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Trees without twin-leaves with smallest number of maximal independent sets

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Abstract: For any n , in the set of n -vertex trees such that any two leaves have no common adjacent vertex, we describe the trees with the smallest number of maximal independent sets.

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1 Introduction

An *independent set* in a graph is an arbitrary set of its pairwise nonadjacent vertices. An independent set in a graph is *maximal* if it is maximal under inclusion. We shall write “i.s.” and “m.i.s.” to abbreviate, respectively, the phrases “independent set(s)” and “maximal independent set(s)”. The number of maximal independent sets in a graph G is usually denoted by $mi(G)$.

The problem of enumeration of i.s. and m.i.s. in various classes of graphs has been extensively studied. The amount of literature on this subject is constantly increasing. In the well-known paper [7], Moon and Moser had evaluated the maximal possible number of m.i.s. in n -vertex graphs and described the corresponding extremal graphs. Such graphs were found to be disconnected. In [3], a similar result for connected graphs was obtained. In [4, 5, 6, 8], the maximal possible numbers of m.i.s. were obtained for triangle-free graphs, unicyclic graphs, bipartite graphs, and for n -vertex trees, respectively.

The lower estimate for the number of i.s. in the class of all n -vertex trees is well known and is attained on the n -path. At present, some lower estimates for the number of i.s. for trees of fixed size are available. For example, in [2] a sharp lower estimate for the number of i.s. in trees of diameter at most 5 was proposed. The paper [1] gives asymptotically attainable lower estimates for the number of i.s. in trees of diameter 6 and 7.

A sharp lower estimate for the number of m.i.s. in the class of all n -vertex trees is the constant 2, which is attained on the $(n - 1)$ -star. Dainyak [1] obtained sharp upper and lower estimates for the number of m.i.s. in trees of fixed diameter. Moreover, his lower bound is also a constant, which depends only on the diameter of the tree. An extensive survey of the results on enumeration of independent sets in graphs and on related topics may be found in [1].

Two leaves of a tree are called *twin-leaves* if they have a common neighbor. The trees with twin-leaves were excluded from consideration because the removal / addition of such leaves from the tree does not alter the number of m.i.s.; the problem of the description of extremal trees of a given size with admissible twin-leaves turns out to be much simpler. Hence in what follows we shall consider trees without twin-leaves. An n -vertex tree T without twin-leaves is called *minimal* if it contains the smallest number of m.i.s. among all such trees. In the present paper we completely describe all minimal n -vertex trees for any n .

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2 Definitions, notation, and transformations of graphs

2.1 Standard definitions and notation

A vertex adjacent to a leaf of a forest is called a *preleaf vertex*. For a two-vertex tree, both its vertices are preleaf vertices.

By P_n we shall denote a simple path on n vertices.

Given a graph G and its vertex v , by $\text{mi}_+(G, v)$ we denote the number of m.i.s. in the graph G which contain the vertex v . For a graph G and its vertex v , by $\text{mi}_-(G, v)$ we denote the number of m.i.s. in the graph G which do not contain the vertex v .

2.2 Transformations of trees and their properties

By a *union* of trees T_1 and T_2 we mean a tree obtained from the disjoint union of the trees T_1 and T_2 by addition of a new vertex of degree two which is adjacent to a preleaf of the tree T_1 and a preleaf of the tree T_2 . The set of all possible unions of trees T_1 and T_2 will be denoted by $u(T_1, T_2)$.

The following result is clear.

Lemma 1. *If in a tree T a preleaf of a vertex v is adjacent to a leaf v' , then $\text{mi}(T) = \text{mi}_+(T, v) + \text{mi}_+(T, v')$.*

Lemma 2. *For any tree $T \in u(T_1, T_2)$,*

$$\text{mi}(T) = \text{mi}(T_1) \cdot \text{mi}(T_2).$$

Proof. Assume that T is obtained from T_1 and T_2 by addition of a vertex w adjacent to a preleaf v_1 of the tree T_1 and a preleaf u_1 of the tree T_2 . We denote by v'_1 the leaf of the tree T_1 adjacent to the vertex v_1 . By u'_1 we denote the leaf in the tree T_2 obtained in the same manner. The following relations hold:

$$\begin{aligned} \text{mi}(T_1) \cdot \text{mi}(T_2) &= (\text{mi}_+(T_1, v_1) + \text{mi}_+(T_1, v'_1)) \cdot (\text{mi}_+(T_2, u_1) + \text{mi}_+(T_2, u'_1)), \\ \text{mi}(T) &= \text{mi}_-(T, w) + \text{mi}_+(T, w) = \text{mi}_-(T, w) + \text{mi}_+(T_1, v'_1) \cdot \text{mi}_+(T_2, u'_1). \end{aligned}$$

Each m.i.s. of the tree T which does not contain the vertex w must contain at least one of the vertices v and u . Hence

$$\begin{aligned} \text{mi}_-(T, w) &= \text{mi}_+(T_1, v_1) \cdot \text{mi}_+(T_2, u_1) + \text{mi}_+(T_1, v_1) \cdot \text{mi}_-(T_2, u_1) + \text{mi}_-(T_1, v_1) \cdot \text{mi}_+(T_2, u_1) \\ &= \text{mi}_+(T_1, v_1) \cdot \text{mi}_+(T_2, u_1) + \text{mi}_+(T_1, v_1) \cdot \text{mi}_+(T_2, u'_1) + \text{mi}_+(T_1, v'_1) \cdot \text{mi}_+(T_2, u_1). \end{aligned}$$

Therefore, $\text{mi}(T) = \text{mi}(T_1) \cdot \text{mi}(T_2)$. □

Assume that F is a forest with s connected components that contains $a_0 \geq 2$ m.i.s. Consider the forest F_k obtained by addition of a k -path with the endpoint x to the forest F and addition of $s' \leq s$ edges such that for any $i \in \overline{1, s}$ there is at most one edge connecting x with the vertices of the i th connected component. We denote by a_k the number of m.i.s. in the forest F_k , write a_{-1} in place of $\text{mi}_+(F_1, x)$, and write a_{-2} in place of $\text{mi}_-(F_1, x)$. We assume that not only the forest F is fixed, but also the vertices of the components of this forest with which x is connected. If F is augmented with paths P_r and P_q is succession and arbitrary and if this gives us a forest, then by $a_{r,q}$ we denote the number of m.i.s. in the resulting graph. The notation $a_{-1,k}$, $a_{k,-1}$, $a_{-1,-1}$ have the same meaning as a_{-1} .

Lemma 3. *The following results hold.*

- I) $a_n < a_{n+1} < 2 \cdot a_n$ for any $n \geq 1$.
- II) $a_{n+2} \leq 2 \cdot a_n$ for any $n \geq 0$.
- III) If F is a tree, then $a_2 \geq \frac{3}{2} \cdot a_0$.
- IV) If each connected component of a forest F contains at least two vertices, then $2 \cdot a_0 > a_1$. If F is a tree and if a neighbor $y \in V(F)$ of a vertex x is not a preleaf, then $a_1 > a_0$.

Proof. I) By Lemma 1, we have $a_{n+1} = a_{n-1} + a_{n-2}$, $a_n = a_{n-2} + a_{n-3}$. Moreover, from Lemma 1 and the inequality $a_0 \geq 2$ it also follows that $a_n > a_{n-2}$, $a_{n-1} > a_{n-3}$, which gives $a_n < a_{n+1}$. We have $a_{n-1} \leq a_n$, and hence $a_{n+1} < 2 \cdot a_n$.

II) By Lemma 1, we have $a_{n+2} = a_n + a_{n-1}$. Next, $a_n \geq a_{n-1}$ for any n , and so $a_{n+2} \leq 2 \cdot a_n$ for $n \geq 0$.

III) Let y be a neighbor of the vertex x in the tree F . By Lemma 1, we have $a_2 = a_0 + a_{-1}$ and $a_0 = \text{mi}_-(F, y) + \text{mi}_+(F, y)$, and besides, $a_{-1} = \text{mi}(F \setminus \{y\}) \geq \max(\text{mi}_+(F, y), \text{mi}_-(F, y))$. As a result, $a_{-1} \geq \frac{a_0}{2}$ and $a_2 \geq 1.5 \cdot a_0$.

IV) Since $a_1 = a_{-1} + a_{-2}$ and $a_{-2} \leq a_0$, $a_{-1} \leq a_0$, we have $2 \cdot a_0 \geq a_1$. The equality here is possible only if $a_0 = a_{-1} = a_{-2}$. By T_1, \dots, T_s we denote all connected components of the forest F , and by z_i the neighbor of the vertex x in the tree T_i . It is clear that $a_0 = \prod_{i=1}^s \text{mi}(T_i)$ and $a_{-2} = \prod_{i=1}^s \text{mi}(T_i) - \prod_{i=1}^s \text{mi}_-(T_i, z_i)$. Therefore, the equality $a_{-2} = a_0$ is possible only if $\prod_{i=1}^s \text{mi}_-(T_i, z_i) = 0$; i.e., when one of the connected components of the forest F contains precisely one vertex. Hence $2 \cdot a_0 > a_1$.

Assume that F is a tree and that a neighbor $y \in V(F)$ of the vertex x is not a preleaf. We denote by T'_1, \dots, T'_p all connected components of the forest $F \setminus \{y\}$, and denote by z'_i the neighbor of the vertex y in the tree T'_i . Hence

$$a_1 = a_{-1} + a_{-2} = \text{mi}(F \setminus \{y\}) + \text{mi}_+(F, y) = \prod_{i=1}^p \text{mi}(T'_i) + \text{mi}_+(F, y),$$

$$a_0 = \text{mi}_-(F, y) + \text{mi}_+(F, y) = \prod_{i=1}^p \text{mi}(T'_i) - \prod_{i=1}^p \text{mi}_-(T'_i, z'_i) + \text{mi}_+(F, y).$$

It is clear that $|V(T'_i)| \geq 2$ and $\text{mi}_-(T'_i, z'_i) > 0$ for any i , because y is not a preleaf of the tree F . Therefore, $a_1 > a_0$. □

2.3 Some additional definitions and notation

By R_n we denote the graph obtained from the path P_n by adding n numbered vertices and n numbered edges, moreover, for any $i \in \overline{1, n}$ the edge with number i connects the i th added vertex and the i th vertex of the path starting from one of the endpoints of the path.

By R'_3 we denote the graph P_6 and by R'_4 we mean the graph obtained by joining the endpoint of the 4-path with the vertex of degree two of the other 4-path. It is clear that $\text{mi}(R_3) = \text{mi}(R'_3) = 5$ and $\text{mi}(R_4) = \text{mi}(R'_4) = 8$.

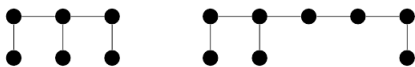


Fig. 1: The graphs R_3 and R'_4 .

By $R_{a,b}$ we denote the tree obtained from R_a and R_b by addition of the vertex adjacent to a vertex of degree two of the tree R_a and to the vertex of degree two of the tree R_b . Similarly, by R_{k_1, k_2, \dots, k_s} we denote the tree consisting of the subtrees $R_{k_1, k_2, \dots, k_{s-1}}$ and R_{k_s} connected in the same manner.

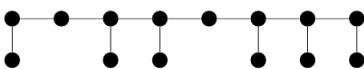


Fig. 2: The tree $R_{1,2,3}$

A subtree T' of a tree T will be called *extreme* if only one vertex of the subtree T' is adjacent to vertices from $V(T) \setminus V(T')$. This vertex of the subtree T' will be called a *contact vertex*. A subtree R_{k_1, k_2, \dots, k_s} will be called *extreme* if among its vertices only a vertex of degree two of its subtree R_{k_s} (if $s = 1$ and $k_1 = 1$, then of degree one) is connected with one or several vertices of the original tree. A path P_l will be called *extreme* if one of its endpoints has degree one, while all the remaining vertices have degree two in the initial tree. Note that it is not envisaged that the concept of an extreme tree will be applied to paths, and hence we will be using the more restrictive definition of an extreme path.

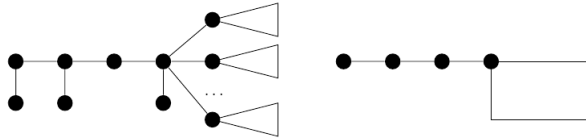


Fig. 3: An extreme subtree $R_{2,1}$ and an extreme 3-path.

We say that an extreme subtree T' of a tree T is *adjacent to an l -path* (x_1, \dots, x_l) if $x_1, \dots, x_l \in V(T) \setminus V(T')$, the vertex x_1 is adjacent to the contact vertex of the subtree T' , and if the degrees of all vertices x_1, \dots, x_l in the tree T are equal to two. Besides, we assume that in the set $V(T) \setminus V(T')$ the contact vertex of the subgraph T' has a unique neighbor — the endpoint of the l -path.

Let T be a tree, T' be an extreme subtree of T , and x be a contact vertex. Next, let T'' be some tree with selected vertex y . We say that we *replace T' by T'' in the tree T* if we remove from T all the elements of the set $V(T')$ and add T'' and all its edges of the form yz , where $z \in V(T) \setminus V(T')$ and $xz \in E(T)$. In what follows such replacements will be applied to some pairs (T', T'') , where T'' is a simple path or a tree of the form R_{k_1, \dots, k_s} , and as a contact vertex y we take either an endpoint of the path or a preleaf of a vertex of degree two (of degree one if $s = 1$ and $k_1 = 1$) of the tree R_{k_1, \dots, k_s} . Besides, such replacements will be applied to trees without twin-leaves in order to preserve the number of vertices and the absence of twin-leaves, and in order to reduce the number of m.i.s.

A tree T will be called T^* -*selected* if T is a union of two its extreme subtrees of which one is isomorphic to T^* . A tree will be called $R_1 \vee R_2$ -*selected* if it is either R_1 -selected or R_2 -selected. The main idea of the present paper is to show that all nontrivial minimal trees are $R_1 \vee R_2$ -selected. This result will enable one to characterize them.

Given a tree T , we construct the tree $Z(T)$ as follows. The vertex set of $Z(T)$ is the set of vertices in T of degree at least three. Two vertices of the tree $Z(T)$ are connected by edge if they are either adjacent in T or the path in T between them consists of some vertices of degree two.

A vertex v of a tree T of degree at least three will be called *extreme* if it is a leaf in the tree $Z(T)$. If in addition v is also an endpoint of one of the paths of largest length in $Z(T)$, then such a vertex is called a *terminal vertex*. It is clear that each extreme vertex is adjacent to at least two extreme paths.

By a *change of an extreme vertex x by a subtree \hat{T} with selected vertex y* in a tree T we mean the removal of some extreme paths adjacent to x (their choice will be clear from the context) and also of the vertex x and all leaves adjacent to it. After this, the tree is augmented with the subtree \hat{T} and its selected vertex is connected with all vertices which were initially adjacent to the vertex x and were not removed from the tree in the process of this transformation. The constraints on (\hat{T}, y) are precisely the same as on (T'', y) . This transformation will be applied in a way to preserve the number of vertices and the absence of twin-leaves, but the number of m.i.s. will be reduced.

3 Structure of minimal trees

In the following two subsections we prove several structural lemmas on the absence of special fragments in minimal trees.

3.1 Some constraints on the extreme subgraphs

Lemma 4. *A minimal tree cannot contain a subgraph of one of the following types:*

- 1) *an extreme 5-path;*
- 2) *an extreme 4-path not adjacent to a preleaf.*

Proof. By a forest F we shall mean the result of removing all vertices of the extreme subgraph under consideration. Assume that some minimal tree contains an extreme 5-path. We replace its first 4-subpath by the subgraph R_2 . It is clear that the result of this transformation does not contain twin-leaves. By Lemma 1, the initial tree contains $a_3 + a_2$ m.i.s., while the result has $a_3 + a_1$ m.i.s. (we apply Lemma 1 to the leaf of the subtree R_2 not adjacent to its contact vertex); moreover, $a_2 > a_1$ by assertion I of Lemma 3.



Fig. 4: Local transformation of the 5-path.

Let us prove the second assertion of the lemma. Assume that some minimal tree contains an extreme 4-path such that the vertex adjacent to this path is not a preleaf vertex. We replace this vertex by the subgraph R_2 . It is clear that result of the transformation does not contain twin-leaves. By Lemma 1 the initial graph contains $a_4 = a_2 + a_1$ m.i.s., while the resulting graph has $a_2 + a_0$ m.i.s. (we applied Lemma 1 to the leaf of the subtree R_2 adjacent to the neighbor of its contact vertex). By assertion IV of Lemma 3, $a_1 > a_0$. \square

Lemma 5. *A minimal tree cannot simultaneously contain:*

- 1) *two extreme 4-paths;*
- 2) *two extreme subgraphs R_3 ,*
- 3) *two extreme subgraphs R_k and R_s , $k, s \in \{2, 3, 4\}$, each of which is adjacent to a 2-path.*

Proof. By a forest F we shall mean the result of removing all vertices of both extreme subgraphs and (in the third case) the four vertices of both 2-paths adjacent to these vertices. Let us prove the first assertion. Assume that a minimal tree contains two extreme 4-paths (in general, such paths may be adjacent to the same vertex). By Lemma 4 (case 2), each of these paths is adjacent to a preleaf vertex. We replace the first 3-subpath of the first path by the subgraph R_2 and replace the first 3-subpath of the second path by the subgraph R_1 . It is clear that result of the transformation does not contain twin-leaves. Then the initial graph contains $a_{4,4}$ m.i.s., while the resulting graph contains $mi(R_1) \cdot mi(R_2) \cdot a_{0,0} = 6 \cdot a_{0,0}$ m.i.s. by Lemma 2.

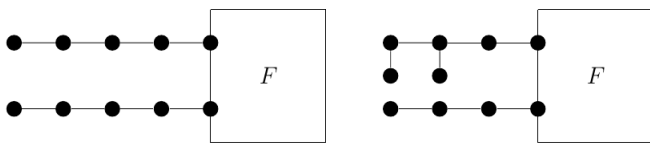


Fig. 5: Local transformation of the two 4-paths.

Moreover, by Lemma 1 and assertion III of Lemma 3,

$$\begin{aligned} a_{4,4} &= a_{2,2} + a_{2,1} + a_{1,2} + a_{1,1} \geq 1.5 \cdot a_{2,0} + 1.5 \cdot a_{0,1} + 1.5 \cdot a_{1,0} + a_{1,1} \\ &\geq 2.25 \cdot a_{0,0} + 1.5 \cdot a_{0,0} + 1.5 \cdot a_{0,0} + a_{0,0} > 6 \cdot a_{0,0}, \end{aligned}$$

hence the number of m.i.s. was reduced.

Let us prove the second assertion. Assume the contrary. We replace the extreme subgraphs by the subgraphs $R_{1,1}$ and $R_{2,1}$. It is clear that the resulting graph does not contain twin-leaves, because they are not contained in the original tree. The initial graph has $4 \cdot a_{2,2} + 2 \cdot a_{0,2} + 2 \cdot a_{2,0} + a_{0,0}$ m.i.s. (we applied Lemma 1 to the “middle” leaves of the subgraphs R_3), while by Lemma 2 the new graph has $\text{mi}(R_1) \cdot \text{mi}(R_2) \cdot a_{2,2} = 6 \cdot a_{2,2}$ m.i.s. By assertion II of Lemma 3,

$$2 \cdot a_{0,2} + 2 \cdot a_{2,0} \geq a_{2,2} + a_{2,2} = 2 \cdot a_{2,2} \geq a_{2,2},$$

and hence the total number of m.i.s. was reduced.

Let us prove the third assertion. Assume on the contrary that there exist extreme subgraphs R_k and R_s , $k, s \in \{2, 3, 4\}$, each of which is adjacent to a 2-path. We may assume that $k = 2$, for otherwise there would exist two extreme subgraphs R_3 .

The case $s = 2$. It may be assumed without loss of generality that $a_{2,1} \leq a_{1,2}$. We replace the first of the extreme subgraphs R_2 by the subgraph $R_{1,1,1}$ and remove all the vertices of the other extreme subgraph R_2 . It is clear that the resulting graph does not contain twin-leaves. The initial graph contains $4 \cdot a_{2,2} + 2 \cdot a_{2,1} + 2 \cdot a_{1,2} + a_{1,1}$ m.i.s., where for evaluation we have applied Lemma 1 to the leaves adjacent to the contact vertices of the extreme subgraphs under consideration. Applying Lemma 2 and Lemma 1 to the leaf $R_{1,1,1}$ adjacent to the contact vertex we find that the resulting graph has $\text{mi}(R_{1,1}) \cdot (a_{2,2} + a_{2,1}) = 4 \cdot (a_{2,2} + a_{2,1})$ m.i.s. So, the number of m.i.s. was reduced.

The case $s = 3$. We replace the extreme subgraph R_3 by the subgraph $R_{2,1,1}$ and remove all the vertices of the extreme subgraph R_2 . It is clear that the resulting graph does not contain twin-leaves. The initial graph contains $6 \cdot a_{2,2} + 4 \cdot a_{2,1} + 3 \cdot a_{1,2} + 2 \cdot a_{1,1}$ m.i.s., where for evaluation we apply Lemma 1 to leaves adjacent to the contact vertices of the subgraphs R_2 and R_3 . Applying Lemma 2 and Lemma 1 to the leaf $R_{2,1,1}$ adjacent to the contact vertex we find that the resulting graph has $\text{mi}(R_{2,1}) \cdot (a_{2,2} + a_{2,1}) = 6 \cdot (a_{2,2} + a_{2,1})$ m.i.s. By assertion I of Lemma 3 we have $2 \cdot a_{1,2} > 2 \cdot a_{1,1} > a_{2,1}$, and hence the total number of m.i.s. was reduced.

The case $s = 4$. We replace the extreme subgraph R_4 by the subgraph $R_{2,2,1}$ and remove all the vertices of the second subgraph. It is clear that the resulting graph does not contain twin-leaves. The initial graph contains $10 \cdot a_{2,2} + 5 \cdot a_{1,2} + 6 \cdot a_{2,1} + 3 \cdot a_{1,1}$ m.i.s., where for evaluation we apply Lemma 1 to the leaves adjacent to the contact vertices of the subgraphs R_2 and R_4 . Applying Lemma 2 and Lemma 1 to the leaf $R_{2,2,2}$ adjacent to the contact vertex we find that the resulting graph has $\text{mi}(R_{2,2}) \cdot (a_{2,2} + a_{2,1}) = 9 \cdot (a_{2,2} + a_{2,1})$ m.i.s. So, it is clear that the total number of m.i.s. was reduced. \square

Lemma 6. *A minimal tree cannot simultaneously contain:*

- 1) an extreme subgraph R_3 and an extreme subgraph R_2 adjacent to a 2-path,
- 2) an extreme subgraph R_2 adjacent to a 2-path and to an extreme 4-path.

Proof. Let us prove the first assertion of the lemma. Assume the contrary. By the forest F we shall mean the result of removing all vertices of the extreme subgraphs R_3 and R_2 and of both vertices of the 2-path adjacent to the extreme subgraph R_2 .

Assume that $a_{0,2} \leq a_{2,0}$. We replace the subgraph R_3 by the subgraph $R_{1,1,2}$ and remove the subgraph R_2 from the graph. It is clear that the resulting graph does not contain twin-leaves. By Lemma 1, the initial graph contains $4 \cdot a_{2,2} + 2 \cdot a_{2,1} + 2 \cdot a_{0,2} + a_{0,1}$ m.i.s., where for evaluation we apply the lemma to the leaf adjacent to the contact vertex of the extreme subgraph R_2 and to the leaf adjacent to a neighbor of the contact vertex of the extreme subgraph R_3 . By Lemmas 2 and 1 the resulting graph has $\text{mi}(R_{1,1}) \cdot (a_{2,2} + a_{0,2}) = 4 \cdot (a_{2,2} + a_{0,2})$ m.i.s., where for evaluation we apply Lemma 1 to the leaf adjacent to a neighbor of the contact vertex of the extreme subgraph $R_{1,1,2}$. So, the number of m.i.s. was reduced.

Now assume that $a_{0,2} > a_{2,0}$. We carry out the following symmetric transformation: we replace R_3 by a 2-path, remove R_2 and the adjacent 2-path (a, b) , and add the graph $R_{1,1,2}$ and the edge xy , where $x \neq a$

is the neighbor of the vertex b and y is the preleaf of degree two belonging to the subgraph R_2 of the graph $R_{1,1,2}$. By Lemmas 2 and 1 the resulting tree has $\text{mi}(R_{1,1}) \cdot (a_{2,2} + a_{2,0}) = 4 \cdot (a_{2,2} + a_{2,0})$ m.i.s. So, the number of m.i.s. was reduced.

Let us prove the second assertion of the lemma. Here, by a forest F we mean the result of removing all vertices of the extreme subgraph R_2 and both vertices of the 2-path adjacent to the extreme subgraph R_2 . Note that one of the endpoints of the extreme 4-path is adjacent to a preleaf by Lemma 4 (case 2). We remove the subgraph R_2 from the graph and replace the three extreme vertices of the 4-paths by the subgraph $R_{2,1}$. The initial graph contains $2 \cdot a_{2,4} + a_{1,4}$ m.i.s. by Lemma 1, which we apply to the neighboring leaf of the contact vertex of the extreme subgraph R_2 . By Lemma 2, the resulting graph contains $\text{mi}(R_{2,1}) \cdot a_{2,0} = 6 \cdot a_{2,0}$ m.i.s. Next, by Lemma 1 and Lemma 3 (assertions II and III) we have

$$2 \cdot a_{2,4} = 2 \cdot a_{2,2} + 2 \cdot a_{2,1} \geq 2 \cdot \frac{3}{2} \cdot a_{2,0} + 2 \cdot a_{2,0} = 5 \cdot a_{2,0},$$

$$a_{1,4} = a_{1,2} + a_{1,1} > 2 \cdot a_{0,0} \geq a_{2,0},$$

and so the number of m.i.s. was reduced. \square

3.2 Some constraints on extreme vertices

Lemma 7. *In a minimal tree each vertex which is simultaneously adjacent to two extreme paths P_k and P_l , where $k \geq l \geq 2$, is adjacent to a leaf.*

Proof. Assume on the contrary that there exists a vertex v which is adjacent to the extreme paths P_l and P_k and which is not adjacent to a leaf. By Lemma 4, $k \leq 3$ and $l \leq 3$. By F we denote the result of removing the vertex v and all vertices of the extreme k -path and l -path from the tree.

The case $k = l = 2$. We remove all vertices of both extreme 2-paths and add the subgraph R_2 , the edge incident to v , and the vertex of degree two of the graph R_2 . Since v is not adjacent to a leaf, the result of the transformation does not contain twin-leaves. By Lemma 1, the initial graph contains $a_1 + 3 \cdot a_0$ m.i.s., while in the resulting graph we have $2 \cdot a_1 + a_0$ m.i.s. (we apply the lemma to the terminals of the extreme 2-paths and to the leaf adjacent to the contact vertex of the subgraph R_2). By Lemma 3 (assertion IV), $2 \cdot a_0 > a_1$.

The case $k = 3, l = 2$. We insert the subgraph R_3 in place of the 6-path with the contact vertex v , which is composed of the vertices of the extreme 3- and 2-paths. Since v is not adjacent to a leaf, the result of the transformation does not contain twin-leaves. By Lemma 1, the initial graph contains $a_4 + 2 \cdot a_0 = a_2 + a_1 + 2 \cdot a_0$ m.i.s., while the resulting graph contains $2 \cdot a_2 + a_0 = a_2 + 2 \cdot a_0 + a_{-1}$ m.i.s. (here the lemma was applied to the terminal of the extreme 2-path and to the leaf adjacent to a neighbor of the contact vertex of the subgraph R_2). Since $a_0 \geq 2$, we have $a_1 > a_{-1}$.

The case $k = l = 3$. We insert the subgraph $R_{2,1}$ in place of the 7-path with the contact vertex v , which is composed of the vertices of the extreme 3-paths. Since v is not adjacent to a leaf, the result of the transformation does not contain twin-leaves. By Lemma 1 (which was applied in succession to the terminals of the extreme 3-paths), the initial graph contains $3 \cdot a_2 + a_1$ m.i.s., while the resulting graph, as given by Lemma 2, has $\text{mi}(R_2) \cdot a_2 = 3 \cdot a_2$ m.i.s.

So, under the assumption that there exists a vertex simultaneously adjacent to two extreme paths and not adjacent to a leaf, we showed in all cases that the number of m.i.s. may be reduced. \square

Lemma 8. *In a minimal non- R_1 -selected tree each extreme vertex has degree at most four.*

Proof. Assume on the contrary that the minimal tree contains an extreme vertex v of degree at least five. Then this vertex is adjacent to three extreme paths P_a, P_b, P_c , where $2 \leq a \leq b \leq c \leq 4$ (see Lemma 4, case 1), and is also adjacent to a leaf by Lemma 7. Since the tree is not R_1 -selected, the vertex v is not adjacent to an extreme 3-path. Moreover, v is adjacent to at most one extreme 4-path by Lemma 5 (case 1). Therefore, the only possible cases are as follows: $a = b = c = 2$ and $a = b = 2, c = 4$. Here by F we mean the result of removing the vertex v , the adjacent leaf, and all vertices of the paths P_a, P_b, P_c .

The case $a = b = c = 2$. We replace the vertex v by the extreme subgraph R_4 . Since v was adjacent to a leaf, the result of the transformation does not contain twin-leaves. By Lemma 1, the initial graph contains $a_2 + 7 \cdot a_0$ m.i.s. (we apply the lemma in succession to the terminal leaves of the three extreme 2-paths), while the resulting graph has $3 \cdot a_2 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf adjacent to a neighbor of the contact vertex of the subtree R_4). Recall that by Lemma 3 (assertion II) we have $a_2 \leq 2 \cdot a_0$. So, the number of m.i.s. was reduced.

The case $a = 2, b = 2, c = 4$. We replace the vertex v by the extreme subgraph $R_{1,1,2}$. Since v was adjacent to a leaf, the result of the transformation does not contain twin-leaves. By Lemma 1, the initial graph contains $2 \cdot a_2 + 10 \cdot a_0$ m.i.s. (we apply the lemma in succession to the terminal leaves of the two extreme 2-paths, and then twice apply the lemma to the vertices of the extreme 4-path), while the resulting graph, as obtained by Lemmas 2 and 1, contains $\text{mi}(R_{1,1}) \cdot (a_2 + a_0) = 4 \cdot (a_2 + a_0)$ m.i.s. So, the number of m.i.s. was reduced.

Thus, under the assumption that there exists an extreme vertex of degree at least five, the number of m.i.s. may be reduced in all possible cases. \square

Lemma 9. *A minimal non- R_1 -selected tree may contain at most one extreme vertex of degree four.*

Proof. Assume that in the minimal tree there exist two extreme vertices of degree four. By Lemma 7, each of such vertices is adjacent to a leaf and to two extreme paths of which each contains at least two vertices. We denote the corresponding extreme paths by P_a, P_b and $P_{a'}, P_{b'}$. From symmetry considerations one may assume that $a \leq b, a' \leq b'$ and $a \leq a'$. Hence, by Lemma 4 (case 1) and Lemma 5 (case 1), it may be assumed that $a = b = a' = b' = 2$ and $a = b = a' = 2, b' = 4$. By F we shall mean the result of removing both extreme vertices, the adjacent leaves, and all vertices of the extreme paths $P_a, P_{a'}, P_b, P_{b'}$.

The case $b' = 2$. We replace one of the extreme vertices by the subgraph $R_{2,1,1}$, and the other one, by a 2-path. Since they were adjacent to leaves, the result of the transformation does not contain twin-leaves. The initial graph contains $9 \cdot a_{0,0} + 3 \cdot a_{2,0} + 3 \cdot a_{0,2} + a_{2,2}$ m.i.s. (Lemma 1 is applied in succession to terminal leaves of the four extreme 2-paths), and by Lemma 2 the resulting graph has $\text{mi}(R_{2,1}) \cdot a_{2,2} = 6 \cdot a_{2,2}$ m.i.s. By Lemma 3 (case II) we have

$$\begin{aligned} 9 \cdot a_{0,0} + 3 \cdot a_{2,0} + 3 \cdot a_{0,2} + a_{2,2} &> 4 \cdot a_{0,0} + 4 \cdot a_{0,0} + 3 \cdot a_{2,0} + 3 \cdot a_{0,2} + a_{2,2} \\ &\geq 2 \cdot a_{2,0} + 2 \cdot a_{0,2} + 3 \cdot a_{2,0} + 3 \cdot a_{0,2} + a_{2,2} = 5 \cdot a_{2,0} + 5 \cdot a_{0,2} + a_{2,2} \\ &\geq \frac{5}{2} \cdot a_{2,2} + \frac{5}{2} \cdot a_{2,2} + a_{2,2} = 6 \cdot a_{2,2}. \end{aligned}$$

The case $b' = 4$. We replace one of the extreme vertices by the subgraph $R_{2,2,1}$, and the other one, by a 2-path. Since they were adjacent to leaves, the result of the transformation does not contain twin-leaves. The initial graph contains $12 \cdot a_{0,0} + 6 \cdot a_{2,0} + 4 \cdot a_{0,2} + 2 \cdot a_{2,2}$ m.i.s. (Lemma 1 is first applied to the terminal leaf of the extreme 4-path), and by Lemma 2 the resulting graph has $\text{mi}(R_{2,2}) \cdot a_{2,2} = 9 \cdot a_{2,2}$ m.i.s. The number of m.i.s. was reduced.

So, under the assumption of the existence of two extreme vertices of degree 4, the number of m.i.s. may be reduced in all the above cases. \square

Lemma 10. *A minimal tree containing an extreme vertex of degree four cannot contain the following subtrees:*

- 1) an extreme 4-path not adjacent to a given extreme vertex,
- 2) an extreme subgraph R_3 ,
- 3) an extreme subgraph R_2 adjacent to a 2-path.

Proof. Consider an arbitrary minimal tree and its extreme vertex of degree four. By Lemma 4 (case 1), Lemma 5 (case 1) and Lemma 7 this vertex must be adjacent to the extreme paths P_a and P_2 , where $a \in \{2, 4\}$, and to a leaf. By F we mean the result of removing the extreme vertex of degree four, the adjacent leaf, all vertices of the extreme paths P_2, P_a , the corresponding extreme subgraph, and (in the third case) the vertices of the 2-path adjacent to the extreme subgraph R_2 .

Let us prove the first assertion of the lemma. The case $a = 4$ is impossible by Lemma 5 (case 1). Consider the case with $a = 2$. We shall assume that some extreme 4-path is adjacent to a nonextreme vertex v . Then v is a preleaf by Lemma 4 (case 2).

We remove all the vertices of the extreme 4-path and replace the extreme vertex of degree four by the subgraph $R_{1,2,1}$. Since the original tree does not contain twin-leaves, the resulting graph also does not contain twin-leaves. So, by Lemma 2, the graph has $\text{mi}(R_{1,2}) \cdot a_{2,0} = 6 \cdot a_{2,0}$ m.i.s. after the transformation, while by Lemma 1 there were $3 \cdot a_{0,4} + a_{2,4}$ m.i.s., where for evaluation the lemma was applied to terminal leaves of the extreme 2-paths. By Lemmas 1 and 3 (assertions II and III)

$$\begin{aligned} 3 \cdot a_{0,4} + a_{2,4} &= 3 \cdot a_{0,2} + 3 \cdot a_{0,1} + a_{2,2} + a_{2,1} \geq 3 \cdot \frac{3}{2} \cdot a_{0,0} + 3 \cdot a_{0,0} + \frac{3}{2} \cdot a_{2,0} + a_{2,0} \\ &= 7.5 \cdot a_{0,0} + 2.5 \cdot a_{2,0} > 3.5 \cdot a_{2,0} + 2.5 \cdot a_{2,0} = 6 \cdot a_{2,0}, \end{aligned}$$

i.e., after the transformation the number of m.i.s. was reduced.

Let us prove the second assertion of the lemma.

The case $a = 2$. We replace the extreme subgraph R_3 by the extreme subgraph R_2 and replace the extreme vertex of degree four by the extreme subgraph R_4 . Since the original tree does not contain twin-leaves, the resulting graph also does not contain twin-leaves. The initial graph has $6 \cdot a_{0,2} + 2 \cdot a_{2,2} + 3 \cdot a_{0,0} + a_{2,0}$ m.i.s. (we apply Lemma 1 to the “middle” leaf of the subgraph R_3 and also to the terminal leaves of 2-paths). As a result, we have $3 \cdot a_{2,2} + 2 \cdot a_{0,2} + 3 \cdot a_{2,0} + 2 \cdot a_{0,0}$ m.i.s. (we apply Lemma 1 to the leaves adjacent to the contact vertices of the subgraphs R_2 and R_4). By Lemma 3 (assertions II–IV),

$$4 \cdot a_{0,2} + a_{0,0} > a_{2,2} + 2 \cdot a_{0,2} + a_{0,0} \geq a_{2,2} + 2 \cdot \frac{3}{2} \cdot a_{0,0} + a_{0,0} = a_{2,2} + 4 \cdot a_{0,0} \geq a_{2,2} + 2 \cdot a_{2,0}.$$

The case $a = 4$. We replace the extreme vertex by the subgraph $R_{1,2}$ and replace the extreme subgraph R_3 by the subgraph $R_{1,2}$. Since the original tree does not contain twin-leaves, the resulting graph also does not contain twin-leaves. The initial graph has $8 \cdot a_{0,2} + 4 \cdot a_{2,2} + 4 \cdot a_{0,0} + 2 \cdot a_{2,0}$ m.i.s. (we first we apply Lemma 1 to the terminal leaf of the extreme 4-paths), while by Lemma 2 the resulting graph has $\text{mi}(R_2) \cdot \text{mi}(R_2) \cdot a_{2,2} = 9 \cdot a_{2,2}$ m.i.s. By Lemma 3 (assertion II)

$$8 \cdot a_{0,2} + 4 \cdot a_{2,2} + 4 \cdot a_{0,0} + 2 \cdot a_{2,0} \geq 4 \cdot a_{2,2} + 4 \cdot a_{2,2} + a_{2,2} + a_{2,2} = 10 \cdot a_{2,2},$$

i.e., after the transformation the number of m.i.s. was reduced.

Let us prove the third assertion of the lemma.

The case $a = 2$. We replace the extreme vertex by the subgraph $R_{1,2,1}$ and remove all vertices of the extreme subgraph R_2 . Since the original tree does not contain twin-leaves, the resulting graph also does not contain twin-leaves. The initial graph contains $2 \cdot a_{2,2} + 3 \cdot a_{0,1} + 6 \cdot a_{0,2} + a_{2,1}$ m.i.s. (we apply Lemma 1 to the leaf vertices of both extreme 2-paths and the leaf of the subgraph R_2 not adjacent to its contact vertex). By Lemma 2, the resulting graph has $\text{mi}(R_{1,2}) \cdot a_{2,2} = 6 \cdot a_{2,2}$ m.i.s. Next, by Lemma 3 (assertion II)

$$2 \cdot a_{2,2} + 3 \cdot a_{0,1} + 6 \cdot a_{0,2} + a_{2,1} > 2 \cdot a_{2,2} + a_{2,1} + 3 \cdot a_{2,2} + a_{2,1} > 6 \cdot a_{2,2}.$$

Hence the number of m.i.s. was reduced.

The case $a = 4$. We replace the extreme vertex by the subgraph $R_{2,2,1}$ and remove all the vertices of the extreme subgraph R_2 . Since the original tree does not contain twin-leaves, the resulting graph also does not contain twin-leaves. By Lemma 1 (which was first applied to the terminal leaf of the extreme 4-path), the initial graph contains $4 \cdot a_{2,2} + 4 \cdot a_{0,1} + 8 \cdot a_{0,2} + 2 \cdot a_{2,1}$ m.i.s., while the resulting graph has $\text{mi}(R_{2,2}) \cdot a_{2,2} = 9 \cdot a_{2,2}$ m.i.s. By Lemma 3 (assertion II)

$$4 \cdot a_{2,2} + 4 \cdot a_{0,1} + 8 \cdot a_{0,2} + 2 \cdot a_{2,1} > 4 \cdot a_{2,2} + 4 \cdot a_{2,2} + a_{2,2} = 9 \cdot a_{2,2},$$

i.e., the number of m.i.s. was reduced. □

3.3 Selection of minimal trees

Lemma 11. *In a minimal tree there are no extreme subgraphs R_k for $k \in \{2, 3, 4\}$ which are adjacent to the path P_l , where $l \geq 3$.*

Proof. Assume the contrary. By F we denote the result of removing all vertices of the extreme subgraph R_k and the 3-subpath P_l adjacent to it. We replace the extreme subgraph R_k and the two first vertices of the l -path by the subgraph R_{k+1} . It is clear that the resulting graph does not contain twin-leaves. According to the Lemma 1 applied in the original graph to the leaf adjacent to the contact vertex of the subgraph R_k , the number of its m.i.s. is $\text{mi}(R_{k-1}) \cdot a_3 + \text{mi}(R_{k-2}) \cdot a_2$. According to the Lemma 1 applied in the resulting graph to the leaf adjacent to a neighbor of the contact vertex of the subgraph R_{k+1} , the number of its m.i.s. is $\text{mi}(R_{k-1}) \cdot a_3 + \text{mi}(R_{k-2}) \cdot a_1$. The number of m.i.s. was reduced, because by Lemma 3 (assertion I) we have $a_2 > a_1$. \square

Lemma 12. *If T'_s is the tree obtained by joining by an edge of a vertex of degree two of the subgraph R_2 and the endpoint x of the path with $s + 1$ vertices, where $s \in \{2, 3, 4\}$, then any minimal tree does not contain an extreme subgraph T'_s with nonpreleaf contact vertex x .*

Proof. By F we shall mean the result of removing all vertices of the subtree T'_s from the minimal tree.

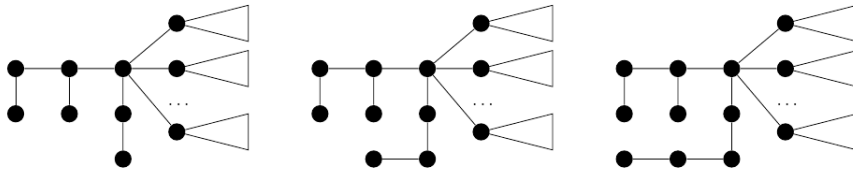


Fig. 6: The trees T'_2 , T'_3 and T'_4 .

The case $s = 2$. We replace T'_2 by the subgraph $R_{2,1}$. The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $2 \cdot a_3 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf adjacent to the contact vertex of the subtree R_2), while by Lemma 2 the resulting graph has $\text{mi}(R_2) \cdot a_2 = 3 \cdot a_2$ m.i.s. Hence by Lemma 3 (assertions I and II) we have $2 \cdot a_3 + 2 \cdot a_0 > 2 \cdot a_2 + 2 \cdot a_0 \geq 3 \cdot a_2$; i.e., the number of m.i.s. was reduced.

The case $s = 3$. We replace T'_3 by the subgraph R_4 . The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $2 \cdot a_4 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf adjacent to the contact vertex of the subtree R_2), while the resulting graph has $3 \cdot a_2 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph R_4 adjacent to a neighbor of the contact vertex). Hence by Lemma 1 and Lemma 3 (assertion I) we have $2 \cdot a_4 + 2 \cdot a_0 = 2 \cdot a_2 + 2 \cdot a_1 + 2 \cdot a_0 > 3 \cdot a_2 + 2 \cdot a_0$.

The case $s = 4$. We replace T'_4 by the subgraph $R_{2,2}$. The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $2 \cdot a_5 + 3 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf adjacent to the contact vertex of the subtree R_2), while by Lemma 2 the resulting graph has $\text{mi}(R_2) \cdot (a_2 + a_0) = 3 \cdot (a_2 + a_0)$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph $R_{2,2}$ adjacent to a neighbor of the contact vertex of this subgraph). Hence by Lemma 1 and Lemma 3 (assertion I), we have $2 \cdot a_5 = 2 \cdot a_3 + 2 \cdot a_2 > 3 \cdot a_2$ i.e., the number of m.i.s. was reduced.

Thus the number of m.i.s. may be reduced in all cases. Therefore, the assumption was false. \square

Lemma 13. *If T''_s is a tree obtained by identifying of one endpoint of a 3-path with a vertex of degree two of the subgraph R_2 and identifying the other endpoint of the 3-path with the endpoint x of a path with $s + 1$ vertices, where $s \in \{2, 3, 4\}$, then each non- R_2 -selected minimal tree does not contain an extreme subgraph T''_s with the contact vertex x .*

Proof. Assume the contrary. Then x is not a preleaf, because the tree is not R_2 -selected. We denote by F the tree from which all vertices of the subtree T''_s were removed. There are three cases to consider.

The case $s = 2$. We replace T''_2 by the subgraph R_4 . The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $a_3 + 2 \cdot a_2 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph R_2 adjacent to the vertex of degree three), the resulting graph having $3 \cdot a_2 + 2 \cdot a_0$ m.i.s.

(we apply Lemma 1 to the leaf of the subgraph R_4 adjacent to a neighbor of the contact vertex). By Lemma 3 (assertion I) we have $a_3 > a_2$, and hence the number of m.i.s. was reduced.

The case $s = 3$. We replace T_3'' by the subgraph $R_{2,2}$. The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $a_4 + 4 \cdot a_2$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph R_2 adjacent to the vertex of degree three), while by Lemma 2 the resulting graph has $\text{mi}(R_2) \cdot (a_2 + a_0) = 3 \cdot (a_2 + a_0)$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph $R_{2,2}$ adjacent to a neighbor of the contact vertex of this subgraph). The number of m.i.s. was reduced, because by Lemma 1 and Lemma 3 (assertion I) we have $a_4 + a_2 = 2 \cdot a_2 + a_1 > 3 \cdot a_0$.

The case $s = 4$. We replace T_4'' by the subgraph $R_{1,1,2}$. The result of the transformation does not contain twin-leaves, because x is not a preleaf. The initial graph contains $a_5 + 4 \cdot a_2 + 2 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf vertex of the graph R_2 adjacent to a vertex of degree three), the resulting graph having $\text{mi}(R_{1,1}) \cdot (a_2 + a_0) = 4 \cdot a_2 + 4 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf of the subgraph $R_{1,1,2}$ adjacent to a neighbor of the contact vertex of this subgraph). By Lemmas 1 and 3 (assertion I) we have $a_5 = a_3 + a_2 > 2 \cdot a_0$, so the number of m.i.s. was reduced.

Thus, the number of m.i.s. may be reduced in all cases. Therefore, the assumption was false. □

Lemma 14. *If T_s'''' is a tree obtained by identifying the endpoints of an $(s + 2)$ -path with vertices of degree two in two copies of the graph R_2 , where $1 \leq s \leq 4$ and x is an arbitrary internal vertex of the $(s + 2)$ -path, then each minimal non- R_2 -selected tree cannot contain an extreme subgraph T_s'''' with the contact vertex x .*

Proof. Assume the contrary. We denote by F the tree from which all vertices of the subtree T_s'''' were removed.

The case $s = 1$. We remove all vertices of the forest $T_1'''' \setminus \{x\}$ and add the subgraph R_4 and the edge incident to x and to a vertex of degree two of the subgraph R_4 . The initial graph contains $4 \cdot a_1 + 5 \cdot a_0$ m.i.s. (here and in what follows we apply Lemma 1 to the leaves of the subgraphs R_2 which are nearest to the vertex x). The resulting graph has $5 \cdot a_1 + 3 \cdot a_0$ m.i.s. (Lemma 1 was applied to the leaf adjacent to the contact vertex of the subtree R_4). It is clear that the transformation does not produce twin-leaves in the tree. By Lemma 3 (assertions I and II) we have $2 \cdot a_0 \geq a_2 > a_1$; i.e., the number of m.i.s. was reduced.

The case $s = 2$. We remove all vertices of the forest $T_2'''' \setminus \{x\}$ and add the graph $R_{2,2}$ and the edge incident to a vertex of degree two of the graph $R_{2,2}$ and to the vertex x . The initial graph contains $4 \cdot a_2 + 2 \cdot a_1 + 3 \cdot a_0$ m.i.s. By Lemma 2, the resulting graph contains $\text{mi}(R_2) \cdot (2 \cdot a_1 + a_0) = 6 \cdot a_1 + 3 \cdot a_0$ m.i.s. (we also apply Lemma 1 to the leaf of the graph $R_{2,2}$ adjacent to its contact vertex). It is clear that the above transformation will not result in twin-leaves in the tree. By Lemma 3 (assertion I) we have $a_2 > a_1$, therefore the number of m.i.s. was reduced.

The case $s = 3$. Suppose that the vertex x is in the middle between the subgraphs R_2 . We replace T_s'''' by $R_{4,1}$. The initial graph contains $8 \cdot a_2 + a_1$ m.i.s., and by Lemma 2 the resulting graph has $\text{mi}(R_4) \cdot a_2 = 8 \cdot a_2$ m.i.s. So, the number of m.i.s. was reduced. Note that in this case the vertex x cannot be a preleaf, because then the tree would be R_2 -selected, and hence the above transformation will not produce twin-leaves in the tree.

The case $s = 3$. Suppose that the vertex x is not in the middle between the subgraphs R_2 . The original graph contains $4 \cdot a_3 + 2 \cdot a_2 + 5 \cdot a_0$ m.i.s. We remove all vertices of the forest $T_3'''' \setminus \{x\}$ and add $R_{1,1,2}$ and the edge incident to a vertex of degree two of the subgraphs R_2 of the graph $R_{1,1,2}$ and to the vertex x . This gives us a tree without twin-leaves. By Lemma 2, the resulting graph contains $\text{mi}(R_{1,1}) \cdot (2 \cdot a_1 + a_0) = 8 \cdot a_1 + 4 \cdot a_0$ m.i.s. (we apply Lemma 1 to the leaf adjacent to the contact vertex of the subtree $R_{1,1,2}$). By Lemmas 1 and 3 (assertions I and II)

$$\begin{aligned} 4 \cdot a_3 + 2 \cdot a_2 + 5 \cdot a_0 &= 4 \cdot a_1 + 5 \cdot a_0 + 2 \cdot a_2 + 4 \cdot a_0 \\ &\geq 4 \cdot a_1 + 2.5 \cdot a_2 + 2 \cdot a_2 + 4 \cdot a_0 = 4.5 \cdot a_2 + 4 \cdot a_1 + 4 \cdot a_0 > 8 \cdot a_1 + 4 \cdot a_0, \end{aligned}$$

i.e., the number of m.i.s. was reduced.

The case $s = 4$. In this case x is not adjacent to contact vertices of the extreme subgraphs R_2 by Lemma 11. We remove all vertices of the forest $T_4'''' \setminus \{x\}$ and add the subgraph $R_{2,3}$ and the edge incident to x and to a vertex of degree two of the subgraph R_3 of the graph $R_{2,3}$. It is clear that the resulting graph has no twin-leaves. The initial graph contains $2 \cdot a_3 + 7 \cdot a_2 + 4 \cdot a_0$ m.i.s. and by Lemma 2 we now have $\text{mi}(R_2) \cdot (3 \cdot a_1 + 2 \cdot a_0) = 9 \cdot a_1 + 6 \cdot a_0$

m.i.s. (we apply Lemma 1 to the leaf adjacent to the contact vertex of the subgraph $R_{2,3}$). By Lemmas 1 and 3 (assertion I)

$$2 \cdot a_3 + 7 \cdot a_2 + 4 \cdot a_0 = 7 \cdot a_2 + 2 \cdot a_1 + 6 \cdot a_0 > 9 \cdot a_1 + 6 \cdot a_0,$$

so the number of m.i.s. was reduced.

Thus the number of m.i.s. may be reduced in all cases. Therefore, the assumption was false. \square

Theorem 1. *A minimal tree T is $R_1 \vee R_2$ -selected if the tree $Z(T)$ contains at least four vertices.*

Proof. Assume that the tree $Z(T)$ is a star. Then this star has at least three leaves. Further, by Lemma 4 (case 1), Lemma 5 (case 1), Lemmas 8, 9, and Lemma 10 (case 1), at least two of these leaves are of degree three in T and are not adjacent to a 4-path. By Lemma 7, these vertices are adjacent to a leaf. We denote by x and y the corresponding leaves of the star $Z(T)$. Since $Z(T)$ is a star, $Z(T)$ is not R_1 -selected and so by Lemma 4 (case 1) each of the second extreme paths has two vertices. Consider the path in the tree T between the vertices x and y . By Lemma 5 (case 2) and Lemma 11, the length of this path is at most five and in this path only one vertex has degree larger two. Now Lemma 14 shows that the tree T is R_2 -selected.

Now assume that the tree $Z(T)$ is not a star. Hence in the tree $Z(T)$ there exist at least two preleaves each of which is adjacent to its set M_i , $i = 1, 2$, of terminal leaves. By Lemma 4 (case 1), Lemma 5 (case 1), Lemmas 7–9, and Lemma 10 (case 1), it may be assumed without loss of generality that each element of the set M_1 has degree three in T and is adjacent to an extreme 2-path and a leaf. By Lemma 11, any such element is at distance at most three from the nearest vertex of degree at most two. If in M_1 there are at least two elements, then we consider a path between them and argue as in the previous case. As a result, we will prove that $Z(T)$ is R_2 -selected.

It remains to consider the case when $M_1 = \{x\}$ and x is at the distance at most 3 in T from the nearest vertex y of degree exceeding two. Then y is a preleaf in the tree $Z(T)$ adjacent to its leaf x . Since $|M_1| = 1$ and x is terminal, then in the tree T all extreme subgraphs which are adjacent to y and which do not contain x are simple paths. Let P_l be one of the extreme paths of this kind. By Lemma 4 (case 1), we have $l \leq 4$. If $\text{dist} = 1$, then by Lemma 12 the vertex y is a preleaf. If $\text{dist} = 2$, then y is not a preleaf and $l \neq 1$, for otherwise T would be R_2 -selected. But this would imply that T is also R_2 -selected by Lemma 13.

It remains to consider the case $\text{dist} = 3$; i.e., when x is in an extreme subgraph R_2 adjacent to a 2-path. If M_2 contains an element of degree four in T , then we get a contradiction with Lemma 10 (case 3). Assume that all elements in M_2 are of degree three in T . By Lemma 6 (case 2) and Lemma 7, they are all adjacent to a leaf and a 2-path. Then it suffices to consider only the case when $M_2 = \{x'\}$. We denote by dist' the distance from x' to the nearest vertex of degree exceeding two. If $\text{dist}' = 2$, then, by Lemmas 12 and 13, the tree T is R_2 -selected. If $\text{dist}' = 1$, then we get a contradiction by Lemmas 12 and 6 (case 1). If $\text{dist}' = 3$, then by Lemma 5 (case 3) we also have a contradiction.

Thus the number of m.i.s. may be reduced in all cases. Therefore, the assumption was false. \square

Theorem 2. *For $n \geq 9$, each minimal n -vertex tree is $R_1 \vee R_2$ -selected.*

Proof. In view of Theorem 1 for the proof of Theorem 2 it suffices to show that all minimal trees T with at least nine vertices and such that the tree $Z(T)$ contains at most three vertices are $R_1 \vee R_2$ -selected.

Assume that tree $Z(T)$ consists of a unique vertex x . By Lemmas 7 and 8, in the initial tree T this vertex is adjacent precisely to one leaf and to at least two paths P_a and P_b , where $a \geq b \geq 2$. By Lemmas 4 (case 1) and 5 (case 1), we have $a \leq 4$, and moreover, $(a, b) \neq (4, 4)$. If $a = 3$ or $b = 3$, then T is R_1 -selected. If $a = 4, b = 2$, then by Lemma 5 (case 1), Lemma 8 and since $n \geq 9$, the vertex x is adjacent to a 4-path, to 2-paths, and to a leaf. But then $\text{mi}(T) = 14$ by Lemma 1, and hence T is not minimal, because we already have $\text{mi}(R_{1,1,2}) = 12$ by Lemma 2.

Assume that the tree $Z(T)$ consists of two vertices. By Lemma 7, each of these vertices is adjacent to a leaf. By Lemmas 8 and 9, each of these vertices has degree $3 \leq d' \leq d \leq 4$ in the initial tree T . The case $d' = d = 4$ is impossible by Lemma 9, and hence we may assume that $d' = 3$. By Lemma 4 (case 1) and Lemma 5 (case 1), among the extreme paths there is at most one 4-path, the remaining path being isomorphic to P_2 . We denote by a the number of vertices in the largest extreme path contained in the tree. Note that in the case $d = a = 4$

an extreme 4-path must be adjacent to a vertex of degree four, for otherwise we would have a contradiction with Lemma 10 (case 1).

Consider several variants depending on the number s of vertices of degree two between extreme vertices. If $s = 1$, then some vertex of the tree T of degree three is adjacent to an extreme 2-path and T is R_2 -selected. If $s \geq 3$, then by Lemma 11, T cannot contain a vertex of degree three which is adjacent to an extreme 2-path. But then each of the extreme vertices is either adjacent to an extreme 4-path or is of degree four, which is impossible. Finally, if $s = 0$ or $s = 2$, then, depending on the values $d \in \{3, 4\}$ and $a \in \{2, 4\}$, the following eight variants are possible.

The variant $s = 0, d = 3, a = 2$. The tree T is isomorphic to the tree R_4 and contains eight vertices.

The variant $s = 0, d = 3, a = 4$. The graph T contains 10 vertices and 13 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,2}) = 12$ by Lemma 2.

The variant $s = 0, d = 4, a = 2$. The graph T contains 10 vertices and 14 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,2}) = 12$ by Lemma 2.

The variant $s = 0, d = 4, a = 4$. The graph T contains 12 vertices and 22 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,3}) = 20$ by Lemma 2.

The variant $s = 2, d = 3, a = 2$. The graph T contains 10 vertices and 13 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,2}) = 12$ by Lemma 2.

The variant $s = 2, d = 3, a = 4$. The graph T contains 12 vertices and 21 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,3}) = 20$ by Lemma 2.

The variant $s = 2, d = 4, a = 2$. The graph T contains 12 vertices and 23 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,3}) = 20$ by Lemma 2.

The variant $s = 2, d = 4, a = 4$. The graph T contains 14 vertices and 36 m.i.s. This tree is not minimal, because we already have $mi(R_{1,1,4}) = 32$ by Lemma 2.

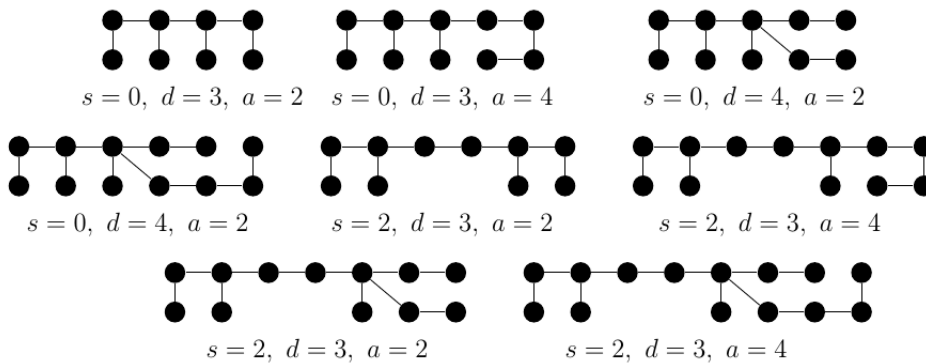


Fig. 7: Variants of graphs with two extreme vertices

Assume that the tree $Z(T)$ consists of three vertices. Then $Z(T)$ is a 3-path. In this case the argument is completely similar to that given in the proof of Theorem 1. □

4 The class of minimal trees

4.1 Totally separated trees and their properties

We define the set $\mathcal{R}(a, b, c, d)$ of trees, where $(c, d) \in \{(0, 0), (1, 0), (0, 1)\}$, as follows. The set $\mathcal{R}(1, 0, 0, 0)$ ($\mathcal{R}(0, 1, 0, 0)$) contains only the tree R_1 (R_2 , respectively). Similarly, the set $\mathcal{R}(0, 0, 1, 0)$ contains only the trees R_3 and R'_3 , and $\mathcal{R}(0, 0, 0, 1)$ contains only the trees R_4 and R'_4 . The set $\mathcal{R}(a_1 + 1, b_1, c_1, d_1)$ consists precisely of such trees T for which there exists a tree $T' \in \mathcal{R}(a_1, b_1, c_1, d_1)$ such that $T \in u(T', R_1)$. The set

$\mathcal{R}(a_2, b_2 + 1, c_2, d_2)$ consists precisely of the trees T for which there exists a tree $T' \in \mathcal{R}(a_2, b_2, c_2, d_2)$ such that $T \in u(T', R_2)$. The elements of the set $\mathcal{R}(a, b, c, d)$, where $a + b + c + d \neq 1$, will be called *totally separated trees*.

Lemma 15. *Let T be a tree in $\mathcal{R}(a, b, c, d)$. Then $|V(T)| = 3 \cdot a + 5 \cdot b + 7 \cdot c + 9 \cdot d - 1$ and $\text{mi}(T) = 2^{a+3d} \cdot 3^b \cdot 5^c$.*

Proof. We argue by induction on the sum $s = a + b + c + d$. The base of the induction $s = 1$ is clear. Assume, for example, that the tree T is R_1 -selected. Then $T \in u(T', R_1)$, where $T' \in \mathcal{R}(a - 1, b, c, d)$. By the induction assumption, the tree T' contains $3 \cdot a + 5 \cdot b + 7 \cdot c + 9 \cdot d - 4$ vertices and $2^{a+3d-1} \cdot 3^b \cdot 5^c$ m.i.s. Then, clearly, the tree T satisfies the hypothesis of this lemma (here we apply Lemma 2). The case when the tree is R_2 -selected is dealt with similarly. \square

We write $\mathcal{R}(a, b, c, d) \succ \mathcal{R}(a', b', c', d')$ if the inequality $\text{mi}(T) > \text{mi}(T')$ holds for any trees $T \in \mathcal{R}(a, b, c, d)$ and $T' \in \mathcal{R}(a', b', c', d')$ with the same number of vertices.

Lemma 16. *If a totally separated tree $T \in \mathcal{R}(a, b, c, d)$ is minimal, then $a \leq 3$ and $ac + ad = 0$.*

Proof. If $c = 1$ and $a \geq 1$, then $\mathcal{R}(a, b, c, d) \succ \mathcal{R}(a - 1, b + 2, c - 1, d)$. If $d = 1$ and $a \geq 1$, then $\mathcal{R}(a, b, c, d) \succ \mathcal{R}(a - 1, b + 1, c + 1, d - 1)$. Hence since the tree T is minimal, we have $a = 0$ or $a \geq 1$, $c = d = 0$. If $c = 0$ and $a \geq 4$, then $\mathcal{R}(a, b, c, d) \succ \mathcal{R}(a - 4, b + 1, c + 1, d)$. Now $a \leq 3$, since the tree T is minimal. \square

The proof of the following result is quite straightforward if we use Lemmas 15 and 16 and consider the cases $a \geq 1$ and $a = 0$ separately.

Lemma 17. *If a minimal n -vertex tree T is totally separated, then:*

- 1) $T \in \mathcal{R}(2, k - 1, 0, 0)$ if $n = 5k$,
- 2) $T \in \mathcal{R}(0, k - 1, 1, 0)$ if $n = 5k + 1$,
- 3) $T \in \mathcal{R}(1, k, 0, 0)$ if $n = 5k + 2$,
- 4) $T \in \mathcal{R}(3, k - 1, 0, 0)$ or $T \in \mathcal{R}(0, k - 1, 0, 1)$ if $n = 5k + 3$,
- 5) $T \in \mathcal{R}(0, k + 1, 0, 0)$ if $n = 5k + 4$.

4.2 Description of minimal trees

We define the class \mathcal{L}_n of n -vertex trees without twin-leaves. For $n \in \{1, 2, 4, 5\}$, the only tree without twin-leaves is the path P_n . For $n = 6, 7, 8$, we set

$$\mathcal{L}_6 = \{R_3, R'_3\}, \mathcal{L}_7 = \{R_{1,2}\}, \mathcal{L}_8 = \{R_4, R'_4\}.$$

Further, for $n \geq 9$, we define

$$\mathcal{L}_n = \begin{cases} \mathcal{R}(2, k - 1, 0, 0) & \text{if } n = 5k, \\ \mathcal{R}(0, k - 1, 1, 0) & \text{if } n = 5k + 1, \\ \mathcal{R}(1, k, 0, 0) & \text{if } n = 5k + 2, \\ \mathcal{R}(3, k - 1, 0, 0) \cup \mathcal{R}(0, k - 1, 0, 1) & \text{if } n = 5k + 3, \\ \mathcal{R}(0, k + 1, 0, 0) & \text{if } n = 5k + 4. \end{cases}$$

Theorem 3. *For any n , the set of minimal n -vertex trees coincides with the set \mathcal{L}_n .*

Proof. A direct verification shows that for $n \leq 8$ the set \mathcal{L}_n contains all minimal trees with n vertices. By Lemma 17, it suffices to show that for $n \geq 9$ each minimal tree is totally separated. We argue by induction on n . The basis of the induction: all n satisfying $n \leq 8$. Assume that T is a minimal tree with $n \geq 9$ vertices. By Theorem 1, the tree T is $R_1 \vee R_2$ -selected.

If T is R_1 -selected, then there exists an $(n-3)$ -vertex tree T' for which $T \in u(T', R_1)$. It is easy to verify that for the minimality of T the tree T' should also be minimal. By the induction assumption $T' \in \mathcal{R}(a_1, b_1, c_1, d_1)$, and hence, $T \in \mathcal{R}(a_1 + 1, b_1, c_1, d_1)$.

If the tree T is R_2 -selected, then there exists a tree T'' with $n - 5$ vertices for which $T \in u(T'', R_2)$. It is easy to check that for the minimality of T the tree T'' should also be minimal. By the induction assumption, $T'' \in \mathcal{R}(a_2, b_2, c_2, d_2)$, which gives $T \in \mathcal{R}(a_2, b_2 + 1, c_2, d_2)$, the result required. \square

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