# Trees with a given number of leaves and the maximal number of maximum independent sets

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**Abstract.** We completely describe the trees with maximal possible number of maximum independent sets among all $n$-vertex trees with exactly $l$ leaves. For all values of the parameters $n$ and $l$ the extremal tree is unique and is the result of merging the endpoints of $l$ simple paths.

**Keywords:** independent set, maximum independent set, maximal independent set, extreme tree

## § 1. Introduction

An *independent set* in a graph is an arbitrary set of its pairwise nonadjacent vertices. We always assume that the empty set is also independent. An independent set in a graph is *maximal* if it is maximal under inclusion A *maximum independent set* is an independent set of the largest size (cardinality). The cardinality of a maximum independent set of a graph $G$ will be denoted by $\alpha(G)$. We shall write "IS", "MLIS" and "MMIS" to abbreviate, respectively, the phrases "independent set(s)", "maximal independent set(s)", and "maximum independent set(s)". The number of all MMIS of a graph $G$ will be denoted by $\xi(G)$.

The problem of enumeration of IS (MLIS or MMIS) in various classes of graphs has been extensively studied. The literature on this subject is constantly updated. In the well-known paper by Moon and Moser [16], the maximal possible number of MLIS and MMIS in $n$-vertex graphs was found and the corresponding extreme graphs were described. These sets were found to be disconnected. In [6], an analogous result was obtained for connected graphs. In [10, 11, 15], the maximal possible numbers of MLIS were obtained for triangle-free graphs, unicyclic graphs, and bipartite graphs, respectively. In [19], the maximal possible number of MLIS in trees was found, and in [17] all the corresponding extreme trees were described.

To date, a large number of papers have been published on the enumeration of IS in trees under various additional constraints. In [8], for any $d$, a complete description was given for the extreme trees maximizing the number of IS in the class of trees in which any vertex has degree at most $d$. Moreover, each extreme tree containing at least $d+1$ vertices must also contain a vertex of degree $d$. A similar problem for MMIS was solved in [1]; the problem for MLIS remains open.

The attainable lower estimates for the number of IS and MLIS in various classes of graphs have been much less studied, since in many cases they are trivial and the corresponding extreme graphs are very simple. So, lower estimate for the number of IS (respectively, MLIS) in the class of all trees is trivial and is attained on a simple path



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(respectively, on a star-graph). Dainyak [5] described all trees of fixed diameter with minimal number of MLIS. Such trees are simple paths whose endpoints are augmented with some leaf vertices which contain twin-leaves. In [2], a more precise lower estimate for the number of MLIS in $n$-vertex trees without twin-leaves was obtained and the corresponding extreme trees were described.

In [9] it was shown that, for any $k > 2$, there exists a $k$-regular graph containing a unique MMIS. Moreover, in [9] an attainable lower estimate for the independence number for graphs with a unique MMIS was derived and a criterion for the uniqueness of an MMIS in a tree was put forward. The survey [12] provides the maximal values of the number of MMIS in $n$-vertex graphs from some classes (in particular, for connected graphs, unicyclic graphs, and triangle-free graphs). In [20], the maximal possible number of MMIS in $n$ vertex trees was found and the corresponding extreme trees were described.

It is clear that a simple path is a unique tree with two leaves. Moreover, $n \geqslant l+1$ for any tree with $n$ vertices and $l$ leaves. Hence in what follows, we will assume that $n > l \geqslant 3$. In [3] and [18], the problem of maximization of the number of IS in $n$-vertex trees with precisely $l$ leaves was solved. It was found that the corresponding extreme tree $T'_{n,l}$ consists of a central vertex augmented with $l-1$ leaves and a simple path $P_{n-l}$. The similar problem for minimum is at present open, but in this direction a result from [7] is worth mentioning on minimization of the number of IS in $n$-vertex trees containing at least $\lfloor \frac{n}{2} \rfloor + 1$ leaves. The problem of maximization of the number of MLIS in $n$-vertex trees with precisely $l$ leaves is open; the corresponding minimization problem is trivial, the corresponding extreme trees coinciding with trees $T'_{n,l}$.

The problem on maximization of the number of IS in $n$-vertex trees of diameter $d$ was solved in many papers (see, for example, in [4, 13, 14]). The corresponding extreme tree was shown to be isomorphic to the tree $T'_{n,n-d+1}$. For MLIS and MMIS this problem remains open.

Рис. 1. The tree $T'_{8,4}$.

In the present paper, for any $n > l \geqslant 3$, we completely describe the trees with maximal possible number of maximum independent sets among the $n$-vertex trees containing precisely $l$ leaves. In what follows, $\mathrm{even}(x)$ will denote the largest even number not exceeding a given real number $x$. By $T_{n,l}$ we will denote an $n$-vertex tree with $l$ leaves containing a maximal possible number of MMIS among all such trees. We shall show that, for any values of the parameters $n$ and $l$, the tree $T_{n,l}$ is unique and is as follows:

(A) If $n \leqslant 2l$, then the tree $T_{n,l}$ consists of a vertex adjacent to $2l-n+1$ leaves and $n-l-1$ paths $P_2$.

(B) If $n > 2l$ and $n = 2k$, then the tree $T_{2k,l}$ is unique and consists of a vertex adjacent to one leave, $r$ paths $P_A$, and $l-r-1$ paths $P_{A+2}$, where $A = \mathrm{even}(\frac{n-2}{l-1})$ and $r = \frac{1}{2}(n-2-(l-1)A)$.

(C) If $n > 2l$ and $n = 2k+1$, then the tree $T_{2k+1,l}$ is unique and consists of a vertex adjacent to two leaves, $r$ paths $P_B$, and $q$ paths $P_{B+2}$, where $B = \mathrm{even}(\frac{n-3}{l-2})$ and $r = \frac{1}{2}(n-3-(l-2)B)$.

Рис. 2. The trees $T_{10,4}$ and $T_{15,5}$.

## § 2. Definitions and notation

As usual, we denote by $P_n$ a simple $n$-vertex path, and by $\deg(x)$ we denote the degree of a vertex $x$. Given a tree $T$ and its vertex $v$, by $\xi_+(T,v)$ we denote the number of MMIS in the tree $T$ containing the vertex $v$, and by $\xi_-(T,v)$ we denote the number of MMIS of the tree $T$ not containing the vertex $v$. A vertex of a tree is called *universal* if it is contained in each MMIS of the tree; a vertex is *empty* if it is not contained in any MMIS of the tree.

By $S_{k_1,\dots,k_l}$ we denote the result of merging of the endpoints of paths of lengths $k_1,\dots,k_l$. We shall assume that $k_1 \geqslant k_2 \geqslant \dots \geqslant k_l$.

Рис. 3. The tree $S_{4,3,2,1,1}$.

A path $(v_1, v_2, \dots, v_k)$ of a tree is called *extreme* if $v_1$ is a leaf of the tree, each of the vertices $v_2,\dots,v_k$ has degree 2 in the tree, and the vertex $v_k$ is adjacent to some vertex of degree $\geqslant 3$. A vertex of a tree is called *extreme* if its degree is $\geqslant 3$ and if all the subtrees adjacent to it are extreme paths (except, possibly, one subtree).

Figure 4 depicts a tree containing two extreme vertices, of which one is adjacent to three extreme paths of zero length and the second one is adjacent to three extreme paths of length one. Note that if a tree contains more than one extreme vertex, then each extreme vertex $u$ of this tree contains a unique neighbor $w$ not ling in the extreme path. Moreover, it is easily seen that if a tree contains at least three leaves, then it is either of the form $S_{k_1,\dots,k_l}$, or it contains at least two extreme vertices.

Рис. 4. An illustration of an extreme vertex and an extreme path.

## § 3. Structure of extreme trees

In this section, it will be shown that, for all admissible $n > l \geqslant 3$, the tree $T_{n,l}$ contains a unique extreme vertex, i.e., it has the form $S_{k_1,k_2,\dots,k_l}$. Before proving this fact, we shall prove some auxiliary results that give various constraints on the structure of the extreme trees $T_{n,l}$.

**Lemma 1.** *If an extreme vertex $u$ of the tree $T_{n,l}$ is universal, then it is not adjacent to an extreme path of even length.*

**Proof.** Assume that the tree $T_{n,l}$ contains an extreme vertex $u$ adjacent to an extreme path $P$ of length $2m$. We denote the vertices of this path by $x_1,\dots,x_{2m+1}$. Consider an arbitrary MMIS $J$ of the tree $T_{n,l}$. It is easily seen that $J$ contains the vertex $u$ and in addition precisely $m$ vertices of the path $P$. Consider the set $J'$ obtained from $J$ by replacing these $m+1$ vertices by the vertices $x_1, x_3, \dots, x_{2m+1}$. it is clear that $J'$ is also an MMIS of the tree $T_{n,l}$. But then the vertex $u$ is not universal, a contradiction.

**Lemma 2.** *If an extreme vertex $u$ of the tree $T_{n,l}$ is empty, then it is adjacent to at least one path of even length.*

**Proof.** Assume that an empty extreme vertex $u$ of degree $d$ is not adjacent to any extreme path of even length. Then it is adjacent to $d-1$ extreme paths of odd length and also to some nonleaf vertex $w$. Since the vertex $u$ is empty, there exists some MMIS $I$ not containing $u$ and not containing the endpoints of all extreme paths of odd length that are adjacent to $u$ in the tree $T_{n,l}$. Hence $I$ contains the vertex $w$, for otherwise $I$ could be augmented with the vertex $u$, which would give an IS of larger cardinality. Next, we replace in $I$ the vertex $w$ by the vertex $u$. The resulting set $I'$ is also an MMIS, but in this case the vertex $u$ is not empty. This contradiction proves the lemma.

**Lemma 3.** *If an extreme vertex $u$ of the tree $T_{n,l}$ is adjacent to at least two extreme paths of even length, then it is empty.*

**Proof.** Assume that an extreme vertex $u$ is not empty and is adjacent to two extreme paths $X$ and $Y$ of even length. We denote their vertices by $x_1, \dots, x_{2a+1}$ and $y_1, \dots, y_{2b+1}$, respectively. Since $u$ is not empty, it is contained in at least one MMIS $I$ of the tree $T_{n,l}$. Hence the set $I$ does not contain the vertices $x_1$ and $y_1$, and therefore, it contains at most $a+b$ vertices from the extreme paths $X$ and $Y$. Consider the set $I'$ containing the vertices $x_1, x_3, \dots, x_{2a+1}$ of the path $X$, the vertices $y_1, y_3, \dots, y_{2b+1}$ of the path $Y$, and all the remaining vertices from the set $I \setminus (V(X) \cup V(Y))$ (except the vertex $u$). It is clear that $I'$ is also an IS, but $I'$ has one more vertex than $I$. Hence $I$ is not an MMIS, a contradiction.

**Lemma 4.** *The tree $T_{n,l}$ does not contain universal extreme vertices.*

**Proof.** Assume that the tree $T_{n,l}$ contains a universal extreme vertex $v$ of degree $d \geqslant 3$. Then by Lemma 1 this vertex is adjacent to $d-1$ extreme paths of odd length. Consider two such paths and denote their vertices by $x_1, \dots, x_{2a}$ and $y_1, \dots, y_{2b}$, respectively. In the tree $T$, the vertices $v, x_2, x_4, \dots, x_{2a}, y_2, y_4, \dots, y_{2b}$ are universal, and the vertices $x_1, y_1, x_3, y_3, \dots, x_{2a-1}, y_{2b-1}$ are empty. We remove from $T_{n,l}$ the edge $y_1 v$ and add the edge $y_1 x_1$. It is clear that this transformation does not change the number of leaves and vertices of the tree. We denote the resulting tree by $T'$. Let us show that $\xi(T') > \xi(T_{n,l})$.

It is clear that each MMIS of the tree $T_{n,l}$ is an IS of the tree $T'$. Hence $\alpha(T_{n,l}) \leqslant \alpha(T')$. On the other hand, each MMIS $I$ of the tree $T'$ contains precisely $a+b$ vertices of the set $S = \{x_1, \dots, x_{2a}, y_1, \dots, y_{2b}\}$. Hence $\alpha(T_{n,l}) = \alpha(T')$.

So, each MMIS of the tree $T$ is an MMIS of the tree $T'$. Adding the vertices $x_2, x_4, \dots,$ $x_{2a}, y_1, y_3, \dots, y_{2b-1}$ to some MMIS of the tree $T_{n,l} \setminus S$, we get some MMIS of the tree $T'$ which is not an MMIS of the tree $T_{n,l}$. Therefore, $\xi(T') > \xi(T_{n,l})$. But this contradicts the assumption.

**Lemma 5.** *If a vertex $v$ of an arbitrary $T$ is not universal, then $\xi_-(T, v) = \xi(T \setminus \{v\})$.*

**Proof.** Let a vertex $v$ be adjacent to vertices $v_1, \dots, v_d$ of connected components $T_1, \dots, T_d$ of the forest $T \setminus \{v\}$. The vertex $v$ is not universal, and hence there exists at least one MMIS of the tree $T$ that contains $v$. Hence $\alpha(T) = \sum_{i=1}^{d} \alpha(T_i)$. Moreover, $\alpha(T \setminus \{v\}) = \sum_{i=1}^{d} \alpha(T_i)$. So, any MMIS of the forest $T \setminus \{v\}$ is also an MMIS in the tree $T$. On the other hand, any MMIS of the tree $T$ not containing the vertex $v$ is an MMIS of the forest $T \setminus \{v\}$. This proves the lemma.

**Lemma 6.** *The strict inequality $\xi(T_{n+2,l}) > \xi(T_{n,l})$ holds.*

**Proof.** We claim that, for each extreme tree $T_{n,l}$, there exists an $(n+2)$-vertex tree $T_{n+2}$ for which the strict inequality $\xi(T_{n+2}) > \xi(T_{n,l})$ holds.

By Lemma 4, the tree $T_{n,l}$ does not contain universal extreme vertices. The following cases are possible: either the tree $T_{n,l}$ contains at least one nonempty extreme vertex, or all the extreme vertices $T_{n,l}$ are empty. In the second case, either there exists at least one empty extreme vertex adjacent to an extreme path of odd length, or there exist two different extreme vertices not adjacent to an extreme path of odd length, or $T_{n,l}$ contains a unique extreme vertex, which is empty and is not adjacent to paths of odd length.

**Case 1.** The tree $T_{n,l}$ contains a nonempty extreme vertex $v$. Then by Lemma 3 this vertex is adjacent to at least one extreme path $X$ of length $2x-1$. We denote by $T_0$ the subtree of the tree $T_{n,l}$ that does not contain the path $X$. We claim that $\xi(T_{n,l}) = \xi_+(T_0, v) + (x+1)\xi_-(T_0, v)$.

Let us first show that $\xi_+(T_0, v) = \xi_+(T_{n,l}, v)$. We denote by $X_0$ the set of $x$ vertices on the path $X$ that lie at distances $2, 4, 6, \dots, 2x$ from the vertex $v$. It is easily seen that each MMIS $J$ of the tree $T$ containing the vertex $v$ can be represented as the union $J_0 \cup X_0$, where $J_0$ is the MMIS of the tree $T_0$ containing the vertex $v$. Conversely, if $J_0$ is some MMIS of the tree $T_0$ containing the vertex $v$, then $J_0 \cup X_0$ is an MMIS of the tree $T_{n,l}$ containing the vertex $v$. Now the required equality follows.

Now let us show that $(x+1)\xi_-(T_0, v) = \xi_-(T_{n,l}, v)$. It is easily seen that the vertex $v$ is not universal in the tree $T_0$. Indeed, if this were so, then the vertex $v$ would be universal in the tree $T_{n,l}$, which is impossible by Lemma 4.

By Lemma 5, we have $\xi_-(T_0, v) = \xi(T_0 \setminus \{v\})$ and

$$\xi_-(T_{n,l}, v) = \xi(T_{n,l} \setminus \{v\}) = \xi(X)\xi(T_0 \setminus \{v\}) = (x+1)\xi(T_0 \setminus \{v\}).$$

Augmenting the endpoint of the path $X$ by two vertices, we get the tree $T_{n+2}$, for which $\xi(T_{n+2}) = \xi_+(T_0, v) + (x+2)\xi_-(T_0, v)$. Hence $\xi(T_{n+2}) > \xi(T_{n,l})$, the result required.

**Case 2a.** The tree $T_{n,l}$ contains at least one empty extreme vertex $v$, which is adjacent to an extreme path of odd length. We denote this path by $X$. Let $2x-1$ be the length of this path. We denote by $T_0$ the subtree obtained by removing this path from $T_{n,l}$. Then by Lemma 5 we have the equality $\xi(T_{n,l}) = \xi_-(T, v) = (x+1)\xi(T_0)$. We augment the endpoint of the path $X$ with two vertices. Then, for the tree $T_{n+2}$ thus obtained, the vertex $v$ is clearly empty. Hence by Lemma 5 we have $\xi(T_{n+2}) = (x+2)\xi(T_0)$, the result required.

**Case 2b.** The tree $T_{n,l}$ contains at least two empty extreme vertices $u$ and $v$ which are not adjacent to an extreme path of odd length. Then each of these vertices is adjacent to at least two extreme paths of even length. We denote by $T_u$ (respectively, $T_v$) the subtree of the tree $T_{n,l}$ consisting of the vertex $u$ (respectively, $v$) and all extreme paths adjacent to this vertex. We denote by $T_0$ the subtree of the tree $T_{n,l}$ containing all the vertices not lying in the subtrees $T_u$ and $T_v$.

Since all the vertices of the subtrees $T_u$ and $T_v$ are either empty or universal in the tree $T_{n,l}$, we have $\xi(T_{n,l}) = \xi(T_0)$. In the subtree $T_u$, we choose one of the extreme paths of even length and increase it by one vertex. Let $T'_u$ be the subtree just obtained. The subtree $T'_v$ is defined in the same way. We denote by $T_{n+1}$ the tree obtained from the tree $T_{n,l}$ by replacing the subtree $T_u$ by $T'_u$. This tree contains just one more vertex than the original tree. We claim that $\xi(T_{n+1}) > \xi(T_{n,l})$. Since in the tree $T'_u$ the vertex $u$ is still adjacent to at least one extreme path of odd length, it is not universal. By Lemma 5,

$$\xi(T_{n+1}) \geqslant \xi_-(T_{n+1}, u) = \xi(T_{n+1} \setminus \{u\}) \geqslant 2\xi(T_0).$$

This last inequality is satisfied, because the vertex $u$ in the tree $T_{n+1}$ is adjacent to at least one extreme path of odd length.

Replacing in the tree $T_{n+1}$ the subtree $T_v$ by the subtree $T'_v$, one can easily show that $\xi(T_{n+2}) \geqslant 2\xi(T_{n+1})$ for the resulting tree $T_{n+2}$. Hence $\xi(T_{n+2}) > \xi(T_{n,l})$, the result required.

**Case 2c.** The tree $T_{n,l}$ contains a unique extreme vertex $v$, which is empty and is adjacent only to extreme paths of odd length. In this case $T_{n,l}$ has the form $S_{k_1,\dots,k_l}$. It is easily seen that in this case all vertices of the tree are either empty or universal, and thence the MMIS of the tree is unique.

We increase by 1 the lengths of two arbitrary extreme paths adjacent to vertex $v$. It is clear that the resulting tree $T_{n+2}$ contains the same number of leaves as the original tree $T_{n,l}$. Moreover, in the tree $T_{n+2}$ the extreme vertex $v$ is adjacent to an extreme path of even length, and hence by Lemma 1 the vertex $v$ cannot be universal in $T_{n+2}$. If the vertex $v$ is empty in $T_{n+2}$, then $\xi(T_{n+2}) = \xi(T_{n+2} \setminus \{v\})$. Since two components of the forest $T_{n+2} \setminus \{v\}$ are paths of odd length, we have $\xi(T_{n+2}) > 1$. If $v$ is not an empty vertex in $T_{n+2}$, then the tree $T_{n+2}$ contains at least two different MMIS, i.e., the number of MMIS is greater than in the original tree $T_{n,l}$.

**Corollary 1.** *Each empty extreme vertex of the tree $T_{n,l}$ is adjacent to at least one leave and is not adjacent to an extreme path of nonzero even length.*

**Proof.** Assume that in the tree $T_{n,l}$ there exists a empty extreme vertex adjacent to an extreme path of even length at least 2. Then the vertices of this path are either empty or universal. We reduce the length of the path by 2. Then the resulting tree $T'$ contains $n-2$ vertices, $l$ leaves, and the same number of MMIS as the original tree. By Lemma 6, there exists an $n$-vertex tree $T''$ containing $l$ leaves and for which the number of MMIS is greater than in the original one, but this contradicts the extremality of the tree $T_{n,l}$.

By Lemma 2, each empty extreme vertex of the tree $T_{n,l}$ is adjacent to at least one extreme path of even length, which by the above is a leaf.

**Lemma 7.** *The tree $T_{n,l}$ contains at most one empty extreme vertex.*

**Proof.** Assume that the tree $T_{n,l}$ contains at least two empty extreme vertices $u$ and $v$. By the first assertion of Corollary 1 to Lemma 6, none of these vertices is adjacent to an extreme even path of nonzero length. We denote by $T_u$ the subtree consisting of the vertex $u$ and all extreme paths adjacent to this vertex. Next, let $u'$ be the vertex adjacent to $u$ and not lying in $T_u$. From the definition of an extreme vertex it follows that $u'$ exists and is unique. In a similar manner, we define the subtree $T_v$ and the vertex $v'$. We denote by $2p_1-1,\ldots,2p_k-1$ the lengths of extreme paths of odd length adjacent to the vertex $u$, and denote by $2q_1-1,\ldots,2q_s-1$ the lengths of extreme paths of odd length adjacent to the vertex $v$. We set $P=\prod_{i=1}^{k}(p_i+1)$ and $Q=\prod_{i=1}^{s}(q_i+1)$. In the case $k=0$ (respectively, $l=0$), we set $P=1$ (respectively, $Q=1$). Moreover, we denote by $T_0$ the subtree of the tree $T_{n,l}$ containing all the vertices not involved in $T_u$ and in $T_v$. From Corollary 1 it easily follows that $\xi(T_{n,l})=PQ\xi(T_0)$. Only the following cases are possible: 1) the vertices $u$ and $v$ are adjacent, 2) the vertices $u$ and $v$ are not adjacent and $\max(\deg(v'),\deg(u'))>2$, 3) the vertices $u$ and $v$ are not adjacent and $\deg(v')=\deg(u')=2$.

**Case 1).** The vertices $u$ and $v$ are adjacent in the tree $T_{n,l}$. In this case, the vertex $u$ coincides with $v'$ and the vertex $v$ is equal to $u'$. Hence the tree $T_0$ is empty and $\xi(T_{n,l})=P\cdot Q$. We remove from $v$ and connect to $u$ all the extreme paths adjacent to $v$, except one leaf $w$. The tree $T'$ just obtained contains the same number of vertices and leaves as the tree $T_{n,l}$. It is easily seen that in this tree $T'$ the vertex $u$ is still empty. Hence $\xi(T')=2PQ$, inasmuch as $u$ is adjacent to the extreme path $vw$ of length 1. Consequently, $\xi(T')>\xi(T_{n,l})$, a contradiction to the assumption.

**Case 2).** The vertices $u$ and $v$ are not adjacent in $T_{n,l}$ and at least one of the vertices $u'$ and $v'$ has degree $>2$ in the tree $T_{n,l}$. We shall assume that $\deg(v')\geqslant 3$. We denote by $w$ one of the leaves adjacent to the vertex $v$. We remove from the tree the vertices $v$ and $w$, attach to the vertex $u$ all the extreme paths which were adjacent to the vertex $v$, and attach to the vertex $u$ an extreme path of length 1. Applying Lemma 5 to the vertex $u$ of the resulting tree $T'$, one cam easily check that after the transformation the number of MMIS is increased by a factor of two.

**Case 3).** The vertices $u$ and $v$ are not adjacent in $T_{n,l}$, moreover, $\deg(u')=\deg(v')=2$. We denote by $w$ one of the leaves adjacent to $v$ in the tree $T_{n,l}$. We remove from the tree $T_{n,l}$ the vertices $v$ and $w$, after which we connect the vertex $u$ with all extreme paths that were connected to the vertex $v$ in the original tree. The resulting tree contains $n-2$ vertices, $l$ leaves, and the same number of MMIS as $T_{n,l}$. Hence by Lemma 6 there exists some tree $T'$ containing $n$ vertices, $l$ leaves, and in which the number of MMIS is strictly greater than in the original tree $T_{n,l}$, which contradicts the extremality of $T_{n,l}$.

**Theorem 1.** *The tree $T_{n,l}$ contains a unique extreme vertex.*

**Proof.** Assume that in the tree $T_{n,l}$ there exist two different extreme vertices $u$ and $v$. We shall show that in this case there always exists a transformation which strictly increases the number of MMIS in the tree, but the number of vertices and leaves remains the same. This will contradict the extremality of $T_{n,l}$.

We shall assume that vertex $u$ is adjacent to $r$ paths of odd length $2p_1-1,\ldots,2p_r-1$, and define $P=\prod_{i=1}^{r}(p_i+1)$. Similarly, the vertex $v$ is adjacent to $s$ extreme paths of odd length $2q_1-1,\ldots,2q_s-1$. We set $Q=\prod_{i=1}^{s}(q_i+1)$. Moreover, we define

$\tilde{P} = \prod_{i=1}^{r-1}(p_i + 1)$ and put $\tilde{Q} = \prod_{i=1}^{s-1}(q_i + 1)$. Hence $P = (p_r + 1)\tilde{P}$ and $Q = (q_s + 1)\tilde{Q}$. It is clear that if the vertex $u$ (respectively, $v$) is adjacent to at least two extreme paths of odd length, then $\tilde{P} > 1$ (respectively, $\tilde{Q} > 1$). In the case $r \geqslant 2$, by the *terminal path* we shall mean the $r$th extreme path of odd length adjacent to the vertex $u$ (and having the length $2p_r - 1$). The terminal path for the vertex $v$ is defined similarly.

Note that if the extreme vertex is not empty, then by Lemma 3 it is adjacent to at most one extreme path of even length.

We remove from the tree all the vertices of the extreme paths that are adjacent to the vertices $u$ and $v$. We denote by $\sigma_{00}$ the number of MMIS of the resulting tree which do not contain the vertices $u$ and $v$. Next, we denote by $\sigma_{10}$ the number of MMIS containing the vertex $u$ and not containing the vertex $v$. Further, $\sigma_{01}$ will denote the number of MMIS not containing the vertex $u$ and containing the vertex $v$. We also denote by $\sigma_{11}$ the number of MMIS containing both vertices $u$ and $v$. Only two cases are possible: either none of the vertices $u$ and $v$ is empty or at least one of the vertices $u$ and $v$ is empty. Let us consider separately each of these cases.

**Case 1.** The vertices $u$ and $v$ are both nonempty. Hence by Lemma 3 each of these vertices is adjacent to at most one extreme path of even length. Next, we will consider three possible variants: both vertices $u$ and $v$ are adjacent to extreme paths of even length, precisely one of them is adjacent to an extreme path of even length, and none of the vertices $u$ and $v$ is adjacent to an extreme path of even length.

**Case 1a.** The vertex $u$ is adjacent to an extreme path $X$ of length $2x - 2 \geqslant 0$, and the vertex $v$ is adjacent to an extreme path $Y$ of length $2y - 2 \geqslant 0$. Then

$$\xi(T_{n,l}) = PQ\sigma_{00} + yP\sigma_{01} + xQ\sigma_{10} + xy\sigma_{11}.$$

For reasons of symmetry, we may assume that $P\sigma_{01} \geqslant Q\sigma_{10}$. If $y < x$, then the paths $X$ and $Y$ can be swapped, thereby increasing the number of MMIS in the tree and not changing the number of its vertices and leaves. Indeed, for the tree $T'$ obtained in this way, we have

$$\xi(T') = PQ\sigma_{00} + xP\sigma_{01} + yQ\sigma_{10} + xy\sigma_{11} > \xi(T).$$

So, we assume that $y \geqslant x$. We disconnect all the extreme paths of odd length from the vertex $v$ and connect them to the vertex $u$. It is clear that after this transformation the number of vertices and the number leaves will remain the same. For the tree $T_1$ thus obtained, we have

$$\xi(T_1) = PQ\sigma_{00} + yPQ\sigma_{01} + x\sigma_{10} + xy\sigma_{11}.$$

From the inequalities $P\sigma_{01} \geqslant Q\sigma_{10} > \sigma_{10}$, $y \geqslant x$, $\min(P, Q) > 1$ we have the strict inequality $yP\sigma_{01} + xQ\sigma_{10} < yPQ\sigma_{01} + x\sigma_{10}$. Hence, the transformation increases the number of MMIS, which contradicts the extremality of the tree $T_{n,l}$.

**Case 1b.** The vertex $u$ is adjacent to an extreme path $X$ of even length $2x - 2 \geqslant 0$, and the vertex $v$ is not adjacent to extreme paths of even length. Hence

$$\xi(T_{n,l}) = PQ\sigma_{00} + P\sigma_{01} + xQ\sigma_{10} + x\sigma_{11}.$$

Assume that $\sigma_{01} > \sigma_{10}$. If, in addition, $P < xQ$, then we swap all the extreme paths adjacent to the vertex $u$ and all the extreme paths adjacent to the vertex $v$. It is easily checked that after this transformation the number of MMIS will increase, because after the transformation the number of MMIS will be equal to

$$PQ\sigma_{00} + xQ\sigma_{01} + P\sigma_{10} + x\sigma_{11}.$$

If now $P \geqslant xQ$, then we connect the vertex $u$ with all the extreme paths of odd length, except the last one, which were connected to the vertex $v$. For the resulting tree $T_2$, we have

$$\xi(T_2) = PQ\sigma_{00} + P\tilde{Q}\sigma_{01} + x(q_s + 1)\sigma_{10} + x\sigma_{11}.$$

Since

$$\sigma_{01} > \sigma_{10},\ P \geqslant xQ > x,\ Q = (q_s + 1)\tilde{Q},\ \tilde{Q} > 1,$$

we have $\xi(T_2) > \xi(T_{n,l})$.

Let us now assume that $\sigma_{01} \leqslant \sigma_{10}$. If, in addition, $P > xQ$, then we swap all the extreme paths adjacent to the vertex $u$ and all the extreme paths adjacent to the vertex $v$. It is easily checked that after this transformation the number of MMIS will not decrease, since after the transformation the number of MMIS is equal to

$$PQ\sigma_{00} + xQ\sigma_{01} + P\sigma_{10} + x\sigma_{11}.$$

If $P \leqslant xQ$, then we augment the vertex $x$ with all the extreme paths of odd length that were adjacent to the vertex $u$. Hence, for the tree $T_3$ thus obtained, we have

$$\xi(T_3) = PQ\sigma_{00} + \sigma_{01} + xPQ\sigma_{10} + x\sigma_{11}.$$

Next, $\min(P, Q) > 1$, $x \geqslant 1$, $\sigma_{01} \leqslant \sigma_{10}$, and so $\xi(T_3) > \xi(T_{n,l})$.

It is easily seen that in the case when the vertex $v$ is adjacent to an extreme path of even length and the vertex $u$ is not adjacent to extreme paths of even length, the arguments are similar.

**Case 1c.** The vertices $u$ and $v$ are not adjacent to an extreme path of even length. Then, clearly, $\min(\tilde{P}, \tilde{Q}) > 1$. For reasons of symmetry, we can assume that $\sigma_{01} \geqslant \sigma_{10}$. We may also assume that $p_r \geqslant q_s$, for otherwise we may swap the corresponding paths — it is easily seen that the number of MMIS will not be reduced. Hence

$$\xi(T_{n,l}) = PQ\sigma_{00} + (p_r + 1)\tilde{P}\sigma_{01} + (q_s + 1)\tilde{Q}\sigma_{10} + \sigma_{11}.$$

We disconnect all the extreme paths of odd length, except the last one, from the vertex $v$ and attach them to the vertex $u$. Hence, for the tree $T_4$ thus obtained. we have

$$\xi(T_4) = PQ\sigma_{00} + (p_r + 1)\tilde{P}\tilde{Q}\sigma_{01} + (q_s + 1)\sigma_{10} + \sigma_{11}.$$

From the inequalities

$$\sigma_{01} \geqslant \sigma_{10}, \quad p_r \geqslant q_s, \min(\tilde{P},\ \tilde{Q}) > 1$$

we have the strict inequality

$$(p_r + 1)\tilde{P}\sigma_{01} + (q_s + 1)\tilde{Q}\sigma_{10} < (p_r + 1)\tilde{P}\tilde{Q}\sigma_{01} + (q_s + 1)\sigma_{10}.$$

Hence $\xi(T_4) > \xi(T_{n,l})$.

**Case 2.** The vertex $u$ is empty, and the vertex $v$ is not empty. By Lemma 3, the vertex $v$ is adjacent to at most one extreme path of even length, and by the first assertion of Corollary 1 to Lemma 6, the vertex $u$ is not adjacent to extreme even paths of nonzero length. We denote by $T''$ the subtree of the tree $T_{n,l}$ not containing the vertex $u$ and all the extreme paths adjacent to $v$ and which also does not contain all the extreme paths adjacent to the vertex $v$. We set $\eta_0 = \xi_-(T'', v)$ and $\eta_1 = \xi_+(T'', v)$. There are two subcases to consider: the vertex $v$ is adjacent to an extreme path of even length and the vertex $v$ is not adjacent to an extreme path of even length.

**Case 2a.** The vertex $v$ is adjacent to an extreme path $X$ of length $2x - 2$. We have

$$\xi(T_{n,l}) = PQ\eta_0 + Px\eta_1.$$

We disconnect all the extreme paths of odd length from the vertex $v$ and connect them to the vertex $u$. For the resulting tree $T_5$, we have

$$\xi(T_5) = PQ\eta_0 + PQx\eta_1.$$

It is clear that $\xi(T_5) > \xi(T_{n,l})$.

**Case 2b.** The vertex $v$ is not adjacent to an extreme path of even length. Then

$$\xi(T_{n,l}) = PQ\eta_0 + P\eta_1.$$

We disconnect all the extreme paths, except the last one, from the vertex $v$ and connect them to the vertex $u$. Hence, for the tree $T_6$ thus obtained, we have

$$\xi(T_6) = PQ\eta_0 + P\tilde{Q}\eta_1.$$

The vertex $v$ is adjacent to at least two extreme even paths, and hence we have $\tilde{Q} > 1$. Therefore, we have the strict inequality $\xi(T_6) > \xi(T_{n,l})$.

## § 4. A complete description of extreme trees

By Theorem 1, any tree $T_{n,l}$ has the form $S_{k_1,\dots,k_l}$, where $k_i \geqslant 1$ for any $i$ and $\sum_{i=1}^{l} k_i = n-1$. In this section, we will find $k_i$ for all $n > l \geqslant 3$.

**Lemma 8.** *No extreme vertex of the tree $T_{n,l}$ can be adjacent to an extreme path of nonzero even length.*

**Proof.** We denote by $v$ an extreme vertex of the tree $T_{n,l}$ of the form $S_{k_1,\dots,k_l}$. Let us prove that $v$ cannot be adjacent to an extreme path of even length at least 2. Assume the contrary. By Lemma 4, the vertex $v$ cannot be universal. By the first assertion of Corollary 1 to Lemma 6, if $v$ is empty, then the condition of the lemma is satisfied and there is nothing to prove.

Assume that the extreme vertex $v$ is not empty and is adjacent to some extreme path $X$ of length $2x \geqslant 2$. By Lemma 3, the vertex $v$ is not adjacent to other extreme paths of even length. Hence it is adjacent to at least $l-1 \geqslant 2$ extreme odd paths. We denote by $Y$ some extreme odd path of length $2y-1$ which is adjacent to $v$, and the lengths of the remaining extreme odd paths we denote by $2q_1-1, 2q_2-1, \dots, 2q_{l-2}-1$. We set $Q = \prod_{i=1}^{l-2}(q_i+1)$. From the condition $l \geqslant 3$, we have the inequality $Q \geqslant 2$.

We have $\xi_+(T,v) = x+1$ and $\xi_-(T,v) = (y+1)Q$. We reduce the length of the path $X$ by 2 vertices and increase the length of the path $Y$ by 2 vertices. It is clear that the resulting tree $T'$ contains the same number of vertices and leaves as the original tree $T_{n,l}$. Since $\xi_+(T',v) = x$ and $\xi_-(T',v) = (y+2)Q$ and since $Q \geqslant 2$, it follows that $\xi(T') > \xi(T_{n,l})$, a contradiction.

**Lemma 9.** *An extreme vertex $v$ of the tree $T_{n,l}$ of the form $S_{k_1,\dots,k_l}$ cannot be adjacent to extreme paths of odd length, whose length differ more than by two.*

**Proof.** Assume that vertex $v$ is adjacent to an extreme path $X$ of length $2x-1$ and an extreme path $Y$ of length $2y-1$, and assume that $x > y+1$. We denote by $2p_1-1, \dots, 2p_s-1$ the lengths of the other extreme paths of odd length adjacent to $v$, and define $P = \prod_{i=1}^{s}(p_i+1)$. If $s=0$, then we put $P=1$. We claim that if the length of $X$ is reduced by 2 and the length of $Y$ is increased by 2, then the number of MMIS in the resulting tree $T'$ will be strictly greater than in the original tree $T_{n,l}$.

If the vertex $v$ is empty, then

$$\xi(T_{n,l}) = (x+1)(y+1)P \text{ and } \xi(T') = x(y+2)P.$$

We have $x > y+1$, and hence $xy + x + y + 1 < xy + 2x$. Therefore, $\xi(T') > \xi(T_{n,l})$.

If the vertex $v$ is not empty, then by Lemma 3 it is adjacent to at most one extreme path of even length, which by Lemma 8 is a leaf. Hence

$$\xi(T_{n,l}) = (x+1)(y+1)P + 1 \quad \text{and} \quad \xi(T') = x(y+2)P + 1,$$

which also implies that $\xi(T_{n,l}) < \xi(T')$.

Thus, for any tree $T_{n,l}$, there exists a natural number $m$ depending on $n$ and $l$ such that $T_{n,l}$ has the form $S_{k_1,\dots,k_l}$, where $k_i \in \{1, 2m, 2m+2\}$ and $1 \leqslant i \leqslant l$. We recall that $\mathrm{even}(x)$ is the largest even number not exceeding a given real number $x$.

**Theorem 2.** (*A*) *If $n \leqslant 2l$, then the tree $T_{n,l}$ is unique and consists of an extreme vertex $v$ adjacent to $2l-n+1$ leaves and $n-l-1$ paths $P_2$.*

(*B*) *If $n > 2l$ and $n = 2k$, then the tree $T_{2k,l}$ is unique and consists of an extreme vertex $v$ adjacent to one leave, $r$ paths $P_A$ and $l-r-1$ paths $P_{A+2}$, where $A = \mathrm{even}(\frac{n-2}{l-1})$ and $r = \frac{1}{2}(n-2-(l-1)A)$.*

(*C*) *If $n > 2l$ and $n = 2k+1$, then the tree $T_{2k+1,l}$ is unique and consists of an extreme vertex $v$ adjacent to two leaves, $r$ paths $P_B$ and $q$ paths $P_{B+2}$, where $B = \mathrm{even}(\frac{n-3}{l-2})$ and $r = \frac{1}{2}(n-3-(l-2)B)$.*

**Proof.** Let us prove the first assertion of the theorem. We claim that tree $T_{n,l}$, for which $n \leqslant 2l$, cannot contain extreme paths of odd length $\geqslant 3$. Indeed, assume that there exists at least one path $X$ of length $2x-1 \geqslant 3$. Then from the inequality $n \leqslant 2l$ it follows that the extreme vertex $v$ is adjacent to at least three leaves. We denote by $2p_1-1, \dots, 2p_s-1$ the lengths of all other (i.e., different from $X$) extreme odd paths of the tree, and put $P = \prod_{i=1}^{s}(p_i+1)$. Then $\xi(T_{n,l}) = (x+1)P$.

We reduce the length of the path $X$ by two vertices, and then replace some two leaves of the tree by two paths of length one. If in the resulting tree $T'$ the extreme vertex is empty, then $\xi(T') = 4xP$, since otherwise $\xi(T') = 4xP+1$. In both cases, the number of MMIS in tree is increased after the transformation, while the number of vertices and leaves will not change. So, the tree $T_{n,l}$ does not contain extreme odd paths of length $> 1$ and extreme even paths of nonzero length. It is clear that $n = l+1+a$ for some $0 \leqslant a < l$. Hence $T_{n,l}$ contains $a$ paths of length 1 and $l-a$ leaves, which implies the first assertion of the theorem.

Let us prove the second assertion of the theorem. We claim that the extreme vertex $v$ of the tree is adjacent precisely to one leave. If $v$ is not adjacent to leaves, then by Lemma 8 all the adjacent extreme paths have odd length. But then $v$ is universal, which is impossible by Lemma 4. Since the number of vertices of the tree is even, the tree contains an odd number of extreme paths from an odd number of vertices, and moreover, by Lemma 8 all such paths are leaves. Assume that the number of such leaves is at least three. Now the inequality $n > 2l$ implies that the tree has at least one extreme path of length $\geqslant 3$. But then one can apply the transformation described in the proof of Lemma 9; this transformation strictly increases the number of MMIS of the tree. But this is a contradiction, and hence, the vertex $v$ is adjacent precisely to one leave. By Lemma 8, there exists a number $m$ such that all extreme paths of odd length adjacent to the vertex $v$ are isomorphic either to the path $P_{2m}$ or to the path $P_{2m+2}$. Hence $2m(l-1) \leqslant n-2$ and $(2m+2)(l-1) > n-2$, which implies the second assertion of the theorem.

The last assertion of the theorem is proved similarly.

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