious that $i_2^-(T,u'') = i_2^-(T',u'')$. Moreover, any 2-DIS of the tree T containing the vertex u'' is a 2-DIS of the tree T' since it does not contain the vertices u and u'. However, the set $\{u'',v\}$ is a 2-DIS of T' but is not a 2-DIS of T, whence $i_2^+(T',u'') > i_2^+(T,u'')$ and $i_2(T') > i_2(T)$; this contradicts the maximality of T.

CASE 3. The tree T has the form $M^{1,1}_{a,b,c,d'}$. Recall that u and v denote its central vertices, and u' and v' denote the leaves adjacent to them. Let us denote the result of removing these leaves from T by $\widehat{T}$. By Lemma 3 we have

$$i_2(T) = i_2(\widehat{T}) + 2^a \cdot 3^b \cdot i_2^-(\widehat{T}_v, v) + 2^c \cdot 3^{d'} \cdot i_2^-(\widehat{T}_u, u) + 2^{a+c} \cdot 3^{b+d'}.$$

Consider the tree T' obtained from the tree T by replacing the edge vv' with $u'v'$. Then

$$i_2(T') = i_2(\widehat{T}) + i_2^+(T',v') + i_2^+(T',u') = i_2(\widehat{T}) + i_2^-(\widehat{T},u) + 2^a \cdot 3^b \cdot i_2^-(\widehat{T}_v, v).$$

Let us show that $i_2(T') > i_2(T)$. Assume that $n \geq 120$; threby $2 \cdot (a+c) + 3 \cdot (b+d') \geq 118$. In this case, we have the inequality

$$\begin{aligned} i_2^-(\widehat{T},u) > i_2^-(\widehat{T}_u,u) \cdot i_2^-(\widehat{T}_v,v) &= 2^{a+c} \cdot 3^{b+d'} \cdot \left(1 + \frac{a}{2} + \frac{b}{3}\right) \cdot \left(1 + \frac{c}{2} + \frac{d'}{3}\right) \\ &> 2^{a+c} \cdot 3^{b+d'} \cdot \left(2 + \frac{a}{2} + \frac{b}{3}\right) = 2^c \cdot 3^{d'} \cdot i_2^-(\widehat{T}_u,u) + 2^{a+c} \cdot 3^{b+d'}. \end{aligned}$$

Thus, $i_2(T) < i_2(T')$; this contradicts the maximality of T.

CASE 4. The tree T has the form $M'_{a,b,c,d'}$. Consider all possible variants and let us show that in each of them T is not maximal.

VARIANT $b \geq 1$. Consider the tree $M_{a+2,b-1,c,d'}$. We have

$$\begin{aligned} i_2(M'_{a,b,c,d'}) &= 2^a \cdot 3^b + 2^c \cdot 3^{d'} \\ &\quad + (2^{a+1} \cdot 3^b + a \cdot 2^{a-1} \cdot 3^b + b \cdot 2^a \cdot 3^{b-1}) \cdot i_2^-(T_v,v), \\ i_2(M_{a+2,b-1,c,d'}) &= 2^{a+2} \cdot 3^{b-1} + 2^c \cdot 3^{d'} \\ &\quad + \left(2^{a+2} \cdot 3^{b-1} + (a+2) \cdot 2^{a+1} \cdot 3^{b-1} + (b-1) \cdot 2^{a+2} \cdot 3^{b-2}\right) \cdot i_2^-(T_v,v). \end{aligned}$$

Then for all $b \geq 1$ one has $i_2(M'_{a,b,c,d'}) < i_2(M_{a+2,b-1,c,d'})$.

VARIANT $a \geq 3,\ b = 0$. Consider the tree $M_{a-1,1,c,d'}$. We have

$$\begin{aligned} i_2(M'_{a,0,c,d'}) &= 2^a + 2^c \cdot 3^{d'} + 2^{a-2} \cdot (2a+8) \cdot i_2^-(T_v,v), \\ i_2(M_{a-1,1,c,d'}) &= 3 \cdot 2^{a-1} + 2^c \cdot 3^{d'} + 2^{a-2} \cdot (3a+5) \cdot i_2^-(T_v,v). \end{aligned}$$

Then for all $a \geq 3$ one has $i_2(M'_{a,0,c,d'}) < i_2(M_{a-1,1,c,d'})$.

VARIANT $a \leq 2,\ b = 0,\ c = 1$. Consider the tree $M'_{a+1,0,0,d'}$. We have

$$\begin{aligned} i_2(M'_{a,0,1,d'}) &= 2^a + 2 \cdot 3^{d'} + 2^{a-1} \cdot 3^{d'-1} \cdot (a+4) \cdot (2d'+9), \\ i_2(M'_{a+1,0,0,d'}) &= 2^{a+1} + 3^{d'} + 2^{a-1} \cdot 3^{d'-1} \cdot (2a+10) \cdot (d'+3). \end{aligned}$$

Then for all $a \leq 2$ and $d' \geq 7$ one has $i_2(M'_{a,0,1,d'}) < i_2(M'_{a+1,0,0,d'})$.

VARIANT $a \leq 2,\ b = 0,\ c = 2$. Consider the tree $M'_{a+2,0,0,d'}$. We have

$$\begin{aligned} i_2(M'_{a,0,2,d'}) &= 2^a + 4 \cdot 3^{d'} + 2^{a-1} \cdot 3^{d'-1} \cdot (a+4) \cdot (4d'+24), \\ i_2(M'_{a+2,0,0,d'}) &= 2^{a+2} + 3^{d'} + 2^{a-1} \cdot 3^{d'-1} \cdot (4a+24) \cdot (d'+3). \end{aligned}$$

Then for all $a \leq 2$ and $d' \geq 7$ one has $i_2(M'_{a,0,2,d'}) < i_2(M'_{a+2,0,0,d'})$.

VARIANT $a \le 2,\ b = 0,\ c \ge 3$. Consider the tree $M'_{a,0,c-3,d'+2}$. We have

$$i_2(M'_{a,0,c,d'}) = 2^a + 2^c \cdot 3^{d'} + 2^{c-4} \cdot 3^{d'-1} \cdot (48 + 24c + 16d') \cdot i_2^-(T_u, u),$$
$$i_2(M'_{a,0,c-3,d'+2}) = 2^a + 2^{c-3} \cdot 3^{d'+2} + 2^{c-4} \cdot 3^{d'-1} \cdot (27c + 18d' + 9) \cdot i_2^-(T_u, u).$$

Since $a \le 2$, one has $3c + 2d' \ge 40$, and hence $i_2(M'_{a,0,c,d'}) > i_2(M'_{a,0,c-3,d'+2})$.

VARIANT $a = 1,\ b = c = 0$. Consider the tree $M_{0,3,0,d'-2}$. We have

$$i_2(M'_{1,0,0,d'}) = 2 + 3^{d'} + 5 \cdot (3^{d'} + d' \cdot 3^{d'-1}),$$
$$i_2(M_{0,3,0,d'-2}) = 27 + 3^{d'-2} + 54 \cdot \big(3^{d'-2} + (d'-2) \cdot 3^{d'-3}\big).$$

Then for all $d' \ge 12$ one has $i_2(M'_{1,0,0,d'}) < i_2(M_{0,3,0,d'-2})$.

VARIANT $a = 2,\ b = c = 0$. Consider the tree $M_{1,3,0,d'-2}$. We have

$$i_2(M'_{2,0,0,d'}) = 4 + 3^{d'} + 12 \cdot (3^{d'} + d' \cdot 3^{d'-1}),$$
$$i_2(M_{1,3,0,d'-2}) = 54 + 3^{d'-2} + 135 \cdot \big(3^{d'-2} + (d'-2) \cdot 3^{d'-3}\big).$$

Then for all $d' \ge 3$ one has $i_2(M'_{2,0,0,d'}) < i_2(M_{1,3,0,d'-2})$.

The proof of Lemma 4 is complete. □

Lemma 5. *Let an $(i_2, 5, n)$-maximal tree T be of the form $M_{a,b,c,d'}$. If $3a + 2b \ge 40$, then $a \le 2$. If, however, $3c + 2d' \ge 40$, then $c \le 2$.*

Proof. Assume that $3a + 2b \ge 40$ and $a \ge 3$. By Lemma 3 we have the relations

$$i_2(M_{a,b,c,d'}) = 2^a \cdot 3^b + 2^c \cdot 3^{d'} + 2^a \cdot 3^b \cdot \left(1 + \frac{a}{2} + \frac{b}{3}\right) \cdot i_2^-(T_v, v),$$
$$i_2(M_{a-3,b+2,c,d'}) = 2^{a-3} \cdot 3^{b+2} + 2^c \cdot 3^{d'} + 2^{a-3} \cdot 3^{b+2} \cdot \left(\frac{1}{6} + \frac{a}{2} + \frac{b}{3}\right) \cdot i_2^-(T_v, v).$$

It is easy to check that the inequality $i_2(M_{a,b,c,d'}) < i_2(M_{a-3,b+2,c,d'})$ holds in the case of $3a + 2b \ge 40$; this contradicts the maximality of T. The case of $3c + 2d' \ge 40$ is treated similarly. The proof of Lemma 5 is complete. □

Lemma 6. *If $n \ge 120$, then each $(i_2, 5, n)$-maximal tree has the form $M_{a,b,c,d'}$ with $|(3a + 2b) - (3c + 2d')| \le 2$.*

Proof. By Lemma 4, each maximal tree has the form $M_{a,b,c,d'}$. Assume that $3a + 2b + 3 \le 3c + 2d'$. If $d' = 0$, then $c \le 13$ by Lemma 5, whence $3a + 2b \le 36$ and $n < 120$; this contradicts the condition in the lemma. If $d' \ge 1$, then consider the tree $M_{a,b+1,c,d'-1}$. We have

$$i_2(M_{a,b,c,d'}) = 2^a \cdot 3^b + 2^c \cdot 3^{d'} + 2^{a+c} \cdot 3^{b+d'} \cdot \left(1 + \frac{a}{2} + \frac{b}{3}\right) \cdot \left(1 + \frac{c}{2} + \frac{d'}{3}\right),$$
$$i_2(M_{a,b+1,c,d'-1}) = 2^a \cdot 3^{b+1} + 2^c \cdot 3^{d'-1} + 2^{a+c} \cdot 3^{b+d'} \cdot \left(\frac{4}{3} + \frac{a}{2} + \frac{b}{3}\right) \cdot \left(\frac{2}{3} + \frac{c}{2} + \frac{d'}{3}\right).$$

These relations imply the inequality

$$i_2(M_{a,b+1,c,d'-1}) - i_2(M_{a,b,c,d'}) > 2^{a+c-1} \cdot 3^{b+d'-2}(3c + 2d' - 3a - 2b - 2) - 2^{c+1} \cdot 3^{d'-1}.$$

We assume that $2a + 3b + 2c + 3d' \ge 118$ and $3c + 2d' \ge 3a + 2b + 3$. Then, as is easy to check, at least one of the inequalities $2^{a-2} \cdot 3^{b-1} \ge 1$ and $3c + 2d' \ge 3a + 2b + 14$ is satisfied, whence

$i_2(M_{a,b+1,c,d'-1}) > i_2(M_{a,b,c,d'})$; this contradicts the extremality of $M_{a,b,c,d'}$. The proof of Lemma 6 is complete. □

Theorem 4. *For all $n \geq 120$, the maximal tree $\widehat{T}_{2,5,n}$ is unique with*

$$\widehat{T}_{2,5,n} = \begin{cases} M_{1,p-1,1,p-1} & \text{if } n = 6p \\ M_{1,p-1,0,p} & \text{if } n = 6p+1 \\ M_{0,p,0,p} & \text{if } n = 6p+2 \\ M_{2,p-2,0,p+1} & \text{if } n = 6p+3 \\ M_{1,p-1,0,p+1} & \text{if } n = 6p+4 \\ M_{0,p+1,0,p} & \text{if } n = 6p+5. \end{cases}$$

Proof. We call a tree of the form $M_{a,b,c,d'}$ *suitable* if the conditions $|(3a+2b)-(3c+2d')| \leq 2$ and $\max(a,c) \leq 2$ are satisfied. Let us show that for $n \geq 120$ the desired tree $\widehat{T}_{2,5,n}$ is suitable. It is sufficient to check the condition $\max(a,c) \leq 2$. If $3a+2b \leq 39$, then $3c+2d' \leq 41$ by Lemma 6. Then $2a+3b+2c+3d' \leq 117$; this contradicts the assumption. The case of $3c+2d' \leq 39$ is treated similarly. If $\min(3a+2b, 3c+2d') \geq 40$, then $\max(a,c) \leq 2$ by Lemma 5; this is what was required. We assume that $c \leq a \leq 2$ and, if $a = c$, then $b \geq d'$ (since the trees $M_{a,b,c,d'}$ and $M_{a,d',c,b}$ coincide in this case).

Case of $n = 6p$. Here the sum $2a+3b+2c+3d'+2$ is a multiple of 3; hence $a+c=2$. There exist three suitable trees: $M_{1,p-1,1,p-1}$, $M_{2,p-2,0,p}$, and $M_{2,p-3,0,p+1}$. Then

$$\begin{aligned} i_2(M_{1,p-1,1,p-1}) &= 4 \cdot 3^{p-1} + (3^p + 2 \cdot (p-1) \cdot 3^{p-2})^2, \\ i_2(M_{2,p-2,0,p}) &= 13 \cdot 3^{p-2} + (8 \cdot 3^{p-2} + 4 \cdot (p-2) \cdot 3^{p-3}) \cdot (3^p + p \cdot 3^{p-1}), \\ i_2(M_{2,p-3,0,p+1}) &= 85 \cdot 3^{p-3} + (8 \cdot 3^{p-3} + 4 \cdot (p-3) \cdot 3^{p-4}) \cdot (4 \cdot 3^p + p \cdot 3^p). \end{aligned}$$

It is easy to check that for all $p \geq 20$ the tree $M_{1,p-1,1,p-1}$ will be the only $(i_2, 5, 6p)$-maximal tree.

Case of $n = 6p+1$. Here $a+c \in \{1,4\}$. There exist two suitable trees: $M_{1,p-1,0,p}$ and $M_{2,p-1,2,p-2}$. It can readily be checked $i_2(M_{1,p-1,0,p}) > i_2(M_{2,p-1,2,p-2})$ for $p \geq 20$.

Case of $n = 6p+2$. In this case $a+c \in \{0,3\}$. There exist two suitable trees: $M_{0,p,0,p}$ and $M_{2,p-2,1,p}$. It can readily be checked that $i_2(M_{0,p,0,p}) > i_2(M_{2,p-2,1,p})$ for $p \geq 20$.

Case of $n = 6p+3$. Here $a+c=2$, the trees $M_{1,p,1,p-1}$ and $M_{2,p-2,0,p+1}$ are suitable, and it can readily be checked that $i_2(M_{2,p-2,0,p+1}) > i_2(M_{1,p,1,p-1})$ for $p \geq 20$.

Case of $n = 6p+4$. In this case $a+c \in \{1,4\}$. There exist two suitable trees: $M_{1,p-1,0,p+1}$ and $M_{2,p-1,2,p-1}$. It can readily be checked that $i_2(M_{1,p-1,0,p+1}) > i_2(M_{2,p-1,2,p-1})$ for $p \geq 20$.

Case of $n = 6p+5$. Here $a+c \in \{0,3\}$, the trees $M_{0,p+1,0,p}$ and $M_{2,p-1,1,p}$ are suitable, and it can readily be checked that $i_2(M_{0,p+1,0,p}) > i_2(M_{2,p-1,1,p})$ for $p \geq 20$.

The proof of Theorem 4 is complete. □

4.2. Variant $d = 5$, $k = 3$

The object of our study is still the tree T of diameter 5 with the central vertices u and v that are adjacent to the vertices $u_1, \dots, u_p$ and $v_1, \dots, v_q$ respectively. Let us introduce the notation $\mathcal{L}_u = \prod_{i=1}^{p} \deg(u_i)$ and $\mathcal{L}_v = \prod_{i=1}^{q} \deg(v_i)$.

Lemma 7. *One has the relation*

$$i_3(T) = 2 + \big(\deg(u) - 1\big) \cdot \mathcal{L}_v + \big(\deg(v) - 1\big) \cdot \mathcal{L}_u + \mathcal{L}_u \cdot \mathcal{L}_v.$$

Proof. It is clear that there exist exactly two 3-DIS's containing at least one of the central vertices of T. In addition, there exist $(\deg(u) - 1) \cdot \mathcal{L}_v$ 3-DIS's containing at least one of the vertices $u_1, \ldots, u_p$ and $(\deg(v) - 1) \cdot \mathcal{L}_u$ of the 3-DIS containing at least one of the vertices $v_1, \ldots, v_q$. Finally, there exist $\mathcal{L}_u \cdot \mathcal{L}_v$ 3-DIS's all of whose elements are diametrical leaves of T. The proof of Lemma 7 is complete. □

Note that for the tree $M_{a,b,c,d'}$ we have the relation

$$i_3(M_{a,b,c,d'}) = 2 + (a+b) \cdot 2^c \cdot 3^{d'} + (c+d') \cdot 2^a \cdot 3^b + 2^{a+c} \cdot 3^{b+d'}.$$

Lemma 8. *Each $(i_3, 5, n)$-maximal tree T has the form $M_{a,b,c,d'}$ with* $\max(a,c) \le 2$.

The **proof** will again be carried out step by step.

STEP 1. Let us show that T has the form $M^{p',q'}_{a,b,c,d'}$. Suppose that this is not the case. Then there exists at least one preleaf vertex u_0 of degree $q_0 \ge 4$ adjacent to one of the central vertices (we assume that to the vertex u). We denote the neighbors of u different from v and u_0 by $u_1, \ldots, u_p$ and the neighbors of v different from u, by $v_1, \ldots, v_q$. Let $\mathcal{L}'_u = \prod_{i=1}^{p} \deg(u_i)$ if $p \ge 1$ and $\mathcal{L}'_u = 1$ if $p = 0$. Let us denote by w_1 and w_2 two arbitrary leaves adjacent to u_0. In the tree T we replace the edges u_0w_1 and u_0w_2 with the edges uw_1 and w_1w_2, and denote the resulting tree by T'. Then

$$\begin{aligned} i_3(T) &= 2 + \big(\deg(u) - 1\big) \cdot \mathcal{L}_v + \big(\deg(v) - 1\big) \cdot q_0 \cdot \mathcal{L}'_u + q_0 \cdot \mathcal{L}'_u \cdot \mathcal{L}_v, \\ i_3(T') &= 2 + \deg(u) \cdot \mathcal{L}_v + \big(\deg(v) - 1\big) \cdot 2 \cdot (q_0 - 2) \cdot \mathcal{L}'_u + 2 \cdot (q_0 - 2) \cdot \mathcal{L}'_u \cdot \mathcal{L}_v. \end{aligned}$$

Since $q_0 \ge 4$, we have $i_3(T') > i_3(T)$ and T is not maximal; this is a contradiction.

STEP 2. Let us show that T has the form $M_{a,b,c,d'}$. Let us assume that this is not the case and that at least one of the central vertices (say, the vertex u) is adjacent to the leaf u'. In the tree T, we consider some diametrical path $u_2u_1uvv_1v_2$. Let us remove the edge uu', add the edge u_1u', and denote the resulting tree by T'. It is clear that $i_3^-(T, u') = i_3^-(T', u')$. Since every 3-DIS of the tree T containing u' does not contain other vertices of the subtree T_u and vertices from the neighborhood $N[v]$, it is a 3-DIS of the tree T' . On the other hand, the set $\{u', v_1\}$ is not a 3-DIS of the tree T, but is a 3-DIS of the tree T', whence $i_3(T) < i_3(T')$; this is a contradiction.

STEP 3. Let us show that $\max(a,c) \le 2$. Assume that $a \ge 3$. Then

$$\begin{aligned} i_3(M_{a,b,c,d'}) &= 2 + (a+b) \cdot 2^c \cdot 3^{d'} + (c+d') \cdot 2^a \cdot 3^b + 2^{a+c} \cdot 3^{b+d'}, \\ i_3(M_{a-3,b+2,c,d'}) &= 2 + (a+b-1) \cdot 2^c \cdot 3^{d'} + (c+d') \cdot 2^{a-3} \cdot 3^{b+2} + 2^{a+c-3} \cdot 3^{b+d'+2}. \end{aligned}$$

It is clear that $i_3(M_{a-3,b+2,c,d'}) > i_3(M_{a,b,c,d'})$ for $a \ge 3$ and $\min(c, d') > 0$; this contradicts the maximality of T. The case of $c \ge 3$ is treated similarly.

The proof of Lemma 8 is complete. □

Lemma 9. *For all $n \ge 13$, each $(i_3, 5, n)$-maximal tree has the form $M_{a,b,c,d'}$ with either* $\min(a,c) = 0$ *and* $\min(b,d') = 1$ *or* $\min(b,d') = 0$.

Proof. Suppose that some maximal tree T has the form $M_{a,b,c,d'}$ and in this case, either $\min(a,c) = 0$ and $\min(b,d') \ge 2$ or $\min(a,b,c,d') \ge 1$ and $\max(a,b,c,d') \ge 2$. Let us introduce the notation

$$j_3(M_{a,b,c,d'}) = i_3(M_{a,b,c,d'}) - 2 - 2^{a+c} \cdot 3^{b+d'} = (a+b) \cdot 2^c \cdot 3^{d'} + (c+d') \cdot 2^a \cdot 3^b.$$

By assumption, the trees $M_{a,b-1,c,d'+1}$ and $M_{a,b+1,c,d'-1}$ exist and have diameter 5. Moreover, since the tree $M_{a,b,c,d'}$ is maximal, we have

$$i_3(M_{a,b,c,d'}) \ge \max\big(i_3(M_{a,b-1,c,d'+1}),\ i_3(M_{a,b+1,c,d'-1})\big),$$

thereby $j_3(M_{a,b,c,d'}) \geq \max(j_3(M_{a,b-1,c,d'+1}),\, j_3(M_{a,b+1,c,d'-1}))$ and the following system of inequalities holds:

$$\begin{cases} 2^c 3^{d'}(a+b) + 2^a 3^b (c+d') \geq 2^c 3^{d'+1}(a+b-1) + 2^a 3^{b-1}(c+d'+1) \\ 2^c 3^{d'}(a+b) + 2^a 3^b (c+d') \geq 2^c 3^{d'-1}(a+b+1) + 2^a 3^{b+1}(c+d'-1). \end{cases}$$

Transforming this system, we obtain

$$\begin{cases} (2c+2d'-1)\cdot 2^a \cdot 3^{b-1} \geq (2a+2b-3)\cdot 2^c \cdot 3^{d'} \\ (2a+2b-1)\cdot 2^c \cdot 3^{d'-1} \geq (2c+2d'-3)\cdot 2^a \cdot 3^b. \end{cases}$$

This implies the inequality

$$\frac{2a+2b-1}{2c+2d'-3} \geq 9 \cdot \frac{2a+2b-3}{2c+2d'-1}.$$

Since $\min(a+b, c+d') \geq 2$, this inequality has solutions only in the case of $a+b = c+d' = 2$. By assumption, this is only possible for $a = c = 0$ and $b = d' = 2$. In this case, $i_3(M_{0,2,0,2}) < i_3(M_{2,0,1,2})$. Thus, every tree $M_{a,b,c,d'}$ that does not satisfy the conditions in the lemma is not maximal, as required. The proof of Lemma 9 is complete. □

Theorem 5. *For all $n \geq 11$, the maximal tree $\widehat{T}_{3,5,n}$ is unique, and moreover,*

$$\widehat{T}_{3,5,n} = \begin{cases} M_{2,0,0,q-2} & \text{if } n = 3q \\ M_{1,0,0,q-1} & \text{if } n = 3q+1 \\ M_{2,0,1,q-2} & \text{if } n = 3q+2. \end{cases}$$

Proof. Let us call a maximal tree *suitable* if it has the form $M_{a,b,c,d'}$, where $c \leq a \leq 2$ and either $\min(a,c) = 0$ and $\min(b,d') = 1$ or $\min(b,d') = 0$. By Lemmas 8 and 9, for $n \geq 13$ the required tree $\widehat{T}_{3,5,n}$ is suitable. We assume that if $a = c$, then $b \leq d'$ (since the trees $M_{a,b,c,d'}$ and $M_{a,d',c,b}$ coincide in this case).

Case of $n = 3q$.

Variant $q = 4$. By Lemma 4, every $(i_3, 5, 12)$-maximal tree has the form $M_{a,b,c,d'}$, where $\max(a,c) \leq 2$. Since the number of vertices in the tree is even, we have $b + d' \in \{0, 2\}$, whence $b + d' = a + c = 2$. Since

$$i_3(M_{2,0,0,2}) > \max\left(i_3(M_{1,1,1,1}),\, i_3(M_{1,0,1,2}),\, i_3(M_{2,1,0,1})\right),$$

the tree $M_{2,0,0,2}$ is the only $(i_3, 5, 12)$-maximal one.

Variant $q \geq 5$. If $a = c = 1$, then the only suitable tree is $M_{1,0,1,q-2}$ with $i_3(M_{1,0,1,q-2}) = 2\cdot 3^{q-1} + 2q$. If $a = 2$ and $c = 0$, then there exist three suitable trees: $M_{2,0,0,q-2}$, $M_{2,q-3,0,1}$, and $M_{2,1,0,q-3}$. In this case, $i_3(M_{2,0,0,q-2}) = 2\cdot 3^{q-1} + 4q - 6$, $i_3(M_{2,q-3,0,1}) = 16\cdot 3^{q-3} + 2q$ and $i_3(M_{2,1,0,q-3}) = 5\cdot 3^{q-2} + 12q - 34$. Since for all $q \geq 5$ we have the inequality

$$i_3(M_{2,0,0,q-2}) > \max\left(i_3(M_{1,0,1,q-2}),\, i_3(M_{2,q-3,0,1}),\, i_3(M_{2,1,0,q-3})\right),$$

the tree $M_{2,0,0,q-2}$ is the only $(i_3, 5, 3q)$-maximal one.

Case of $n = 3q+1$. If $a = 1$ and $c = 0$, then there exist three suitable trees: $M_{1,0,0,q-1}$, $M_{1,q-2,0,1}$, and $M_{1,1,0,q-2}$, while $i_3(M_{1,0,0,q-1}) = 3^q + 2q$, $i_3(M_{1,q-2,0,1}) = 8\cdot 3^{q-2} + 2q$ and $i_3(M_{1,1,0,q-2}) = 8\cdot 3^{q-2} + 6q - 10$. If $a = c = 2$, then the only suitable tree is $M_{2,0,2,q-3}$ with $i_3(M_{2,0,2,q-3}) = 8\cdot 3^{q-2} + 4q - 2$. Since for $q \geq 4$ we have

$$i_3(M_{1,0,0,q-1}) > \max\left(i_3(M_{1,q-2,0,1}),\, i_3(M_{1,1,0,q-2}),\, i_3(M_{2,0,2,q-3})\right),$$

the tree $M_{1,0,0,q-1}$ is the only $(i_3, 5, 3q+1)$-maximal one.

Case of $n = 3q + 2$.

Variant $q = 3$. By Lemma 8, every $(i_3, 5, 11)$-maximal tree has the form $M_{a,b,c,d'}$, where $\max(a, c) \le 2$. Since the number of vertices in the tree is odd, we have $b + d'\{1, 3\}$; then $a + c \in \{0, 3\}$. We conclude that

$$i_3(M_{2,0,1,1}) > \max\left(i_3(M_{0,1,0,2}),\ i_3(M_{2,1,1,0})\right),$$

and hence the tree $M_{2,0,1,1}$ is the only $(i_3, 5, 11)$-maximal one.

Variant $q \ge 4$. If $a = c = 0$, then the only suitable tree is $M_{0,1,0,q-1}$ with $i_3(M_{0,1,0,q-1}) = 4 \cdot 3^{q-1} + 3q - 1$. If $a = 2$ and $c = 1$, then there exist two suitable trees: $M_{2,q-2,1,0}$ and $M_{2,0,1,q-2}$, while $i_3(M_{2,q-2,1,0}) = 4 \cdot 3^{q-1} + 2q + 2$ and $i_3(M_{2,0,1,q-2}) = 4 \cdot 3^{q-1} + 4q - 2$. Since

$$i_3(M_{2,0,1,q-2}) > \max\left(i_3(M_{0,1,0,q-1}),\ i_3(M_{2,q-2,1,0})\right),$$

the tree $M_{2,0,1,q-2}$ is the only $(i_3, 5, 3q + 2)$-maximal one.

The proof of Theorem 5 is complete. □

Note that the condition in the theorem is not satisfied for $n = 10$, since $i_3(M_{2,0,2,0}) > i_3(M_{1,0,0,2})$.

5. CASE OF (i_k, d, n)-MINIMAL TREES

Recall that the problem of describing (i_1, d, n)-minimal trees remains open for $d \ge 8$. In this section, for all $1 < k < d < n$, a (i_k, d, n)-minimal tree $T_{k,d,n}$ is constructed and all triples (k, d, n) for which it is unique are indicated. In addition, all minimal trees are described in the case of $1 < k < d \le 5$.

It follows from the definition of k-DIS that for $n, k \ge 1$ we have the relation

$$i_k(P_n) = i_k(P_{n-1}) + i_k(P_{n-k-1}),$$

where $i_k(P_{-s}) = 1$ for $0 \le s \le k$. Note that $i_k(P_n) = n + 1$ for $0 \le n \le k + 1$.

Lemma 10. *Let $k \ge 2$ and $1 \le m \le n - 1$. Then*

$$i_k(P_n) < i_k(P_m) \cdot i_k(P_{n-m}).$$

Proof. Induction on n for a fixed $k \ge 2$. The basis of induction $n \le k + 1$ is obvious. By the induction assumption, the following relations hold:

$$\frac{i_k(P_{n-1})}{i_k(P_{n-m-1})} \le i_k(P_m), \quad \frac{i_k(P_{n-k-1})}{i_k(P_{n-m-k-1})} \le i_k(P_m).$$

The first inequality becomes an equality only in the case of $m = n - 1$, but then, obviously, the second inequality is strict. Thus, we have the strict inequality

$$\frac{i_k(P_n)}{i_k(P_{n-m})} = \frac{i_k(P_{n-1}) + i_k(P_{n-k-1})}{i_k(P_{n-m-1}) + i_k(P_{n-m-k-1})} < i_k(P_m).$$

The proof of Lemma 10 is complete. □

We denote by $T_{k,d,n}$ the tree obtained from the path P_{d+1} by joining $n - d - 1$ leaves either to its kth vertex from the end if $d > 2k - 2$ or to its central vertex if $d \le 2k - 2$. Let us define the tree $T'_{k,d,n}$ as follows. If d is even, then $T'_{k,d,n}$ is obtained from the path P_{d+1} by attaching $n - d - 1$ leaves to one of the vertices adjacent to the central path vertex (see Fig. 3). If d is odd, then $T'_{k,d,n}$ is obtained from the path P_{d+1} by attaching a leaf to one of its central vertices and $n - d - 2$ leaves, to the other of its central vertices.

Theorem 6. *For all $1 < k < d < n$, the tree $T_{k,d,n}$ is (i_k, d, n)-minimal. Moreover, it is the only minimal one if and only if one of the following conditions is satisfied*:

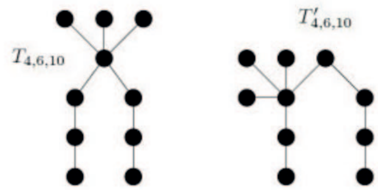

Fig. 3. Trees $T_{4,6,10}$ and $T'_{4,6,10}$.

1. $n = d + 1$.
2. $n = d + 2$ *and* $d \geq 2k - 3$.
3. $n \geq d + 3$ *and either* $d = 2k - 2$ *or* $d \geq 3k - 3$.

Proof. Consider three cases.

CASE OF $n = d + 1$. The only $(d + 1)$-vertex tree of diameter d is the path P_{d+1}, which coincides with the tree $T_{k,d,d+1}$. Thus, this is the only $(i_k, d, d + 1)$-minimal tree.

CASE OF $n \geq d + 3$. Consider two variants.

VARIANT $d \leq 2k - 2$. By the definition of the tree $T_{k,d,n}$, all of its leaves that do not lie on the diametrical path are adjacent to one of the central vertices. Then each of these leaves is located at a distance of at most k from all other vertices of the tree and

$$i_k(T_{k,d,n}) = i_k(P_{d+1}) + (n - d - 1).$$

Let us prove that $i_k(T) \geq i_k(T_{k,d,n})$ for any n-vertex tree T of diameter d. Let us fix some diametrical path P in the tree T. It is clear that T contains exactly $i_k(P_{d+1})$ k-DIS's containing only vertices of P and at least $n-d-1$ k-DIS's containing at least one vertex not from P, which would immediately imply the required inequality.

If $d = 2k - 2$, then the equality $i_k(T) = i_k(T_{k,d,n})$ is possible only if all vertices of T not belonging to P are leaves adjacent to the central vertex of T. Since for even value of d the central vertex is unique, the tree $T_{k,d,n}$ is the only minimal one. If $d < 2k - 2$, then $i_k(T_{k,d,n}) = i_k(T'_{k,d,n})$, and the trees $T_{k,d,n}$ and $T'_{k,d,n}$ do not match. This means that the tree $T_{k,d,n}$ is not the only minimal one.

VARIANT $d > 2k - 2$. Since for each leaf of the tree $T_{k,d,n}$ not lying on its diametrical path, vertices at a distance more than k from it form the path P_{d-2k+2}, we have the relation

$$i_k(T'_{k,d,n}) = i_k(P_{d+1}) + (n - d - 1) \cdot i_k(P_{d-2k+2}).$$

Let us prove that $i_k(T) \geq i_k(T_{k,d,n})$ for any n-vertex tree T of diameter d. Let us fix some diametrical path P in T. For any vertex u that is not on P, there exist at least $d - 2k + 2$ vertices in P at a distance of more than k from u. Moreover, such vertices form either one simple path or two simple paths. Then by Lemma 10 we have

$$\begin{aligned} i_k(T) &\geq i_k(P_{d+1}) + (n - d - 1) \cdot \min_{0 \leq m \leq d-2k+2} (i_k(P_m) \cdot i_k(P_{d-2k+2-m})) \\ &= i_k(P_{d+1}) + (n - d - 1) \cdot i_k(P_{d-2k+2}) = i_k(T_{k,d,n}). \end{aligned}$$

The equality $i_k(T) = i_k(T_{k,d,n})$ means that every vertex T not lying on P is a leaf located at a distance k from one of the endpoints of P, and all such leaves are located at a distance of at most k from each other. For $d > 2k - 2$, the path P contains two different vertices located at a distance of $k - 1$ from one of its endpoints; we denote them by v_1 and v_2. Then every leaf T not lying on P is adjacent to one of these vertices. Moreover, if T is not isomorphic to $T_{k,d,n}$, then $\min(\deg(v_1), \deg(v_2)) \geq 3$. Since the distance between v_1 and v_2 does not exceed $k - 2$, the path P contains at most $3k - 3$ vertices and T has a diameter of at most $3k - 4$. This means that for $d \geq 3k - 3$ the tree $T_{k,d,n}$ is unique; this is what was required.

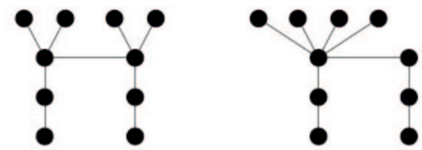

Fig. 4. Two pairwise nonisomorphic $(i_3, 5, 10)$-minimal trees.

Case of $n = d + 2$.

Variant $d > 2k - 2$. It follows from the reasoning in the previous case that the only $(i_k, d, d+2)$-minimal tree is obtained from the path P_{d+1} by attaching a leaf to its kth vertex from the end. This means that it coincides with the tree $T_{k,d,d+2}$.

Variant $d \in \{2k-2, 2k-3\}$. It is clear that $i_k(T_{k,d,d+2}) = i_k(P_{d+1}) + 1$. Consider an arbitrary $(d+2)$-vertex tree T of diameter d. It consists of a diametrical path P_{d+1} and some leaf u not lying on it. Moreover, if T does not coincide with $T_{k,d,d+2}$, then the leaf u is not adjacent to the central vertex of the path, meaning that $i_k^+(T, u) > 1$ and $i_k(T) > i_k(T_{k,d,d+2})$; then the tree $T_{k,d,d+2}$ is the only minimal one.

Variant $d < 2k - 3$. Let us denote by $T''_{k,d,d+2}$ the tree obtained from the path P_d by attaching a leaf to its vertex that is adjacent to one of the central vertices. Then $i_k(T_{k,d,d+2}) = i_k(T''_{k,d,d+2}) = i_k(P_{d+1}) + 1$ and the tree $T_{k,d,d+2}$ is minimal but not unique.

The proof of Theorem 6 is complete. □

Let us give an explicit description of all (i_k, d, n)-minimal trees in the case of $1 < k < d \le 5$.

Corollary 1. *For all $n \ge 4$, the only $(i_2, 3, n)$-minimal tree is the graph $S_{3,n}$ with $i_2(S_{3,n}) = 2n - 2$.*

Corollary 2. *For all $n \ge 5$, the following assertions hold true.*

1. *The only $(i_2, 4, n)$-minimal tree is the graph $S_{4,n}$ with $i_2(S_{4,n}) = 3n - 6$.*
2. *The only $(i_3, 4, n)$-minimal tree is $M_{2,0}^{n-5}$ with $i_3(M_{2,0}^{n-5}) = n + 2$.*

Corollary 3. *For all $n \ge 6$, the following assertions hold true.*

1. *The only $(i_2, 5, n)$-minimal tree is the graph $S_{5,n}$ with $i_2(S_{5,n}) = 4n - 11$.*
2. *For $k \in \{3, 4\}$ each $(i_k, 5, n)$-maximal tree has the form $M_{1,0,1,0}^{p,q}$, where $p + q = n - 6$, with $i_3\big(M_{1,0,1,0}^{p,q}\big) = 2n - 2$ and $i_4\big(M_{1,0,1,0}^{p,q}\big) = n + 2$.*

Note that the number of pairwise nonisomorphic $(i_k, 5, n)$-maximal trees for $k \in \{3, 4\}$ grows linearly with n (see Fig. 4).

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