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On the Number of Minimum Dominating Sets in Trees

D. S. Taletskii[1*]

[1] *National Research University Higher School of Economics in Nizhny Novgorod, Nizhny Novgorod, 603155 Russia*

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Abstract—The class of trees in which the degree of each vertex does not exceed an integer d is considered. It is shown that, for $d = 4$, each n-vertex tree in this class contains at most $(\sqrt{2})^n$ minimum dominating sets (MDS), and the structure of trees containing precisely $(\sqrt{2})^n$ MDS is described. On the other hand, for $d = 5$, an n-vertex tree containing more than $(1/3) \cdot 1.415^n$ MDS is constructed for each $n \geq 1$. It is shown that each n-vertex tree contains fewer than 1.4205^n MDS.

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1. INTRODUCTION

A *dominating set* in a graph is a subset D of its vertices such that any vertex not belonging to D is adjacent to at least one vertex in D. A dominating set is said to be *minimum* if it is of minimum cardinality. The *domination number* $\gamma(G)$ of a graph G is defined to be the cardinality of its minimum dominating set. We use the abbreviations "DS" and "MDS" for "dominating set" and "minimum dominating set," respectively.

It is known that any graph contains an odd number of DS [1]. In 2006, Bród and Skupień [2] described trees containing the maximum and the minimum number of DS in the class of all n-vertex trees. The star S_n is the unique n-vertex tree containing the maximum possible number of DS. However, there exist exponentially many n-vertex trees containing the minimum possible number of DS. Later, Wagner [3] generalized this result to some other classes of graphs. In the 2022 paper [4], for all $k \geq 2$, the structure of trees containing the maximum and the minimum number of k-DS (that is, subsets D_k of tree vertices such that each vertex not belonging to D_k is adjacent to at least k vertices in D_k) was described.

To date, relatively few estimates of the number of MDS in trees and forests are known. In [5], three equivalent conditions under which a tree contains a unique MDS were given. The question of whether a tree with domination number γ can contain more than 2^γ MDS remained open until 2017, when Bień gave an example of such a tree in [6]. On the other hand, in [7], Alvarado et al. proved that a forest with domination number γ contains at most 2.4606^γ MDS.

In this paper, we obtain new bounds for the maximum possible number of MDS in an n-vertex tree. We show that if the maximum degree d of a vertex in a tree is at most 4, then the tree contains at most $(\sqrt{2})^n$ MDS. Interestingly, this is false already for $d = 5$. For any $n \geq 1$, we give an example of a tree T_n containing more than $(1/3) \cdot 1.415^n$ MDS. Moreover, we prove that each n-vertex tree contains fewer than 1.4205^n MDS.

[*]E-mail: dmitalmail@gmail.com

2. DEFINITIONS AND NOTATION

As usual, we denote the vertex and edge sets of a simple undirected graph G by $V(G)$ and $E(G)$, respectively. Given a vertex $v \in V(G)$, by $\deg_G(v)$ we denote its degree and by $N_G[v]$, its *closed neighborhood*, i.e., the set consisting of this vertex and all vertices adjacent to it. In the case where the choice of a graph G is clear from the context, we denote the degree and the closed neighborhood of a vertex v by $\deg(v)$ and $N[v]$, respectively. We use $\Delta(G)$ to denote the maximum degree of a vertex in a graph G.

A *tree* is a connected graph without cycles. A vertex of degree 1 in a tree is called a *leaf*. We refer to a vertex as a *support vertex* or a *support* if it is adjacent to at least one leaf. *Attaching a support of degree* 2 to a vertex v in a tree is inserting vertices u_1 and u_2 and the edges u_1u_2 and u_2v in this tree. We say that a tree is *splittable* if it is possible to delete an edge from this tree so that the number of MDS in the resulting forest remains the same; otherwise, the tree is said to be *unsplittable*. The *diameter* $\operatorname{diam}(T)$ of a tree T equals the longest possible distance between its vertices. A simple path $X = x_1x_2x_3\dots$ in a tree T is said to be *diametrical* if it consists of $\operatorname{diam}(T)+1$ pairwise distinct vertices. Obviously, the end vertices of each diametrical path in a tree are leaves.

Let $\partial_M(G)$ denote the number of MDS in a graph G. By $\partial_M^+(G,v)$ (by $\partial_M^-(G,v)$) we denote the number of those MDS in G which contain (respectively, do not contain) the vertex v. We say that a vertex v in a graph G is *universal* if $\partial_M^+(G,v) = \partial_M(G)$ and *idle* if $\partial_M^-(G,v) = \partial_M(G)$.

Let D be an MDS in a tree T. By $\phi(D)$ we denote the set obtained by replacing all leaves of T in D by supports adjacent to them. It is easy to see that the set $\phi(D)$ is determined uniquely and is an MDS as well.

We use $W_{a,b}$ to denote the tree obtained from a path (v_1, v_2, v_3) by attaching $a \ge 0$ supports of degree 2 to the vertex v_1 and $b \ge 0$ supports of degree 2 to the vertex v_3. It is easy to check that

$$\partial_M(W_{a,b}) = \partial_M^+(W_{a,b}, v_1) + \partial_M^+(W_{a,b}, v_2) + \partial_M^+(W_{a,b}, v_3) = 2^a(2^b-1) + 2^{a+b} + 2^b(2^a-1).$$

Suppose that a tree T contains a subtree $W_{a,b}$, where $a \ge 1$ and $b \ge 0$. We say that this subtree is *extreme* if its vertex adjacent to b supports of degree 2 is the only vertex adjacent to other vertices of T (an example is shown in Fig. 1). We refer to this vertex as the *contact* vertex of the extreme subtree.

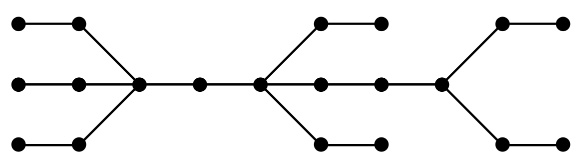

Fig. 1. An example of a tree with two extreme subtrees $W_{3,2}$ and $W_{2,0}$.

We say that a set D *dominates* a vertex v in a tree T if

$$N[v] \cap D \neq \varnothing.$$

By $\widehat{\partial}_M(W_{a,b})$ we denote the number of sets of cardinality $\gamma(W_{a,b})$ in a subtree $W_{a,b}$ which dominate all vertices of this subtree, except, possibly, a contact vertex. It is easy to see that

$$\widehat{\partial}_M(W_{a,b}) = \partial_M(W_{a,b}) + 2^a.$$

Obviously,

$$\frac{\partial_M(W_{3,b})}{\widehat{\partial}_M(W_{3,b})} \ge \frac{\partial_M(W_{3,0})}{\widehat{\partial}_M(W_{3,0})} = \frac{15}{23}.$$

We say that an n-vertex tree is *maximal* if it contains the maximum possible number of MDS among all n-vertex trees. Similarly, we say that an n-vertex tree is *k-maximal* (where $k \ge 2$) if it contains the maximum possible number of MDS among all trees in which the degrees of all vertices are at most k. Note that if a tree T is not $\Delta(T)$-maximal then it is not maximal, but the converse is generally false.

3. PRELIMINARY RESULTS

3.1. Universal, Idle, and Support Vertices

Lemma 1. *If a tree T contains a vertex v adjacent to at least two leaves u_1 and u_2, then the vertex v is universal and the leaves u_1 and u_2 are idle.*

Proof. Suppose that the vertex v is not universal. Then there exists a MDS D not containing v. Therefore, $u_1, u_2 \in D$. Consider the set $D' = (D \cup \{v\}) \setminus \{u_1, u_2\}$. Obviously, if D is dominating in T, then so is D'; therefore, D is not a minimum dominating set. This contradiction shows that the vertex v is universal, and hence the leaves u_1 and u_2 are idle. □

Lemma 2. *For any tree T and any vertex v of T which is not a leaf or a support, the following assertions hold*:

(1) *If all neighbors of v are supports, then the vertex v is idle.*

(2) *If all neighbors of v except w are supports and the vertex w is adjacent to at least one support, then the vertex v is idle.*

Proof. Let us prove the first assertion of the lemma; the proof of the second is similar. Suppose that the vertex v is not idle; then there exists an MDS D containing v. Consider the set $\phi(D)$, which is also an MDS in T. This set contains the vertex v and all vertices adjacent to it. Obviously, the set $\phi(D) \setminus \{v\}$ is dominating in T and its cardinality is smaller than that of D. This contradiction shows that the vertex v is idle, as required. □

Lemma 3. *If a tree T contains at least one universal or idle vertex, then there exists a forest F such that*

$$|V(F)| \le |V(T)|, \qquad \Delta(F) \le \Delta(T), \qquad \partial_M(F) > \partial_M(T).$$

Proof. Suppose that a tree T contains a universal vertex v. Obviously, $\deg(v) \ge 2$. Let us show that, in this case, v is adjacent to at least two idle vertices. Suppose that this is not the case. Let $w_1, w_2, \dots, w_k$ be the neighbors of v. Suppose that all of them, except possibly w_1, are not idle. Then there exists at least one MDS D containing the vertex v and the vertices $w_2, \dots, w_k$. Obviously, $D' = (D \setminus \{v\}) \cup \{w_1\}$ is also an MDS, so that the vertex w_1 is not idle. This contradiction proves that the vertex v is adjacent to at least two idle vertices $w'_1, w'_2, \dots, w'_m$. Let us delete the vertices $w'_2, \dots, w'_m$ and all edges incident to them from T and denote the forest thus obtained by F. Obviously,

$$|V(F)| < |V(T)|, \qquad \Delta(F) \le \Delta(T).$$

Moreover, each MDS of the tree T is an MDS of the forest F, whence $\partial_M(T) \le \partial_M(F)$. Consider an MDS D' of the forest T containing all vertices of the set $N[v] \setminus \{w'_1, \dots, w'_k\}$. It is easy to see that the set $(D' \setminus \{v\}) \cup \{w'_1\}$ is an MDS for F, which implies $\partial_M(F) > \partial_M(T)$, as required.

Now suppose that a tree T having no universal vertices contains an idle vertex u. Since T has no universal vertices, it follows that u is adjacent to at least two vertices $u_1, \dots, u_k$ that are not idle. For each $1 \le i \le k$, let T_i denote the maximal (by inclusion) subtree containing u_i and not containing u, and let F_0 denote the maximal (by inclusion) forest not containing u and the vertices of the subtrees $T_1, \dots, T_k$. Note that if the forest F_0 is nonempty, then each of its connected components contains precisely one idle vertex adjacent to u in the tree T. Let F denote the three T from which the vertex u is deleted. Obviously, $\Delta(F) \le \Delta(T)$. It is easy to see that $\gamma(T) = \gamma(F)$. Indeed, since the vertex u is idle in T, it follows that $\gamma(T) \ge \gamma(F)$. But if $\gamma(T) > \gamma(F)$, then, for any MDS D of the forest F, the set $D \cup \{u\}$ is an MDS in T, so that the vertex u is not idle. This contradiction shows that

$$\partial_M(F) = \partial_M(F_0) \cdot \prod_{i=1}^{k} \partial_M(T_i),\ \partial_M(T) = \partial_M(F_0) \cdot \left(\prod_{i=1}^{k} \partial_M(T_i) - \prod_{i=1}^{k} \partial_M^-(T_i, u_i)\right).$$

Note that, for any $1 \le i \le k$, the vertex u_i is not universal in T_i (otherwise, it would be universal in T, which contradicts the assumption). Thus, $\prod_{i=1}^{k} \partial_M^-(T_i, u_i) > 0$, whence $\partial_M(F) > \partial_M(T)$, as required. □

Lemma 4. *If a tree T contains adjacent support vertices v_1 and v_2, then $\partial_M(T) = \partial_M(T - v_1v_2)$.*

Proof. Let us denote by $N_l[v_1]$ (by $N_l[v_2]$) the set consisting of the vertex v_1 (respectively, v_2) and all leaves adjacent to it, and let F denote the forest obtained from T by deleting the edge v_1v_2. It is easy to see that, both in the tree T and in the forest F, each MDS contains precisely one vertex from each of the sets $N_l[v_1]$ and $N_l[v_2]$; thus, each MDS of the tree T is an MDS of the forest F, and vice versa. Therefore, $\partial_M(F) = \partial_M(T)$, as required. □

Lemma 5. *Let T be an n-vertex tree. If there exists an n-vertex forest F without isolated vertices such that*

$$\partial_M(F) > \partial_M(T), \qquad \Delta(F) \le \Delta(T),$$

then the tree T is not $\Delta(T)$-maximal.

Proof. Let us show that if such a forest F exists, then there exists an n-vertex tree T' such that $\Delta(T') \le \max(3, \Delta(F))$ and $\partial_M(T') > \partial_M(T)$. If F is a tree, then we set $T' = F$. Suppose that F contains at least two connected components T_1 and T_2 each of which contains at least two vertices. Note that each tree with at least two vertices contains either a support vertex of degree at most 2 or a support vertex adjacent to at least two leaves (for example, such are the penultimate vertices of a diametrical path in the tree). Let us show that, in each of the following three cases, the connected components T_1 and T_2 can be joined in such a way that the number of MDS in the resulting tree $T_{1,2}$ is not smaller than in the initial forest $T_1 \cup T_2$.

Case 1. Each of the components T_1 and T_2 contains at least one support vertex of degree at most 2 (we assume that the path P_2 consists of two support vertices of degree 1). We choose such support vertices $u \in V(T_1)$ and $v \in V(T_2)$ and draw an edge uv. By the preceding lemma, adding this edge does not affect the number of MDS. Moreover, as is easy to see, we have

$$\Delta(T_{1,2}) \le \max(3, \Delta(T_1), \Delta(T_2)).$$

Case 2. The trees T_1 and T_2 contain vertices u and v each of which is adjacent to at least two leaves. We choose leaves u' and v' adjacent to the vertices u and v, respectively, and draw an edge $u'v'$. Obviously, $\Delta(T_{1,2}) = \max(\Delta(T_1), \Delta(T_2))$. By Lemma 2, the vertices u' and v' are idle in the tree $T_{1,2}$. Thus,

$$\partial_M(T_{1,2}) = \partial_M(T_1 \cup T_2),$$

as desired.

Case 3. One of the subtrees (let it be T_1) contains a support u of degree at most 2, and the other subtree contains a support v adjacent to at least two leaves v' and v''. Let us draw an edge uv' and show that $\partial_M(T_{1,2}) \ge \partial_M(T_1 \cup T_2)$. By Lemma 2, the vertex v' is idle in the tree $T_{1,2}$. By Lemma 1, the vertex v is universal in the forest $T_1 \cup T_2$. Therefore, $\partial_M(T_{1,2}) \ge \partial_M^+(T_{1,2}, v) = \partial_M(T_1 \cup T_2)$, as desired.

Thus, replacing the forest $T_1 \cup T_2$ by the tree $T_{1,2}$, we have turned the forest F into a forest F_1 containing one connected component fewer than F; moreover, $\partial_M(F_1) \ge \partial_M(F)$. If F_1 is a tree, then we set $T' = F_1$. Otherwise, we will repeat the procedute until we obtain a tree F_k; then we set $T' = F_k$. Since $\Delta(F_k) \le \Delta(T)$ and $\partial_M(F_k) > \partial_M(T)$, it follows that the condition in the lemma is satisfied. □

Corollary 1. *For any n-vertex tree T, the following assertions hold*:

(1) *If T contains at least one universal or idle vertex, then there exists an n'-vertex tree T' such that $n' < n$, $\Delta(T') \le \Delta(T)$, and $\partial_M(T')^{1/n'} > \partial_M(T)^{1/n}$.*

(2) *If T is splittable, then there exists an n'-vertex tree T' such that $n' < n$, $\Delta(T') \le \Delta(T)$, and $\partial_M(T')^{1/n'} \ge \partial_M(T)^{1/n}$.*

Proof. The first assertion readily follows from Lemmas 3 and 5. The second one is an obvious consequence of the definition of a splittable tree. □

3.2. An $\mathcal{S}$-Partition of a Tree

The following structural lemma plays the key role in obtaining upper bounds for the number of MDS in 4-maximal and maximal trees.

Lemma 6. *If a tree T contains no idle vertices, then there exists a unique partition $\mathcal{S}(T)$ of the set $V(T)$ into disjoint subsets with the following properties*:

(1) $\gamma(T) = |\mathcal{S}(T)|$, *and any MDS of the tree T contains precisely one vertex in each element of the partition $\mathcal{S}(T)$*;

(2) *for any element $S' \in \mathcal{S}(T)$, there exists a vertex $v' \in V(T)$ such that $N[v'] = S'$.*

Proof. We prove the lemma by induction on the number n of vertices. The base case $n \le 5$ is obvious. Let us show that the lemma is true for $n \ge 6$ and $\operatorname{diam}(T) \le 4$. If all nonleaf vertices of T are supports, then each support is adjacent to precisely one leaf (otherwise, the tree contains idle leaves) and each element of $\mathcal{S}(T)$ consists of a support and a leaf adjacent to it. It is easy to see that such a partition satisfies the assumptions of the lemma and is unique. If T contains a vertex v which is not a leaf or a support, then, as is easy to see, such a vertex is unique and all of its neighbors are supports. Thus, by Lemma 2, the vertex v is idle, which contradicts the assumption.

Now suppose that $n \ge 6$ and $\operatorname{diam}(T) \ge 5$. Let $X = x_1x_2x_3x_4x_5\dots$ be a diametrical path in T. Note that $\deg(x_2) = 2$. Indeed, otherwise the vertex x_2 is adjacent to at least two leaf vertices; they are idle by Lemma 1, which contradicts the assumption. Depending on $\deg(x_3)$, $\deg(x_4)$, and $\deg(x_5)$, there are the following possible cases.

Case 1: $\deg(x_3) \ge 3$. In this case, the vertex x_3 is either support or adjacent to at least one support vertex x_2' different from x_2 and x_4. Let us delete the vertices x_1 and x_2 from T, denote the resulting tree by T_1, and show that if T does not contain idle vertices, then neither does T_1.

Subcase 1, a: the vertex x_3 is a support in T_1. In this case, for any MDS D of the tree T, the set $D \setminus \{x_1, x_2\}$ is an MDS of the tree T_1. Therefore, T_1 contains no idle vertices.

Subcase 1 b: the vertex x_3 is not a support. Then it is adjacent to at least one support vertex x_2' different from x_2 and x_4. Since T contains no idle vertices and the path X is diametrical, it follows that $\deg(x_2') = 2$. Suppose that a vertex $x' \in V(T_1)$ different from x_1' and x_2' is idle in T_1 (note at once that the vertex x_2' is a support in T_1 and therefore cannot be idle). Then there exists an MDS D in T which contains the vertices x_2, x_2', and x'. Thus, the set $D \setminus \{x_2\}$ is an MDS for the tree T_1, and the vertex x' is not idle in T_1. We have obtained a contradiction. Now suppose that the vertex x_1' is idle in T_1. Since the tree T contains no idle vertices, it follows that the vertex x_3 is contained in some MDS D_3 of T. Obviously, the set $D_3 \setminus \{x_1, x_2\}$ is an MDS for the tree T_1. If D_3 contains x_1', then x_1' is not idle in T_1, which contradicts the assumption. If D_3 does not contain x_1', then the set $(D_3 \cup \{x_1'\}) \setminus \{x_2'\}$ contains x_1' and is an MDS for T_1, and hence the vertex x_1' is not idle in T_1. We have again obtained a contradiction.

Thus, the tree T_1 contains no idle vertices, and, by the induction hypothesis, there exists a unique partition $\mathcal{S}(T_1)$ of T_1 satisfying the conditions in the lemma. It is easy to see that the partition $\mathcal{S}(T) = \mathcal{S}(T_1) \cup \{\{x_1, x_2\}\}$ satisfies these conditions as well and is unique for T, as required.

Case 2: $\deg(x_3) = 2$ and $\deg(x_4) \ge 3$. The following subcases are possible.

Subcase 2, a: the vertex x_4 is a support. By Lemma 2, the vertex x_3 is idle, which contradicts the assumption.

Subcase 2, b: the vertex x_4 is adjacent to at least one support x_3' different from the vertices x_3 and x_5. By Lemma 2, the vertex x_3 is idle, which contradicts the assumption.

Subcase 2, c: the vertex x_4 is adjacent to some vertices $w_1, w_2, \dots, w_s$ different from x_3 and x_5 and not being supports (here $s \ge 1$). Since the path X is diametrical and T contains no idle vertices, it follows that all neighbors of the vertices $w_1, w_2, \dots, w_s$ different from x_4 are supports of degree 2. We delete the vertices x_1, x_2, and x_3 from T and denote the resulting tree by T_2. Let us show that if T does not contain idle vertices, then neither does T_2. Suppose that, on the contrary, T_2 contains an idle vertex x'. Then there exists an MDS D of T containing x'. Obviously, the set $D' = (D \setminus \{x_1\}) \cup \{x_2\}$ is an MDS of T as well. Moreover, D' cannot contain both vertices x_3 and x_4. If D' contains x_3, then we consider the set $D'' = (D' \setminus \{x_3\}) \cup \{x_4\}$; otherwise, we set $D'' = D'$. Obviously, D'' is an MDS for T. Therefore, $D'' \setminus \{x_2\}$ is an MDS for T_2 and contains x'. We have obtained a contradiction.

Thus, the tree T_2 contains no idle vertices. Therefore, by the induction hypothesis, there exists a unique partition $\mathcal{S}(T_2)$ of T_2 satisfying the conditions in the lemma. Let us show that

$$N_{T_2}[x_4] = \{x_4, x_5, w_1, \dots, w_s\} \in \mathcal{S}(T_2).$$

Recall that all neighbors of the vertices $w_1, w_2, \dots, w_s$ different from x_4 are supports of degree 2. It is easy to see that each MDS of T_2 contains at most one vertex in the set $N_{T_2}[x_4]$. Indeed, suppose that there exists an MDS D containing at least two vertices in $N_{T_2}[x_4]$. Then the set $(\phi(D) \setminus N_{T_2}[x_4]) \cup \{x_5\}$ is dominating in T_2, which contradicts the minimality of D. Therefore, each MDS of T_2 contains precisely one vertex from the set $N_{T_2}[x_4]$, and, by assumption, each vertex in $N_{T_2}[x_4]$ is not idle, as required.

Consider the partition

$$\mathcal{S}(T) = (\mathcal{S}(T_2) \setminus \{N_{T_2}[x_4]\}) \cup \{\{x_1, x_2\}, N_T[x_4]\}.$$

Obviously, this is a unique partition satisfying the conditions in the lemma for the tree T, as required.

Case 3: $\deg(x_3) = \deg(x_4) = 2$, $\deg(x_5) \geq 3$. The following subcases are possible.

Subcase 3, a: the vertex x_5 is a support. By Lemma 2, the vertices x_3 and x_4 are idle, which contradicts the assumption.

Subcase 3, b: there exists a vertex u adjacent to x_5 and to $\deg(u) - 1$ leaves. In this case, $\deg(u) = 2$, because the tree has no idle vertices. Consider the tree T_3 obtained from T by deleting the vertex u and a leaf u' adjacent to it. Let us show that if T does not contain idle vertices, then neither does T_3. Suppose that, on the contrary, there exists a vertex v' which is idle in T_3 and not idle in T. It is easy to see that, both in T_3 and in T, each MDS contains precisely two vertices from the set $\mathcal{X}_5 = \{x_1, x_2, x_3, x_4, x_5\}$. Suppose that $x' \notin \mathcal{X}_5$. Then there exists an MDS D' in the tree T which contains the vertices x_2, x_5, and x'. It is easy to see that the set $D' \setminus \{u, u'\}$ contains the vertex x' and is an MDS for the tree T_3. We have obtained a contradiction. Now suppose that there exists a vertex $x' \in \mathcal{X}_5$ which is idle in T_3. Then there exists an MDS D'' in T which contains the vertices x_6 and x' (indeed, if each MDS of T containing x_6 does not contain x', then the vertex x' is idle, which is impossible). It is easy to see that the set $D'' \setminus \{u, u'\}$ contains x' and is an MDS in T_3. We have again obtained a contradiction.

Thus, T_3 contains no idle vertices and, by the induction hypothesis, there exists a unique partition $\mathcal{S}(T_3)$. The partition $\mathcal{S}(T_3) \cup \{\{u, u'\}\}$ is unique in T, as required.

Subcase 3, c: there exists a path (u_1, u_2, u_3, x_5) such that the vertex u_1 is a leaf, the vertex u_2 is adjacent to $\deg(u_2) - 1$ leaves, and the vertex u_3 is different from x_4 and x_6 and all of its neighbors different from x_5 are either leaves or supports. If u_3 is a support, then we argue as in Subcase 1, a. Let us prove that if u_3 is not a support, then it is idle in T. It suffices to show that each MDS in the tree contains at most one vertex in the set $\{x_3, x_4, x_5, u_3\}$. Suppose that there exists an MDS D containing at least two vertices in this set. It is easy to see that $D' = (\phi(D) \setminus \{x_3, x_4, x_5, u_3\}) \cup \{x_5\}$ is an MDS and $|D'| < |\phi(D)| = |D|$; this is a contradiction. On the other hand, each MDS of the tree T must contain at least one vertex in the closed neighborhood $N[x_4]$, which does not contain u_3. Thus, the vertex u_3 is idle, which contradicts the assumption of the lemma.

Subcase 3, d: there exists a path $(w_1, w_2, w_3, w_4, x_5)$ such that the vertex w_4 is different from the vertices x_4 and x_6. If, moreover, $\max(\deg(w_2), \deg(w_3), \deg(w_4)) > 2$, then we rename the vertices and argue as in Cases 1 and 2. If $\deg(w_2) = \deg(w_3) = \deg(w_4) = 2$, then, clearly, the vertices in the set $\{x_3, x_4, w_3, w_4\}$ are idle in T. Indeed, each MDS of T must contain at least one vertex from the neighborhoods $N[x_4]$ and $N[u_4]$. On the other hand, according to the considerations in the previous subcase, each MDS contains at most one vertex in the set $\{x_3, x_4, x_5, w_3, w_4\}$. Thus, T contains an idle vertex, which contradicts the assumption of the lemma.

Case 4: $\deg(x_2) = \deg(x_3) = \deg(x_4) = \deg(x_5) = 2$. Consider the tree T_4 obtained from T by deleting the vertices x_1, x_2, and x_3. Let us prove that if T does not contain idle vertices, then neither does T_4. First, we show that $\gamma(T) = \gamma(T_4) + 1$. On the one hand, each MDS of T contains a vertex in the set $\{x_1, x_2\}$, whence $\gamma(T) \geq \gamma(T_4) + 1$. On the other hand, given any MDS D' of T_4, the set $D' \cup \{x_2\}$ is an MDS of T, whence $\gamma(T) \leq \gamma(T_4) + 1$.

Suppose that some vertex x' is idle in T_4 but not idle in T. Then there exists an MDS D of T which contains x'. Consider the set $D' = D \setminus \{x_1, x_2\}$. Obviously, D' contains at most one vertex in the set $\{x_3, x_4\}$. If D' contains the vertex x_3, then we consider the set $D'' = (D' \setminus \{x_3\}) \cup \{x_4\}$; otherwise, we set $D'' = D'$. In any case, D'' is an MDS of T_4 and hence contains the vertex x'. This contradiction shows that the tree T_4 contains no idle vertices.

By the induction hypothesis, there exists a unique partition $\mathcal{S}(T_4)$ of T_4. Obviously, it includes the set $\{x_4, x_5\}$. It is easy to see that the partition

$$\mathcal{S}(T) = \big(\mathcal{S}(T_4) \setminus \{\{x_4, x_5\}\}\big) \cup \big\{\{x_1, x_2\}, \{x_3, x_4, x_5\}\big\}$$

is a unique appropriate partition of the tree T. This completes the proof of the lemma. $\square$

Corollary 2. *For any tree T without idle vertices, the following assertions hold*:

(1) *If an element S' of the partition $\mathcal{S}(T)$ contains at least three vertices, then none of them is a leaf or a support in T.*

(2) *If $S'' \in \mathcal{S}(T)$ contains two vertices, then one of them is a leaf and the other is a support adjacent to it.*

(3) *If the tree T contains at least two vertices, then so does each element of the partition $\mathcal{S}(T)$.*

Proof. Let us prove the first assertion. Suppose that some element S' with $|S'| \geq 3$ contains a leaf u'. In this case, S' also contains the vertex u adjacent to it. Since $\partial^+_M(T, u') + \partial^+_M(T, u) = \partial_M(T)$, it follows that all vertices in $S' \setminus \{u, u'\}$ are idle in T, which is impossible. If S' contains a support w but does not contain a leaf w' adjacent to w, then the vertex w' does not belong to any element of the partition $\mathcal{S}(T)$, because it is not universal. This contradiction shows that all elements of S' are neither leaves nor supports, as required.

The second and third assertions readily follow from assertion (2) of Lemma 6. $\square$

4. THE CASE OF 4-MAXIMAL TREES

Lemma 7. *Given any $n \geq 3$, if an n-vertex tree T without idle vertices is 4-maximal, then each element of the partition $\mathcal{S}(T)$ contains at most three vertices.*

Proof. Suppose that the lemma is false for some 4-maximal tree T. Since $\Delta(T) \leq 4$, it follows that each element of $\mathcal{S}(T)$ contains at most five vertices. There are two possible cases.

Case 1: there exist vertices $w, w_1, w_2, w_3 \in V(T)$ such that

$$\{w, w_1, w_2, w_3\} = N[w] \in \mathcal{S}(T).$$

For each $1 \leq i \leq 3$, let T_i denote the maximal (by inclusion) subtree of T containing the vertices w and w_i and not containing the other neighbors of w, and let T_i' be the tree obtained by attaching a leaf w_0 to the vertex w of the tree T_i. Finally, let F_i denote the forest obtained from T_i by deleting the vertices w and w_i and all edges incident to them. For any $1 \leq i \leq 3$, the forest F_i is nonempty and contains no isolated vertices, because, by Corollary 2, none of the vertices in the neighborhood $N[w]$ is a leaf or a support.

Let us introduce the notation

$$A_i^+ = \partial_+(T_i, w_i), \qquad A_i = \partial(F_i), \qquad A_i^- = \partial_+(T_i', w_0).$$

We have

$$\begin{aligned}\partial_M(T) &= \partial^+_M(T, w) + \partial^+_M(T, w_1) + \partial^+_M(T, w_2) + \partial^+_M(T, w_3)\\ &= A_1A_2A_3 + A_1^+A_2^-A_3^- + A_1^-A_2^+A_3^- + A_1^-A_2^-A_3^+.\end{aligned}$$

We delete the vertices w and w_3 from the tree T and attach leaves w_1' and w_2' to the vertices w_1 and w_2, respectively (see Fig. 2). Let us denote the resulting forest by F, and let T_1'' (T_2'') be the connected component of F containing the vertex w_1 (respectively, w_2).

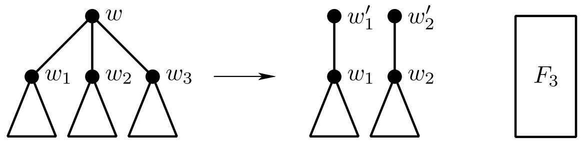

Fig. 2. The transformation in Case 1.

Then $F = T_1'' \cup T_2'' \cup F_3$. We have

$$\begin{aligned}\partial_M(F) &= \big(\partial_M^+(T_1'', w_1) + \partial_M^+(T_1'', w_1')\big) \cdot \big(\partial_M^+(T_2'', w_2) + \partial_M^+(T_2'', w_2')\big) \cdot \partial_M(F_3) \\ &= (A_1^+ + A_1) \cdot (A_2^+ + A_2) \cdot A_3 = A_1^+ A_2^+ A_3 + A_1^+ A_2 A_3 + A_1 A_2^+ A_3 + A_1 A_2 A_3.\end{aligned}$$

Since the tree T contains no universal vertices, it follows that, for each $1 \le i \le 3$, there exists an MDS of F_i which contains none of the vertices adjacent to w_i in the tree T. Thus, for each $1 \le i \le 3$, the strict inequality $A_i > A_i^-$ holds. Moreover, we have $A_i^+ \ge A_i$. We can assume that $A_1^+/A_1 \ge A_2^+/A_2 \ge A_3^+/A_3$. Then $A_1^+ A_2^+ A_3 \ge A_1 A_2 A_3^+ > A_1^- A_2^- A_3^+$, whence $\partial_M(F) > \partial_M(T)$. Therefore, by Lemma 5, the tree T is not 4-maximal. We have arrived at a contradiction.

Case 2: there exist vertices $w, w_1, w_2, w_3, w_4 \in V(T)$ such that

$$\{w, w_1, w_2, w_3, w_4\} = N[w] \in \mathcal{S}(T).$$

For each $1 \le i \le 4$, we define subgraphs T_i, T_i', and F_i and introduce the notation A_i^+, A_i, and A_i^- as in the preceding case. We have

$$\partial_M(T) = A_1A_2A_3A_4 + A_1^+A_2^-A_3^-A_4^- + A_1^-A_2^+A_3^-A_4^- + A_1^-A_2^-A_3^+A_4^- + A_1^-A_2^-A_3^-A_4^+.$$

From the tree T we delete the vertex w_4, all edges incident to it, and the edge ww_3; after that, we attach a leaf w_3' to the vertex w_3. In the resulting forest F, by T' we denote the connected component containing the vertices w, w_1, and w_2 and by T'', the connected component containing the vertices w_3 and w_3'. Note that $F = T' \cup T'' \cup F_4$. We have

$$\begin{aligned}\partial_M(F) &= \big(\partial_M^+(T', w) + \partial_M^+(T', w_1) + \partial_M^+(T', w_2)\big) \\ &\quad \times \big(\partial_M^+(T'', w_3) + \partial_M^+(T'', w_3')\big) \cdot \partial_M(F_4) \\ &= (A_1A_2 + A_1^+A_2^- + A_1^-A_2^+) \cdot (A_3^+ + A_3) \cdot A_4.\end{aligned}$$

We can assume that $A_1^+/A_1^- \ge A_3^+/A_3^- \ge A_4^+/A_4^- > A_4^+/A_4$, in which case the strict inequality $A_1^+A_2^-A_3^+A_4 > A_1^-A_2^-A_3^-A_4^+$ holds. Therefore, $\partial_M(F) > \partial_M(T)$ and the tree T is not 4-maximal by Lemma 5. This contradiction proves Lemma 7. $\square$

Theorem 1. *For any $n \ge 4$, each 4-maximal n-vertex tree T contains at most $(\sqrt{2})^n$ MDS. The equality $\partial_M(T) = (\sqrt{2})^n$ is attained if and only if $n = 2l$ and T contains precisely l support vertices each of which is adjacent to a unique leaf.*

Proof. It is easy to check that the theorem is true for $n < 6$. Suppose that $n \ge 6$ and there exist trees for which it is false; let T be such a tree with the least number of vertices. By Corollary 1, if T contains a universal or an idle vertex, then it contains fewer that $(\sqrt{2})^n$ MDS. Similarly, it is easy to check that if T is splittable, then, by Corollary 1, it satisfies the condition in the theorem, which contradicts the assumption. Thus, by Lemma 6, there exists a unique $\mathcal{S}$-partition $\mathcal{S}(T)$. Since the tree T is unsplittable, it contains no adjacent support vertices, and the partition $\mathcal{S}(T)$ contains at least one element S' comprising precisely three vertices (the case $|S'| > 3$ is impossible by the previous lemma). According to Corollary 1, all vertices in S' are neither leaves nor supports, whence $\operatorname{diam}(T) \ge 6$.

Let $X = x_1x_2x_3x_4x_5x_6\dots$ be a diametrical path in T (an example is shown in Fig. 3). If the vertex x_3 is a support, then T contains a pair of adjacent supports x_2 and x_3 and the tree T is splittable by Lemma 4, which contradicts the assumption. Since T has no idle vertices, it follows that each support in T is adjacent to a unique leaf. Thus, all neighbors of x_3 different from x_4 are supports of degree 2. In view of Lemmas 6 and 7, we have $x_3 \in N[x_4] = \{x_3, x_4, x_5\} \in \mathcal{S}(T)$.

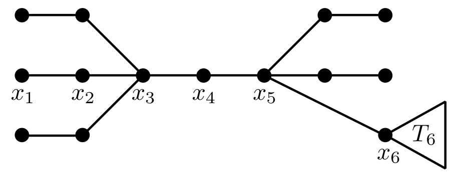

Fig. 3. The form of the tree T for $a = 3$ and $b = 2$.

Let us prove that if $\deg(x_5) \geq 3$, then all vertices in the set $N[x_5] \setminus \{x_4, x_5, x_6\}$ are supports of degree 2. Suppose that this set is nonempty, and let w denote one of the vertices contained in it. If w is not a support, then there exist vertices w_0 and w_1 such that

$$\{w, w_0, w_1\} = N[w_0] \in \mathcal{S}(T).$$

By Corollary 1, the vertex w_1 is neither a leaf nor a support; hence there exists a path (w_1, u', u'') in T in which the vertex u' is different from w_0. It follows that the path $u''u'w_1w_0wx_5x_6\ldots$ is longer than X. We have obtained a contradiction. Suppose that the vertex w is adjacent to the leaf w' and $\deg(w) \geq 3$. Let u denote a neighbor of w different from x_5 and w'. If u is a support, then the tree T is splittable by Lemma 4. If u is not a support, then there exist vertices u_0 and u_1 such that $\{u, u_0, u_1\} = N[u_0] \in \mathcal{S}(T)$. The path $u_1u_0uwx_5\ldots$ is of the same length as X, but the vertex u_1 is not a leaf by Corollary 2. We have again obtained a contradiction.

Thus, the vertices x_3 and x_5 are adjacent to $a = \deg(x_3) - 1$ and $b = \deg(x_5) - 2$ supports of degree 2, respectively. Let T' be the tree obtained from T by deleting these supports, the leaves adjacent to them, and the vertex x_3, and let T_6 denote the tree obtained from T' by deleting the vertices x_4 and x_5. By the induction hypothesis,

$$\partial_M(T') \leq 2^{|V(T')|/2} = 2^{(n-2a-2b-1)/2}.$$

We have

$$\partial_M(T') = \partial_M^+(T', x_4) + \partial_M^+(T', x_5), \qquad \partial_M(T) = \partial_M^+(T, x_3) + \partial_M^+(T, x_4) + \partial_M^+(T, x_5),$$
$$\partial_M^+(T, x_4) = 2^{a+b} \cdot \partial_M^+(T', x_4), \qquad \partial_M^+(T, x_5) = (2^a - 1) \cdot 2^b \cdot \partial_M^+(T', x_5),$$
$$\partial_M^+(T, x_3) = 2^a \cdot (2^b - 1) \cdot \partial_M(T_6) + 2^a \cdot \partial_M^+(T_6, x_6).$$

It is easy to show that if $a, b \in \{1, 2\}$, then the relations $\partial_M^+(T_6, x_6) \leq \partial_M(T_6)$, $\partial_M(T_6) = \partial_M^+(T', x_4)$, and $\partial_M^+(T', x_4) \leq \partial_M^+(T', x_5)$ imply the inequality

$$2^{a+b+1/2} \cdot (\partial_M^+(T', x_4) + \partial_M^+(T', x_5)) > \partial_M^+(T, x_3) + \partial_M^+(T, x_4) + \partial_M^+(T, x_5).$$

If $a = 3$, then, for this inequality to hold, it is also required that $\partial_M^+(T_6, x_6)/\partial_M(T_6) \leq 3/4$. The purpose of the further considerations is to prove this relation. We consider four cases, depending on whether the vertices x_6 and x_7 or their neighbors are supports in the tree T.

Case 1: there exist vertices w and w' such that $\{x_6, w, w'\} = N[w] \in \mathcal{S}(T)$. Note that the vertex w may or may not coincide with the vertex x_7.

Subcase 1, a: all neighbors of x_6 different from x_5 and w are supports of degree 2 (in particular, it is possible that $\deg_T(x_6) = 2$). Obviously, we have $\partial_M^+(T_6, x_6) \leq \partial_M^+(T_6, w)$, whence $\partial_M^+(T_6, x_6)/\partial_M(T_6) \leq 1/2$.

Subcase 1, b: the vertex x_6 is adjacent to some vertex x_5' different from x_5 and w and not being a support and, possibly, to a support x_5'' of degree 2. Then there exist vertices x_3' and x_4' such that $\{x_3', x_4', x_5'\} = N_T[x_4'] \in \mathcal{S}(T)$. Let T_5' be the maximal (by inclusion) subtree of T containing x_5' and not containing x_6. It is easy to see that the tree T_5' is the extreme subgraph $W_{a',b'}$ of T_6 with contact vertex x_5', where $a' = \deg(x_3') - 1$ and $b' = \deg(x_5') - 2$. We can assume that $a' = 3$ (otherwise, we consider the diametrical path passing through the vertices x_5' and x_6, rename the tree vertices, and apply the above argument to this path). Let T_6' be the maximal (by inclusion) subtree of T_6 containing the vertex x_6 and not containing the vertex x_5'. Then

$$\partial^+_M(T_6, x_6) = \partial^+_M(T_6', x_6) \cdot \widehat{\partial}_M(W_{a',b'}), \qquad \partial^+_M(T_6, w) = \partial^+_M(T_6', w) \cdot \partial_M(W_{a',b'}).$$

As in the preceding subcase, we have $\partial^+_M(T_6', x_6) \le \partial^+_M(T_6', w)$. Since

$$\partial_M(W_{3,b'})/\widehat{\partial}_M(W_{3,b'}) \ge 15/23,$$

it follows that $\partial^+_M(T', x_6)/\partial_M(T_6) \le 3/4$.

Note that, in the subcases considered above, the argument remains valid in the cases where the supports adjacent to x_6 are of degree greated than 2. We will use this observation in considering Subcase 3, b.

Subcase 1, c: the vertex x_6 is adjacent to two vertices x_5' and x_5'' different from x_5 and w and not being supports. It follows from considerations in Subcase 1, b that x_5' and x_5'' are the contact vertices of extreme subgraphs $W_{3,b'}$ and $W_{3,b''}$ of T_6, where $b' = \deg(x_5') - 2$ and $b'' = \deg(x_5'') - 2$. Let T_6'' denote the maximal (by inclusion) subtree of T containing the vertex x_6 and not containing the vertices x_5' and x_5''. Then

$$\partial_M(T_6, x_6) = \widehat{\partial}_M(W_{3,b'}) \cdot \widehat{\partial}_M(W_{3,b''}) \cdot \partial_M(T_6'', x_6),$$
$$\partial_M(T_6, w) = \partial_M(W_{3,b'}) \cdot \partial_M(W_{3,b''}) \cdot \partial_M(T_6'', w),$$
$$\partial^+_M(T_6, w) \ge \frac{\partial_M(W_{3,b'})}{\widehat{\partial}_M(W_{3,b'})} \cdot \frac{\partial_M(W_{3,b''})}{\widehat{\partial}_M(W_{3,b''})} \cdot \partial^+_M(T_6, x_6) > \frac{1}{3} \cdot \partial^+_M(T_6, x_6).$$

Therefore, we have $\partial^+_M(T_6, x_6)/\partial_M(T_6) \le 3/4$. This completes the consideration of Case 1.

In Cases 2–4, we assume that the vertex x_6 is a support and adjacent to a leaf vertex l_6, to the vertices x_5 and x_7, and possibly to a vertex x_5' different from x_5, l_6, and x_7. If the vertex x_5' is present, then it is the contact vertex of some extreme subgraph $W_{3,b'}$, where $b' = \deg(x_5') - 2$. Since $\partial_M(T_6) = \partial^+_M(T_6, x_6) + \partial^+_M(T_6, l_6)$, it suffices to prove that either $\partial^+_M(T_6, x_6) \le 3\partial^+_M(T_6, l_6)$ or the tree T is not 4-maximal.

Case 2: the vertices x_7 and x_8 belong to distinct elements of the partition $\mathcal{S}(T)$. The vertex x_7 is not a support, because the tree T is unsplittable. Thus, there exist vertices u and u' such that $\{x_7, u, u'\} = N[u] \in \mathcal{S}(T)$. Since the path X is diametrical and T contains no idle vertices, it follows that all neighbors of u' different from u are support vertices of degree 2. Depending on $\deg_T(x_6)$, two subcases are possible.

Subcase 2, a: $\deg_T(x_6) = 3$. Let us show that $\partial^+_M(T_6, x_6) < 3\partial^+_M(T_6, l_6)$. We denote by T_7 the maximal (by inclusion) subtree of T_6 containing the vertex x_7 and not containing the vertex x_6. Let F_7 be the forest obtained from T_7 by deleting the vertex x_7 and all edges incident to it. We have

$$\partial^+_M(T_6, l_6) = \partial_M(T_7) = \partial^+_M(T_7, x_7) + \partial^+_M(T_7, u) + \partial^+_M(T_7, u'),$$
$$\partial^+_M(T_6, x_6) = \partial^+_M(T_7, x_7) + \partial^+_M(F_7, u) + \partial^+_M(F_7, u').$$

Note that $\partial^+_M(F_7, u') = \partial^+_M(F_7, u)$, because all neighbors of the vertex u' except u are supports of degree 2. It is easy to see that

$$\partial^+_M(F_7, u) = \partial^+_M(T_7, u) = \partial_M(T_7 \setminus N[u]).$$

Therefore,

$$\partial^+_M(T_6, x_6) = \partial^+_M(T_7, x_7) + 2\partial^+_M(T_7, u) < 2\partial^+_M(T_6, l_6).$$

Subcase 2, b: $\deg_T(x_6) = 4$. The tree T_6 contains a vertex x_5' adjacent to x_6 and contact for an extreme subgraph $W_{3,b'}$, where $b' = \deg(x_5') - 2$. The same argument as in Subcase 2, a yields

$$\partial^+_M(T_6, l_6) = \partial_M(W_{3,b'}) \cdot (\partial^+_M(T_7, x_7) + \partial^+_M(T_7, u) + \partial^+_M(T_7, u')),$$
$$\partial^+_M(T_6, x_6) = \widehat{\partial}_M(W_{3,b'}) \cdot (\partial^+_M(T_7, x_7) + 2\partial^+_M(T_7, u)).$$

It is easy to check that $\partial_M^+(T_7,u) \le 2\partial_M^+(T_7,x_7)$ (this inequality may turn into an equality only if $\deg(u')=2$). The inequality $\partial_M(W_{3,b'})/\widehat{\partial}_M(W_{3,b'}) \ge 15/23$ implies $\partial_M^+(T_6,x_6) < 3\partial_M^+(T_6,l_6)$, as required.

Case 3: the vertices x_7 and x_8 belong to the same element of the partition, and $\deg(x_7)>2$. In this case, $N[x_8]=\{x_7,x_8,x_9\}\in\mathcal{S}(T)$.

Subcase 3, a: the vertex x_7 is adjacent to at least one support vertex x_7' (possibly, $\deg(x_7')>2$). We denote the unique leaf adjacent to x_7' by l_7'. Let us show that $\partial_M^+(T_6,x_6) < 3\partial_M^+(T_6,l_6)$ in this case. We denote by T_7 the maximal (by inclusion) subtree of T containing x_7 and not containing x_6 and by F_7 the forest obtained from T_7 by removing the vertex x_7 and all edges incident to it. We have

$$\partial_M^+(T_6,l_6)=\partial_M^+(T_7,x_7)+\partial_M^+(T_7,x_8)+\partial_M^+(T_7,x_9).$$

On the other hand,

$$\partial_M^+(T_6,x_6)=\partial_M^+(T_7,x_7)+\partial_M^+(T_7,x_8)+\partial_M^+(F_7,x_9).$$

Since $\partial_M^+(T_7,x_7')\ge\partial_M^+(T_7,l_7')$, it follows that $\partial_M^+(F_7,x_9)\le 2\partial_M^+(T_7,x_9)$, whence

$$\partial_M^+(T_6,x_6)<2\partial_M^+(T_6,l_6),$$

as required.

Subcase 3, b: the vertex x_7 is adjacent to a vertex x_6' different from x_8 and not being a support. Suppose that there exists a diametrical path $X''=x_1''x_2''x_3''x_4''x_5''x_6'x_7\dots$. Since x_6' is not a support, we can consider the path X'' instead of x and apply the argument of Case 1. If such a path does not exist, then, as is easy to see, the vertex x_6' itself is the contact vertex of some extreme subgraph $W_{a',b'}$. Hence there exists a path $X'''=x_2'''x_3'''x_4'''x_5'''x_6'x_7\dots$ containing $\operatorname{diam}(T)$ vertices. It is easy to check that the argument of Case 1 applies to the path X''' (the role of x_6 is played by the vertex x_7, which is not a support).

Case 4: the vertices x_7 and x_8 belong to the same element of the partition and $\deg(x_7)=2$. In this case, $N[x_8]=\{x_7,x_8,x_9\}\in\mathcal{S}(T)$. Let T_6' denote the maximal (by inclusion) subtree of T containing the vertex x_6 and not containing the vertex x_7. For $m\in\{7,8,9\}$, we denote by T_m the maximal (by inclusion) subtree of T containing the vertex x_m and not containing x_{m-1}.

Subcase 4, a: $\deg(x_6)=3$. The structure of the tree T is shown in Fig. 4.

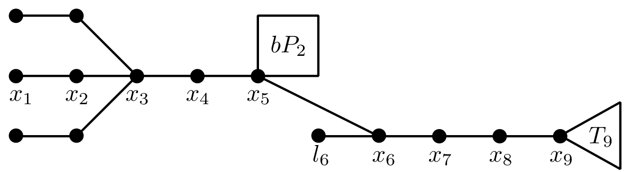

Fig. 4. The structure of the tree T in Subcase 4, a.

We have

$$\partial_M(T)=\partial_M^+(T,x_7)+\partial_M^+(T,x_8)+\partial_M^+(T,x_9),$$
$$\partial_M^+(T,x_7)=\partial_M^+(T_7,x_7)\cdot\partial_M(T_6')=\partial_M^+(T_7,x_7)\cdot\partial_M(W_{3,b+1}),$$
$$\partial_M^+(T,x_8)=\partial_M^+(T_7,x_8)\cdot\partial_M(T_6')=\partial_M^+(T_7,x_8)\cdot\partial_M(W_{3,b+1}),$$
$$\partial_M^+(T,x_9)=\partial_M^+(T_8,x_9)\cdot\partial_M^+(T_6',x_6)=\partial_M^+(T_8,x_9)\cdot\widehat{\partial}_M(W_{3,b}).$$

Recall that

$$\partial_M(W_{3,b})=2^{3+b}+(2^3-1)2^b+2^3(2^b-1),\qquad \widehat{\partial}_M(W_{3,b})=\partial_M(W_{3,b})+2^b.$$

We remove the edge x_7x_8 from the tree T and replace the connected component containing x_7 by the forest $(6+b)P_2$. Let us denote the forest thus obtained by F. We have

$$\partial_M(F)=2^{6+b}(\partial_M^+(T_8,x_8)+\partial_M^+(T_8,x_9)).$$

Moreover,

$$\partial^+_M(T_7,x_7) \le \partial^+_M(T_7,x_8) = \partial^+_M(T_8,x_8) \le \partial^+_M(T_8,x_9).$$

It is easy to check that the strict inequality $\partial_M(F) > \partial_M(T)$ holds. Thus, by Lemma 5, the tree T is not 4-maximal. We have arrived at a contradiction.

Subcase 4, b: $\deg(x_6) = 4$. In this case, the vertex x_6 is adjacent to a vertex x_5' different from x_5, x_6, and l_6. Since the tree T is unsplittable, it follows that x_5' is the contact vertex of a subgraph $W_{3,b'}$, where $b' = \deg(x_5') - 2$. Therefore,

$$\begin{aligned}
\partial_M(T) &= \partial^+_M(T,x_7) + \partial^+_M(T,x_8) + \partial^+_M(T,x_9),\\
\partial^+_M(T,x_7) &= \partial^+_M(T_7,x_7)\cdot\partial_M(T_6) = \partial^+_M(T_7,x_7)\cdot\big(\partial^+_M(T_6,l_6) + \partial^+_M(T_6,x_6)\big)\\
&= \partial^+_M(T_7,x_7)\cdot\big(\partial_M(W_{3,b})\cdot\partial_M(W_{3,b'}) + \widehat{\partial}_M(W_{3,b})\cdot\widehat{\partial}_M(W_{3,b'})\big),\\
\partial^+_M(T,x_8) &= \partial^+_M(T_7,x_8)\cdot\big(\partial_M(W_{3,b})\cdot\partial_M(W_{3,b'}) + \widehat{\partial}_M(W_{3,b})\cdot\widehat{\partial}_M(W_{3,b'})\big),\\
\partial^+_M(T,x_9) &= \partial^+_M(T_8,x_9)\cdot\partial^+_M(T_6,x_6) = \partial^+_M(T_8,x_9)\cdot\widehat{\partial}_M(W_{3,b})\cdot\widehat{\partial}_M(W_{3,b'}).
\end{aligned}$$

Let us delete the vertices x_6 and l_6 from the tree. In the forest thus obtained, we replace the connected components containing the vertices x_5 and x_5' by the forest $(7+b+b')P_2$. Moreover, to the vertex x_7 we attach three supports of degree 2. We denote the connected component containing x_7 in the resulting n-vertex forest F by T'.

We have

$$\begin{gathered}
\partial_M(F) = 2^{7+b+b'}(\partial^+_M(T',x_7) + \partial^+_M(T',x_8) + \partial^+_M(T',x_9)),\\
\partial_M(T',x_7) = 8\cdot\partial^+_M(T_7,x_7),\ \partial_M(T',x_8) = 8\cdot\partial^+_M(T_7,x_8),\ \partial_M(T',x_9) = 7\cdot\partial^+_M(T_8,x_9).
\end{gathered}$$

It is easy to check that $\partial_M(F) > \partial_M(T)$ for any $b, b' \in \{0,1,2\}$. By Lemma 5, the tree T is not 4-maximal. This contradiction proves the theorem. □

5. BOUNDS FOR THE MAXIMUM POSSIBLE NUMBER OF MDS IN n-VERTEX TREES

5.1. A Lower Bound

Recall that the 19-vertex tree $W_{4,4}$ is obtained by attaching four supports of degree 2 to each endvertex of the path P_3 (see Fig. 5). For this tree, the inequality $\partial_M(W_{4,4}) = 736 > (\sqrt{2})^{19}$ holds. We set $\theta = 736^{1/19} = 1.415\dots$.

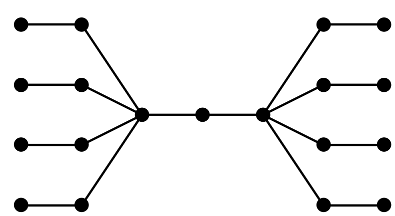

Fig. 5. The tree $W_{4,4}$.

Theorem 2. *For any $n \ge 1$, there exists an n-vertex tree T_n such that*

$$\Delta(T) \le 5, \qquad \partial(T_n) > \frac{1}{3}\cdot 1.415^n.$$

Proof. First, we show that the theorem is true for $n = 19k$. Let us arbitrarily join supports of degree 2 from different connected components in the forest $kW_{4,4}$ until we obtain a tree T_{19k}. It follows from the proof of Lemma 5 that $\Delta(T_n) = 5$ and

$$\partial_M(T_{19k}) = \partial_M(kW_{4,4}) = \theta^n > \frac{1}{3} \cdot 1.415^n.$$

Now suppose that $n = 19k + r$, where $k \geq 0$ and $1 \leq r < 19$. If r is even, then we set

$$F_n = kW_{5,5} \cup \frac{r}{2} P_2.$$

If r is odd and $k = 0$, then we set

$$F_n = P_r \quad \text{for } r < 7, \qquad F_n = P_7 \cup \frac{r-7}{2} P_2 \quad \text{for } r \geq 7.$$

Finally, if r is odd and $k > 0$, then we set

$$F_n = (k-1)W_{5,5} \cup \left(10 + \frac{r-1}{2}\right) P_2.$$

Let us arbitrarily join supports of degree at most 2 from different connected components of F_n until we obtain a tree T_n. It follows from the proof of Lemma 5 that $\Delta(T_n) \leq 5$ and $\partial_M(T_n) = \partial_M(F_n)$. It is easy to check that $\partial_M(T_n) > (1/3) \cdot \theta^n$ for all $n < 19$. Note that $(\sqrt{2})^p/\theta^p > 1/3$ for all integer p in the interval $[1, 36]$. Therefore, as is easy to see, for all integer $n = 19k + r \geq 19$ we have

$$\frac{\partial_M(T_n)}{\theta^n} \geq \frac{\theta^{19(k-1)} \cdot (\sqrt{2})^{19+r}}{\theta^{19k+r}} > \frac{1}{3},$$

whence

$$\partial_M(T_n) > \frac{1}{3} \cdot 1.415^n.$$

This completes the proof of the theorem. $\square$

5.2. *An Upper Bound*

Apparently, maximal trees have complex structure, which is hard to describe. Using the notion of an $\mathcal{S}$-partition, we obtain a nontrivial upper bound for the number of MDS in an n-vertex tree.

Lemma 8. *Let T be a maximal n-vertex tree containing no idle vertices. Then each element of the partition $\mathcal{S}(T)$ contains at most three vertices.*

Proof. Suppose that, for some maximal tree T, there exists an element $S' \in \mathcal{S}(T)$ containing $k > 3$ vertices. If $k \in \{4, 5\}$, then we apply the argument of Lemma 7. Suppose that $k = 2p + \delta$, where $p \geq 3$ and $\delta \in \{0, 1\}$. In this case, there exist vertices $w, w_1, \dots, w_{k-1}$ such that

$$\{w, w_1, \dots, w_{k-1}\} = N[w] \in \mathcal{S}(T).$$

For each $1 \leq i \leq k-1$, we define subgraphs T_i, T_i', and F_i and quantities A_i, A_i^+, and A_i^- in the same way as in Lemma 7. Recall that $A_i^- < A_i \leq A_i^+$.

We introduce the notation

$$A_* = \prod_{i=1}^{k-1} A_i, \qquad A_*^+ = \prod_{i=1}^{k-1} A_i^+, \qquad A_*^- = \prod_{i=1}^{k-1} A_i^-,$$

$$A_{\mathrm{I}}^+ = \prod_{i=1}^{p} A_i^+ \cdot \prod_{j=p+1}^{k-1} A_j, \qquad A_{\mathrm{II}}^+ = \prod_{i=1}^{p} A_i \cdot \prod_{j=p+1}^{k-1} A_j^+.$$

Note that $\partial_M(T) = A_* + A_*^- \cdot \sum_{i=1}^{k-1}(A_i^+/A_i^-)$. Moreover, for any positive integer s such that $s \le p$ we have $A_*^- \cdot A_s^+/A_s^- < A_{\mathrm{I}}^+$. If $p < s \le k-1$, then $A_*^- \cdot A_s^+/A_s^- < A_{\mathrm{II}}^+$. Finally, for each $1 \le s \le k-1$ we have $A_*^- \cdot A_s^+/A_s^- < A_*^+$.

The case of $\delta = 1$. Consider the forest $F' = (p-2)P_2 \cup T_{\mathrm{I}}' \cup T_{\mathrm{II}}'$, in which the component T_{I}' is obtained by attaching forests $F_1, \dots, F_p$ to the end vertex of the path P_2 (here and in what follows, we assume that a vertex w_i of the path is joined to those vertices of the forest F_i which were adjacent to w_i in tree T and no other vertices) and the component T_{II}' is obtained by attaching forests $F_{p+1}, \dots, F_{2p}$ to the end of the path P_2. We have

$$\partial_M(F') = 2^{p-2}(A_* + A_{\mathrm{I}}^+ + A_{\mathrm{II}}^+ + A_*^+).$$

It is easy to check that $\partial_M(T) < \partial_M(F')$. By Lemma 5, the tree T is not maximal, which contradicts the assumption.

The case of $\delta = 0$. Consider the forest $F'' = (p-3)P_2 \cup T''$ in which the component T'' is obtained by attaching forests $F_1, \dots, F_p$ to one of the supports in the path P_7 and forests $F_{p+1}, \dots, F_{2p-1}$ to the other supports in this path. We have

$$\partial_M(F'') = 2^{p-3}(A_* + 2A_{\mathrm{I}}^+ + 2A_{\mathrm{II}}^+ + 3A_*^+), \qquad \partial_M(T) < \partial_M(F'').$$

By Lemma 5, the tree T is not maximal, which contradicts the assumption. □

Theorem 3. *For any n-vertex tree T,*

$$\partial_M(T) < 1.4205^n.$$

Proof. Obviously, the theorem is true for $n < 6$. Suppose that $n \ge 6$ and there exist n-vertex trees containing at least 1.4205^n MDS. Choose a tree T with the least number of vertices among them (we can assume that T is maximal). By Corollary 1, T is unsplittable and contains no idle vertices. Hence, by Lemma 6, there exists a unique $\mathcal{S}$-partition $\mathcal{S}(T)$, and by Lemma 8, each element of this partition contains two or three vertices. Consider a diametrical path $X = x_1x_2x_3x_4x_5\dots$ in T. Since T is unsplittable, it follows that $\{x_3, x_4, x_5\} = N[x_4] \in \mathcal{S}(T)$, $\deg(x_4) = 2$, and the vertices x_3 and x_5 are adjacent to $a = \deg(x_3) - 1$ and $b = \deg(x_5) - 2$ supports of degree 2, respectively. Let T' denote the tree obtained from T by deleting all supports of degree 2 adjacent to vertices x_3 and x_5, all leaves adjacent to them, and the vertex x_3. By assumption, $\partial_M(T') < 1.4205^{|V(T')|}$, whence

$$\partial_M(T) > 1.4205^{2a+2b+1} \cdot \partial_M(T').$$

Moreover,

$$\begin{aligned}\partial_M(T) &= \partial_M^+(T, x_3) + \partial_M^+(T, x_4) + \partial_M^+(T, x_5) \le 2\partial_M^+(T, x_4) + \partial_M^+(T, x_5)\\ &= 2^{a+b+1} \cdot \partial_M^+(T', x_4) + (2^a - 1) \cdot 2^b \cdot \partial_M^+(T', x_5),\\ \partial_M(T') &= \partial_M^+(T', x_4) + \partial_M^+(T', x_5).\end{aligned}$$

Let us show that

$$2^{a+b+1} \cdot \partial_M^+(T', x_4) + (2^a - 1) \cdot 2^b \cdot \partial_M^+(T', x_5) < 1.4205^{2a+2b+1}(\partial_M^+(T', x_4) + \partial_M^+(T', x_5)).$$

Obviously, for any $a, b \ge 0$ we have $1.4205^{2a+2b+1} > (2^a - 1)2^b$. Moreover, since the vertex x_4 of the tree T' is a leaf, it follows that $\partial_M^+(T', x_4) \le \partial_M^+(T', x_5)$. Thus, it suffices to consider the case where $\partial_M^+(T', x_4) = \partial_M^+(T', x_5)$. Let us show that

$$2^{a+b+1} + 2^{a+b} - 2^b < 2 \cdot 1.4205^{2a+2b+1}.$$

We divide both sides of the inequality by 2 and consider the function

$$f(x, y) = 1.4205^{2x+2y+1} - 3 \cdot 2^{x+y-1} + 2^{y-1}.$$

It is easy to check that $\min_{x,y \ge 0} f(x, y) > 0$, whence

$$\partial_M(T) < 1.4205^{2a+2b+1} \cdot \partial_M(T').$$

This contradiction shows that there exist no n-vertex trees containing at least 1.4205^n MDS, which completes the proof of the theorem. □

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