# On the Number of Minimum Total Dominating Sets in Trees 

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#### Abstract

The minimum total dominating set (MTDS) of a graph is a vertex subset $D$ of minimum cardinality such that every vertex of the graph is adjacent to at least one vertex of $D$. In this paper we obtain a sharp upper bound for the number of MTDSs in the class of $n$-vertex 2 -caterpillars. We also show that for all $n \geq 1$ every $n$-vertex tree has less than $(\sqrt{2})^{n}$ MTDSs.


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## INTRODUCTION

The dominating set of a graph is a vertex subset $D$ such that any vertex not in $D$ is adjacent to at least one vertex in $D$. The total dominating set of a graph is a vertex subset $D^{\prime}$ such that any vertex of the graph is adjacent to at least one vertex in $D^{\prime}$. The dominating set is called minimum if it is of the least cardinality. We use the abbreviations DS, MDS, TDS, and MTDS for the terms "dominating set," "minimum dominating set," "total dominating set," and "minimum total dominating set," respectively. The total dominance number $\gamma_{t}(G)$ of a graph $G$ is the cardinality of each of its MTDSs. Let $\vartheta(G)$ denote the number of all MTDSs in the graph $G$.

In 2006, Bród and Skupień [1] described trees containing the maximum and minimum number of DMs among all $n$-vertex trees. Later, Krzywkowski and Wagner[2] described trees and connected graphs containing the minimum number of TDSs. The question of whether a tree with dominance number $\gamma$ can contain more than $2^{\gamma}$ MDSs remained open until 2017, when an example of such a tree was given in [3]. On the other hand, Alvarado et al. [4] showed that every tree with dominance number $\gamma$ contains at most $2.4606^{\gamma}$ MDSs. For all $k \geq 2$, the paper [5] describes trees that contain the maximum and minimum number of $k$-DSs (i.e., sets $D_{k}$ such that each vertex of a tree not in $D_{k}$ is adjacent to at least $k$ vertices in $D_{k}$ ).

To date, the question of the structure of trees containing the maximum possible number of MDSs and MTDSs remains open. It was shown in [6] in 2019 that each $n$-vertex tree contains less than $95^{n / 13}$ minimal (i.e., inclusion-minimal) DSs. In addition, an example of an $n$-vertex tree containing more than $0.649 \times 95^{n / 13}$ minimal DSs is given for any $n \geq 1$. The methods proposed in [6] can also be applied to other classes of graphs, but using them to enumerate sets of fixed cardinality (including MDSs and MTDSs) is not possible in the opinion of the present author.

In 2019, Henning et al. [7] obtained three upper bounds for the number of MTDSs in trees and forests. Namely, for an $n$-vertex forest $F$ with total dominance number $\gamma_{t}$, they proved the inequality

$$
\vartheta(F) \leq \min \left((8 \sqrt{e})^{\gamma_{t}}\left(\frac{n-\gamma_{t} / 2}{\gamma_{t} / 2}\right)^{\gamma_{t} / 2},(1+\sqrt{2})^{n-\gamma_{t}}, 1.4865^{n}\right)
$$

In the present paper, we prove the strict inequality $\vartheta(T)<(\sqrt{2})^{n}$ for all $n$-vertex trees. In addition, a sharp upper bound for the number of MTDSs for the class of $n$-vertex 2-caterpillars is obtained

## 1. SOME DEFINITIONS AND NOTATION

As usual, the vertex and edge sets of a simple undirected graph $G$ are denoted by $V(G)$ and $E(G)$, respectively. The open neighborhood $N(v)$ of a vertex $v$ is the set consisting of all adjacent vertices, and the the closed neighborhood $N[v]$ is the set $N(v) \cup\{v\}$.

Let $G \backslash V_{0}$ denote the subgraph of $G$ induced by the vertices of the set $V(G) \backslash V_{0}$. In the case of $V_{0}=\{v\}$, we will use the notation $G \backslash v$ instead of $G \backslash\{v\}$. Let $G-e$ denote the graph obtained by removing the edge $e \in E(G)$ from the graph $G$.

A tree vertex is called a preleaf if it is adjacent to at least one leaf. Let us say that a tree vertex is preterminal if all but one of its neighbors are leaves. The diameter $\operatorname{diam}(T)$ of a tree $T$ is the maximum possible distance between its vertices. A simple path $P=v_{1} v_{2} \ldots v_{m}$ of a tree $T$ is said to be diametrical if it consists of $\operatorname{diam}(T)+1$ pairwise distinct vertices. A tree is called a $k$-caterpillar if the distance from each of its vertices to some simple path, called the backbone, is at most $k$. We assume that the backbone of a $k$-caterpillar is a diametrical path. The star graph $S_{m}$ is the $(m+1)$-vertex tree containing a vertex of degree $m$ (here $m \geq 0$ ).

By $\overline{a, b}$ we denote the set of all integers in the interval $[a ; b]$. Let $P=v_{1} v_{2} \ldots v_{m}$ be chosen in the tree $T$. For each $i \in 2, \ldots, m$, denote by $T_{i}$ the inclusion-maximal subtree $T$ that contains $v_{i}$ and does not contain $v_{i-1}$. We assume that the subtree $T_{1}$ coincides with $T$. We set $\widehat{T}_{i}=T_{i} \backslash T_{i+1}$. By $\mathcal{D}_{T, P}\left(v_{i}\right)$ we denote the distance in the tree $\widehat{T}_{i}$ from the vertex $v_{i}$ to the nearest leaf other than $v_{i}$. If $\widehat{T}_{i}$ consists of one vertex, then we set $\mathcal{D}_{T, P}\left(v_{i}\right)=0$. Note that if the vertex $v$ lies on the backbone of a $k$-caterpillar, then $\mathcal{D}_{T, P}(v) \leq k$. In the case where the choice of the tree $T$ and the path $P$ is clear from the context, we use the notation $\mathcal{D}(v)$ instead of $\mathcal{D}_{T, P}(v)$.

Recall that $\vartheta(G)$ denotes the number of MTDSs in a graph $G$. We assume that $\vartheta\left(K_{1}\right)=0$. The numbers of MTDSs in $G$ containing and not containing a vertex $v$ will be denoted by $\vartheta_{+}(G, v)$ and $\vartheta_{-}(G, v)$, respectively. A vertex $v$ of the graph $G$ is said to be universal if $\vartheta_{+}(G, v)=\vartheta(G)$ and idle if $\vartheta_{-}(G, v)=\vartheta(G)$. As usual, $G_{1} \cup G_{2}$ denotes the graph with vertex set $V\left(G_{1}\right) \cup V\left(G_{2}\right)$ and edge set $E\left(G_{1}\right) \cup E\left(G_{2}\right)$. It is easy to see that $\vartheta\left(G_{1} \cup G_{2}\right)=\vartheta\left(G_{1}\right) \vartheta\left(G_{2}\right)$ for disjoint graphs $G_{1}$ and $G_{2}$.

We say that a tree $T$ separable if it is possible to remove an edge from it in such a way that the number of MTDSs in the resulting forest remains the same and inseparable otherwise. We say that an $n$-vertex tree (2-caterpillar) is maximal if it contains the maximum possible number of MTDSs among all $n$-vertex trees ( $n$-vertex 2 -caterpillars, respectively).

Let a vertex $v \in V(T)$ be chosen in a tree $T$. Denote by $\widehat{\gamma}_{t}(T, v)$ the cardinality of the smallest vertex subset $D \subseteq V(T)$ such that every vertex in $V(T)$, except possibly $v$, is adjacent to at least one vertex in $D$. It is easily seen that the inequality $\gamma_{t}(T)-1 \leq \widehat{\gamma}_{t}(T, v) \leq \gamma_{t}(T)$ holds. Denote by $\widehat{\vartheta}(T, v)$ the number of subsets $D \subseteq V(T)$ of cardinality $\widehat{\gamma}_{t}(T, v)$ such that each vertex $V(T)$, possibly except for the vertex $v$, is adjacent to at least one vertex in $D$. Note that if $\widehat{\gamma}_{t}(T, v)=\gamma_{t}(T)$, then $\widehat{\vartheta}(T, v) \geq \vartheta(T)$, because in this case each MTDS $T$ has cardinality $\widehat{\gamma}_{t}(T, v)$. We define the quantities $\widehat{\vartheta}_{+}(T, v)$ and $\widehat{\vartheta}_{-}(T, v)$ by analogy with $\vartheta_{+}(T, v)$ and $\vartheta_{-}(T, v)$.

Let a set $D$ be a $\operatorname{TDS}$ of a tree $T$, and let $\operatorname{diam}(T) \geq 3$. Denote by $L(T)$ the set of leaves of $T$ whose neighbors are preterminal vertices. Consider the mapping $\varphi: L(T) \rightarrow V(T)$ taking each leaf $l \in L(T)$ to the only nonleaf vertex at distance 2 from it. Denote by $\varphi(D)$ the set obtained by replacing each leaf $l \in L(T)$ in $D$ by the vertex $\varphi(l)$. Since $D$ contains all preleaves of $T$, it follows that $\varphi(D)$ is a TDS, while $|\varphi(D)| \leq|D|$. Thus, for any MTDS $D$ the set $\varphi(D)$ is an MTDS as well.

We say that a vertex $v$ of a tree $T$ is $\varphi$-universal if $v \in \varphi(D)$ for any MTDS $D \subseteq V(T)$. Note that every universal vertex is $\varphi$-universal, and every nonleaf vertex adjacent to at least one preterminal vertex is $\varphi$-universal.

Figure 1 shows a tree that is a 2 -caterpillar and its diametrical path $v_{1} v_{2} \ldots v_{9}$ is the backbone of the caterpillar. Note that $\mathcal{D}\left(v_{4}\right)=0, \mathcal{D}\left(v_{2}\right)=1$, and $\mathcal{D}\left(v_{5}\right)=2$. In addition, the nonleaf vertices $v_{3}, v_{5}, v_{6}$, and $v_{7}$ (and only they) are adjacent to preterminal vertices, and so they are $\varphi$-universal.


Fig. 1. Example of 2-caterpillar with backbone $v_{1} v_{2} \ldots v_{9}$.

## 2. PRELIMINARIES

### 2.1. Class of Elementary Forests

We say that a forest $F$ is elementary if each of its connected components is a star graph. We say that an elementary $n$-vertex forest is maximal if it contains the maximum possible number of MTDSs among all such forests. It is clear that $\vartheta\left(S_{k}\right)=k$ for all $k \geq 0$.

Lemma 1. For $n=4 k+r \geq 12, r \in\{0,1,2,3\}$, the $n$-vertex maximal elementary forest is unique, is isomorphic to the forest $F_{n}=(k-r) S_{3} \cup r S_{4}$, and contains $f(n)=4^{r} \cdot 3^{k-r}$ MTDSs.

Proof. Let a star $S_{k}$ be the least connected component of a forest $F$. If $F$ contains a star $S_{m}$ such that $k+1<m$, then the subgraph $S_{k} \cup S_{m}$ can be replaced by the subgraph $S_{k+1} \cup S_{m-1}$ and the number of MTDSs of the forest $F$ will increase, which contradicts its maximality. Then for some integers $a \geq 1$ and $b \geq 0$ the equality $F=a S_{k} \cup b S_{k+1}$ holds. Let us show that for any $n$-vertex forest $F$ not isomorphic to $F_{n}$, there exists a replacement of some of its subgraphs by a forest with the same number of vertices and a larger number of MTDSs.
Case of $k=0$. Replace the entire forest $F$ with the tree $S_{n-1}$.
CASE $k=1$. Replace the entire forest $F$ with the forest $(b-1) S_{k+1} \cup S_{(a+1)(k+1)}$.
CASE OF $k=2$. If $F$ contains the forest $2 S_{2}$, then replace it with the tree $S_{5}$. Otherwise, $F$ contains the forest $S_{2} \cup 2 S_{3}$; replace it with the forest $S_{4} \cup S_{5}$.
Case of $k=3$. If $b \leq 4$, then the condition of the lemma is satisfied; otherwise, replace the forest $4 S_{4}$ with the forest $5 S_{3}$.
CASE OF $k=4$. If $a \leq 3$ and $b=0$, then the condition of the lemma is satisfied. Otherwise, $F$ contains one of the forests $4 S_{4}, 2 S_{4} \cup S_{5}$, or $2 S_{5}$; replace them with the forests $5 S_{3}, 4 S_{3}$, or $3 S_{3}$, respectively.
Case of $k=5$. If $F$ contains the forest $2 S_{5}$, then replace it with the forest $3 S_{3}$. Otherwise, $F$ contains the forest $S_{5} \cup S_{6}$; replace it with the forest $2 S_{3} \cup S_{4}$.
CASE OF $k=6$. If $F$ contains the forest $2 S_{6}$, then replace it with the forest $S_{3} \cup 2 S_{4}$. Otherwise, $F$ contains the tree $S_{7}$; replace it with the forest $S_{2} \cup S_{4}$.
CASE of $k \geq 7$. Replace the tree $S_{k}$ with the forest $S_{2} \cup S_{k-3}$.
Thus, for any $n \geq 12$ and any $n$-vertex forest $F$ other than $F_{n}$, there exists at least one replacement that increases the number of MTDSs in it. The proof of Lemma 1 is complete.

Note that for $n \in\{4,5,8,9,10\}$ the maximal forest is unique and isomorphic to $F_{n}$, for $n=11$ the only maximal forest is $S_{4} \cup S_{5}$, and for $n \in\{1,2,3,6,7\}$ the tree $S_{n-1}$ is a maximal forest (possibly not the only one). Thus, for all positive integers $n$, the inequality $\vartheta\left(F_{n}\right) \leq f(n)$ holds, which is strict for $n \in\{1,2,3,6,7,11\}$.

### 2.2. Universal and Idle Vertices

Lemma 2. If a tree $T$ contains two adjacent nonleaf vertices $u$ and $v$ such that $u$ is idle and $v$ is either idle or universal, then $T$ is separable.

Proof. If the vertex $v$ is idle, then remove the edge $u v$ and denote the resulting forest by $F_{1}$. Obviously, $\gamma_{t}\left(F_{1}\right) \geq \gamma_{t}(T)$. On the other hand, each MTDS of the tree $T$ does not contain the vertices $u$ and $v$, and so it is a TDS in the forest $F_{1}$, whence $\gamma_{t}\left(F_{1}\right) \leq \gamma_{t}(T)$. Then $\gamma_{t}\left(F_{1}\right)=\gamma_{t}(T)$, with each MTDS of the tree $T$ being an MTDS of the forest $F$ and vice versa, whence $\vartheta\left(F_{1}\right)=\vartheta(T)$.

If, however, the vertex $v$ is universal, then we remove all the edges incident to the vertex $u$ except for the edge $u v$, and denote the resulting forest by $F_{2}$. As in the previous case, it is easy to check that the equalities $\gamma_{t}\left(F_{2}\right)=\gamma_{t}(T)$ and $\vartheta\left(F_{2}\right)=\vartheta(T)$ hold. The proof of Lemma 2 is complete.

Lemma 3. If a tree $T$ contains universal vertices $u$ and $v$ such that $\operatorname{dist}(u, v)=3$, then $T$ is separable.

Proof. By assumption, there exist vertices $u^{\prime}$ and $v^{\prime}$ in $T$ such that there exists a path $u u^{\prime} v^{\prime} v$. Let us denote by $F$ the forest obtained by removing the edge $u^{\prime} v^{\prime}$ from $T$ and show that $\vartheta(T)=\vartheta(F)$. Obviously, $\gamma_{t}(F) \geq \gamma_{t}(T)$. Let us prove that if $D^{\prime}$ is an MTDS $T$, then it is an MTDS of $F$. Since the vertices $u$ and $v$ are in $D^{\prime}$, it follows that each of the vertices $u^{\prime}$ and $v^{\prime}$ in the forest $F$ has a neighbor in $D^{\prime}$. Thus, $D^{\prime}$ is a TDS in the forest $F$, whence $\gamma_{t}(F)=\gamma_{t}(T)$ and $\vartheta(F) \geq \vartheta(T)$. On the other hand, since $\gamma_{t}(F)=\gamma_{t}(T)$, it follows that each MTDS of the forest $F$ is an MTDS for the tree $T$, whence $\vartheta(F)=\vartheta(T)$, as desired. The proof of Lemma 3 is complete.

Lemma 4. The following statements are true for any tree $T$.

1. If $T$ contains a vertex $v$ adjacent to a leaf $v^{\prime}$ and also to a preterminal vertex $u$, then $\vartheta\left(T_{1}\right) \geq \vartheta(T)$, where $T_{1}$ is the tree obtained by removing the leaf $v^{\prime}$ from $T$.
2. If $T$ contains a vertex $v$ adjacent to at least two preterminal vertices $u_{1}$ and $u_{2}$, then $\vartheta\left(T_{2}\right) \geq \vartheta(T)$, where $T_{2}$ is the tree obtained by removing the vertex $u_{2}$ and all leaves adjacent to it from $T$.
Proof. Let us prove the first assertion of the lemma. Since the vertex $v^{\prime}$ is a leaf in $T$, it follows that $\gamma_{t}\left(T_{1}\right) \leq \gamma_{t}(T)$. On the other hand, $v$ is $\varphi$-universal in $T_{1}$. Then there exists an MTDS $D \ni v$ of the tree $T_{1}$. It is obvious that $D$ is also a TDS for $T$, whence $\gamma_{t}\left(T_{1}\right)=\gamma_{t}(T)$, and each MTDS of $T$ is also an MTDS for $T_{1}$, whence $\vartheta\left(T_{1}\right) \geq \vartheta(T)$, as desired.

The second assertion can be proved in a similar way. The proof of Lemma 4 is complete.
Lemma 5. Let a tree $T$ contain a vertex $u$ that is not a preleaf. If all neighbors of $u$ are adjacent to at least one $\varphi$-universal vertex, then $u$ is idle.

Proof. Assume, on the contrary, that there exists an MTDS $D$ containing $u$. Consider the set $\varphi(D)$. By assumption, all vertices of the open neighborhood $N(u)$ have at least one neighbor in $\varphi(D)$ distinct from $u$, and at least one of these vertices is itself included in $\varphi(D)$. Then the set $\varphi(D) \backslash\{u\}$ is also a TDS, which contradicts the minimality of $D$. The proof of Lemma 5 is complete.

Lemma 6. If a tree $T$ contains an idle nonleaf vertex $u$ not adjacent to universal vertices and $\gamma_{t}(T \backslash u)=\gamma_{t}(T)$, then $\vartheta(T \backslash u)>\vartheta(T)$.

Proof. Let $u_{1}, u_{2}, \ldots, u_{k}$ be the neighbors of the vertex $u$ in $T$. Denote by $T_{i}^{*}$ the inclusionmaximal subtree of $T$ containing vertex $u_{i}$ and not containing $u$. Since the vertex $u$ is idle and $\gamma_{t}(T \backslash u)=\gamma_{t}(T)$, for any MTDS $D$ of the tree $T$ the set $D \operatorname{cap} V\left(T_{i}^{*}\right)$ is an MTDS of the tree $T_{i}^{*}$. Since for any $i \in 1, \ldots, k$ there exists an MTDS $D_{i}$ of the tree $T$ that does not contain $v_{i}$, it follows that the set $D_{i} \cap V\left(T_{i}\right)$ is an MTDS of the tree $T_{i}$ and does not contain $v_{i}$, whence $\vartheta_{-}\left(T_{i}, v_{i}\right)>0$. Thus, we have the inequality

$$
\vartheta(T)=\prod_{i=1}^{k} \vartheta\left(T_{i}^{*}\right)-\prod_{i=1}^{k} \vartheta_{-}\left(T_{i}^{*}, v_{i}\right)<\prod_{i=1}^{k} \vartheta\left(T_{i}^{*}\right)=\vartheta(T \backslash u) .
$$

The proof of Lemma 6 is complete.
Lemmas 2 and 6 imply the following assertion.
Corollary 1. For any $n, k \geq 1$, if an $n$-vertex tree $T$ is a $k$-caterpillar and contains an idle nonleaf vertex $u$ such that $\gamma_{t}(T \backslash u)=\gamma_{t}(T)$, then either $T$ is separable or it is neither a maximal tree nor a maximal $k$-caterpillar.

This assertion will apply both to 2 -caterpillars and to arbitrary trees.

## 3. CLASS OF 2-CATERPILLARS

Lemma 7. For $n \geq 3$, for any $n$-vertex 2 -caterpillar $T$ there exists an $(n+1)$-vertex 2 -caterpillar $T^{\prime}$ such that $\vartheta(T)<\vartheta\left(T^{\prime}\right)$.

Proof. The proof is carried out by induction on the number $n$ of vertices. One can readily verify that the assertion of the lemma is true for $n \in 3, \ldots, 6$. Assume that for $n \geq 7$ there exists some maximal $n$-vertex 2 -caterpillar $T$ for which the assertion is false but for any $\overline{2}$-caterpillar $T^{\prime \prime}$ with fewer vertices the strict inequality $\vartheta\left(T^{\prime \prime}\right)<\vartheta(T)$ holds.

Assume that $\operatorname{diam}(T) \leq 4$. If $\operatorname{diam}(T)=2$, then $T$ is isomorphic to $S_{n-1}$. If $\operatorname{diam}(T)=3$, then $T$ contains exactly two nonleaf vertices, with $\gamma_{t}(T)=2$ and $\vartheta(T)=1$. However, if $\operatorname{diam}(T)=4$, then the central vertex $T$ is universal, whence $\vartheta(T)=1$. Thus, the inequality $\vartheta(T) \leq \vartheta\left(S_{n-1}\right)<\vartheta\left(S_{n}\right)$ holds; this is impossible by assumption.

Assume that $\operatorname{diam}(T) \geq 5$. Denote by $v_{1} v_{2} \ldots v_{k}$ the backbone of $T$. The following cases are possible.
CASE 1. In $T$ there exists at least one nonidle leaf $l$ adjacent to some vertex $u$. We attach a new leaf $l^{\prime}$ to $u$ and denote the resulting tree by $T^{\prime}$. Then $\vartheta\left(T^{\prime}\right)=\vartheta_{-}(T, l)+2 \vartheta_{+}(T, l)>\vartheta(T)$; this is a contradiction.
When considering cases $2-4$, we will assume that all leaves $T$ are idle and the vertex $v_{3}$ is universal (since all neighbors of $v_{2}$ except for $v_{3}$ are idle leaves).
CASE 2. The inequality $\operatorname{deg}\left(v_{3}\right) \geq 3$ holds. By Lemma 4 , in the tree $T$ there exists a subtree $T^{\prime}$ such that $\vartheta\left(T^{\prime}\right) \geq \vartheta(T)$; a contradiction.
When considering cases 3 and 4 , we assume that $\operatorname{deg}\left(v_{3}\right)=2$.
CASE 3. The vertex $v_{4}$ is universal or idle. If $v_{4}$ is universal, then for any MTDS $D$ of the tree $T$ the set $D \backslash\left\{v_{2}\right\}$ is an MTDS of the tree $T_{2}$, whence $\vartheta(T) \leq \vartheta\left(T_{2}\right)$; a contradiction. If, however, $v_{4}$ is idle, then $\operatorname{deg}\left(v_{4}\right)=2$, because otherwise $v_{4}$ would be $\varphi$-universal. Then for any MTDS $D$ of the tree $T$ the set $D \backslash\left\{v_{2}, v_{3}\right\}$ is an MTDS in $T_{5}$, whence $\vartheta(T) \leq \vartheta\left(T_{5}\right)$; a contradiction.
Case 4. The vertex $v_{4}$ is not universal and not idle. Assume that $\operatorname{deg}\left(v_{4}\right) \geq 3$. Then $v_{4}$ is not a preleaf and is adjacent to at least one preterminal vertex all whose other neighbors are idle leaves. However, $v_{4}$ is universal, which is impossible; therefore, $\operatorname{deg}\left(v_{4}\right)=2$. Assume that the vertex $v_{5}$ is not idle. Then for any MTDS $D \ni v_{5}$ the set $\left(D \backslash\left\{v_{3}\right\}\right) \cup\left\{v_{1}\right\}$ is also an MTDS; this contradicts the universality of $v_{3}$. Thus, $v_{5}$ is idle and $\operatorname{deg}\left(v_{5}\right)=2$. Let us show that $\operatorname{deg}\left(v_{6}\right)=2$. Let $\operatorname{deg}\left(v_{6}\right)>2$. Then the vertex $v_{6}$ is $\varphi$-universal and by Lemma 5 the vertex $v_{4}$ is idle, which is impossible. Since $v_{5}$ is idle and $\operatorname{deg}\left(v_{6}\right)=2$, it follows that $v_{7}$ is universal.
Note that the inequality $\vartheta_{+}\left(T, v_{4}\right) \leq \vartheta_{+}\left(T, v_{6}\right)$ holds, because each MTDS of $T$ contains exactly one of the vertices $v_{4}$ or $v_{6}$; moreover, if the MTDS $D$ contains $v_{4}$, then the set $\left(D \backslash\left\{v_{4}\right\}\right) \cup\left\{v_{6}\right\}$ is an MTDS as well. Consider an $n$-vertex forest $S_{3} \cup T_{5}$ and denote by $T^{\prime}$ the tree obtained by adding a leaf of the tree $S_{3}$ to the vertex $v_{7}$ of the tree $T_{5}$. Obviously, $T^{\prime}$ is a separable 2-caterpillar. Then

$$
\vartheta\left(T^{\prime}\right)=3 \vartheta\left(T_{5}\right) \geq 3 \vartheta_{+}\left(T, v_{6}\right)>\vartheta_{+}\left(T, v_{4}\right)+\vartheta_{+}\left(T, v_{6}\right)=\vartheta(T) .
$$

Thus, $T$ is not a maximal 2-caterpillar; this contradicts the assumption.
The proof of Lemma 7 is complete.
Theorem 1. For $n \geq 12$, every maximal $n$-vertex 2 -caterpillar $T$ contains a maximal elementary forest $F_{n}$ as a spanning subgraph. The equality $\vartheta(T)=f(n)$ holds.

Proof. It follows from the reasoning in the previous lemma that if $\operatorname{diam}(T) \leq 4$, then $\vartheta(T) \leq \vartheta\left(S_{n-1}\right) \leq f(n)$. The equality $\vartheta(T)=f(n)$ is possible only if $T$ is isomorphic to $S_{3}$ or $S_{4}$. Thus, we will assume that $n \geq 6$ and $\operatorname{diam}(T) \geq 5$.

By $v_{1}, \ldots, v_{k}$ we denote the backbone of $T$ and by $p$, the index of the leftmost vertex of the backbone that is different from $v_{2}$ and has degree greater than 2 (if $T=P_{n}$, then we set $p=k+1$ ). Denote by $q$ the number of the second vertex on the left of the backbone with this property (if there is no such vertex, then we set $q=k+1$ ). We assume that if $T$ is different from $P_{n}$, then $p \leq\left\lfloor\frac{k+1}{2}\right\rfloor$ (otherwise, we will rename the vertices of the backbone in reverse order).

Assume that there exists a maximal 2-caterpillar $T$ that either contains more than $f(n)$ MTDSs or contains exactly $f(n)$ MTDSs and does not contain the forest $F_{n}$ as a spanning subgraph. We can assume that $T$ is inseparable, because there are no 2-caterpillars with fewer vertices that have this property. Denote by $a$ the number of leaves adjacent to $v_{2}$ (that is, $a=\operatorname{deg}\left(v_{2}\right)+1$ ). Let us consider several cases depending on the value of $p$.
CASE $p=3$. By Lemmas 4 and 7 , the tree $T$ is not a maximal 2-caterpillar; a contradiction.
CASE $p=4$. If $\mathcal{D}\left(v_{4}\right)=2$, then the vertex $v_{4}$ is adjacent to some preleaf $u_{4}$ that does not lie on the backbone $T$. Then $\operatorname{dist}\left(v_{2}, u_{4}\right)=3$ and $T$ is separable by Lemma 3 ; a contradiction. Now let $\mathcal{D}\left(v_{4}\right)=1$. Let us show that in this case all leaves adjacent to $v_{4}$ are idle. Assume that this is not true and there exists some MTDS $D$ containing a leaf $v_{4}^{\prime}$ adjacent to $v_{4}$. Then the set $\varphi(D) \backslash\left\{v_{4}^{\prime}\right\}$ is also a TDS and is less than $D$ in cardinality; a contradiction. Since $T$ is maximal, by Lemma 7 the vertex $v_{4}$ is adjacent to the only idle leaf $v_{4}^{\prime}$. Consider several cases depending on the value of the quantity $q$.
CASE OF $p=4$ AND $q=5$. If $\mathcal{D}\left(v_{5}\right)=1$, then $v_{5}$ is universal and $T$ is separable, because $\operatorname{dist}\left(v_{2}, v_{5}\right)=3$. If $\mathcal{D}\left(v_{5}\right)=2$, then we remove the vertices $v_{4}$ and $v_{4}^{\prime}$ from the tree and denote the resulting forest by $F$. The equality $\gamma_{t}(F)+1=\gamma_{t}(T)$ holds, and for any MTDS $D$ of the tree $T$, the set $D \backslash\left\{v_{4}\right\}$ is an MTDS of the forest $F$. Moreover, each connected component of $F$ is a 2 -caterpillar. Then

$$
f(n)>f(a+2) f(n-a-4) \geq \vartheta(F) \geq \vartheta(T)
$$

this contradicts the assumption about the maximality of $T$.
CASE OF $p=4$ AND $q=6$. If $\mathcal{D}\left(v_{6}\right)=2$ and $v_{6}$ is adjacent to some preleaf $u_{6}$, then $\operatorname{dist}\left(v_{4}, u_{6}\right)=3$ and $T$ is separable. If $\mathcal{D}\left(v_{6}\right)=1$, then we act by analogy with the previous case. Let us remove the vertices $v_{4}$ and $v_{4}^{\prime}$ from the tree and denote the resulting forest by $F$. Then for any MTDS $D$ of the tree $T$ the set $D \backslash\left\{v_{4}\right\}$ is an MTDS of the forest $F$, whence $f(n)>\vartheta(F) \geq \vartheta(T)$; a contradiction.
CASE OF $p=4$ AND $q=7$. If $\mathcal{D}\left(v_{7}\right)=1$, then $v_{7}$ is universal and $T$ is separable, because $\operatorname{dist}\left(v_{4}, v_{7}\right)=3$. Let $\mathcal{D}\left(v_{7}\right)=2$ and $v_{7}$ be adjacent to some preterminal vertex $u_{7}$ not lying on the backbone $T$. The vertices $v_{4}$ and $u_{7}$ are universal, while vertices $v_{3}$ and $v_{7}$ are $\varphi$-universal. Then by Lemma 5 the vertices $v_{5}$ and $v_{6}$ are idle and $T$ is separable by Lemma 2; a contradiction.
CASE OF $p=4$ AND $q=8$. Since the vertex $v_{8}$ is either universal or $\varphi$-universal, it follows by Lemma 5 that the vertex $v_{6}$ is idle. One can readily verify that $\gamma_{t}(T)=\gamma_{t}\left(T_{6}\right)+3$. Then each MTDS of $T$ containing the vertex $v_{7}$ contains $v_{3}$ and does not contain $v_{5}$, whence $\vartheta(T)=\vartheta_{+}\left(T, v_{5}\right)+\vartheta_{+}\left(T, v_{7}\right)$ and $\vartheta_{+}\left(T, v_{7}\right) \leq \vartheta\left(T_{6}\right)$. If the vertex $v_{5}$ is idle, then $T$ is separable by Lemma 2; a contradiction. However, if $v_{5}$ is not idle, then $\vartheta_{+}\left(T, v_{5}\right)=(a+1) \vartheta_{-}\left(T_{7}, v_{7}\right)$, because if some MTDS of $T$ contains the vertex $v_{5}$, then it also contains exactly one vertex from the open neighborhood $N\left(v_{2}\right)$. Thus,

$$
\vartheta(T)=\vartheta_{+}\left(T, v_{7}\right)+\vartheta_{+}\left(T, v_{5}\right) \leq \vartheta\left(T_{6}\right)+(a+1) \vartheta_{-}\left(T_{7}, v_{7}\right)
$$

Since $f(n-a-5) \geq \vartheta\left(T_{6}\right)$ and $f(n-a-6) \geq \vartheta_{-}\left(T_{7}, v_{7}\right) \geq \vartheta\left(T_{7}\right)$, we have

$$
f(n)>f(n-a-5)+(a+1) f(n-a-6) \geq \vartheta(T)
$$

this contradicts the assumption about the maximality of $T$.


Fig. 2. Structure of the 2-caterpillar $T$ for $p=4, q \geq 9$, and $a=2$.

CASE of $p=4$ And $q \geq 9$. In this case, $T$ has the structure shown in Fig. 2. Suppose that $\gamma_{t}\left(T_{9}\right)>\widehat{\gamma}_{t}\left(T_{9}, v_{9}\right)$. Then $v_{8}$ is universal and $v_{6}$ is idle by Lemma 5. If the MTDS $D$ contains the vertex $v_{5}$, then it does not contain $v_{7}$; otherwise the set $\varphi(D) \backslash\left\{v_{5}\right\}$ would be a TDS as well, which is impossible. If $D$ contains $v_{7}$, then it does not contain $v_{5}$ and hence contains $v_{3}$. Then

$$
\begin{aligned}
\vartheta(T) & =\vartheta_{+}\left(T, v_{5}\right)+\vartheta_{+}\left(T, v_{7}\right)=(a+1) \vartheta_{-}\left(T_{7}, v_{7}\right)+\vartheta_{+}\left(T_{6}, v_{8}\right) \\
& \leq(a+1) \vartheta\left(T_{7}\right)+\vartheta\left(T_{6}\right) \leq(a+1) f(n-a-6)+f(n-a-5)<f(n) .
\end{aligned}
$$

Assume that $\gamma_{t}\left(T_{9}\right)=\widehat{\gamma}_{t}\left(T_{9}, v_{9}\right)$. We introduce the notation

$$
A_{1}=\vartheta_{+}\left(T_{9}, v_{9}\right), \quad A_{2}=\vartheta\left(T_{9}\right), \quad B_{1}=\widehat{\vartheta}_{+}\left(T_{9}, v_{9}\right), \quad B_{2}=\widehat{\vartheta}\left(T_{9}, v_{9}\right) .
$$

Note that $A_{1} \leq A_{2}$ and $B_{1} \leq B_{2}$. Moreover, since $\gamma_{t}\left(T_{9}\right)=\widehat{\gamma}_{t}\left(T_{9}, v_{9}\right)$, it follows that $A_{2} \leq B_{2}$. Assume that there exists an MTDS $D$ containing at least three vertices in the set $\left\{v_{5}, v_{6}, v_{7}, v_{8}\right\}$. Then the set

$$
\left(\varphi(D) \backslash\left\{v_{5}, v_{6}, v_{7}, v_{8}\right\}\right) \cup\left\{v_{7}, v_{8}\right\}
$$

is an MTDS as well and is less than $D$ in terms of cardinality; a contradiction. Thus, for any MTDS $D$ the intersection $D \cap\left\{v_{5}, v_{6}, v_{7}, v_{8}\right\}$ coincides with one of the sets $\left\{v_{5}, v_{6}\right\},\left\{v_{6}, v_{7}\right\}$, $\left\{v_{5}, v_{8}\right\}$, or $\left\{v_{7}, v_{8}\right\}$. Then

$$
\vartheta(T)=(a+1) A_{1}+A_{2}+(a+1) B_{1}+B_{2} .
$$

Denote by $T_{6}^{\prime}$ the tree obtained from $T_{6}$ by adding the leaf $v_{7}^{\prime}$ to the vertex $v_{7}$. Then the forest $F=S_{a+3} \cup T_{6}^{\prime}$ satisfies the relation

$$
\begin{aligned}
f(n) \geq \vartheta(F) & =(a+3)\left(\vartheta_{+}\left(T_{6}^{\prime}, v_{6}\right)+\vartheta_{+}\left(T_{6}^{\prime}, v_{7}^{\prime}\right)+\vartheta_{+}\left(T_{6}^{\prime}, v_{8}\right)\right) \\
& =(a+3)\left(2 \vartheta_{+}\left(T_{6}^{\prime}, v_{6}\right)+\vartheta_{+}\left(T_{6}^{\prime}, v_{8}\right)\right)=(a+3)\left(2 A_{2}+B_{2}\right)>\vartheta(T)
\end{aligned}
$$

this contradicts the assumption about the maximality of $T$.
CASE OF $p=5$. If $\mathcal{D}\left(v_{5}\right)=1$, then the vertex $v_{5}$ is universal and $T$ is separable, because $\operatorname{dist}\left(v_{2}, v_{5}\right)=3$. However, if $\mathcal{D}\left(v_{5}\right)=2$, then $v_{5}$ is adjacent to some preterminal vertex $u_{5}$ that does not lie on the backbone of $T$. By Lemma 5 , the vertex $v_{4}$ is idle in $T$, and by Corollary $1, T$ is either separable or nonmaximal; a contradiction.
Case of $p=6$. The vertex $v_{6}$ is $\varphi$-universal. Then the vertex $v_{4}$ is idle by Lemma 5 , and by Corollary $1, T$ is either separable or nonmaximal; a contradiction.
Case of $p=7$. It is clear that the vertices $v_{3}$ and $v_{7}$ are $\varphi$-universal. Then by Lemma 5 the vertex $v_{5}$ is idle. Therefore, $v_{3}$ and $v_{7}$ are universal. Each MTDS $T$ contains exactly one vertex from the set $\left\{v_{4}, v_{6}\right\}$ (because if the TDS $D$ contains both vertices, then the set $D \backslash\left\{v_{4}\right\}$ is also a TDS). Moreover, $\vartheta_{+}\left(T, v_{4}\right) \leq \vartheta_{+}\left(T, v_{6}\right)$, because for any MTDS $D^{\prime}$ the set $\left(D^{\prime} \backslash\left\{v_{4}\right\}\right) \cup\left\{v_{6}\right\}$ is an MTDS as well. Then

$$
\vartheta(T)=\vartheta_{+}\left(T, v_{4}\right)+\vartheta_{+}\left(T, v_{6}\right) \leq 2 \vartheta\left(T_{5}\right) \leq 2 f(n-a-3)<f(n) .
$$

CASE $p \geq 8$. We argue by analogy with the case of $p=4$ and $q \geq 9$. If $\gamma_{t}\left(T_{8}\right)>\widehat{\gamma}_{t}\left(T_{8}, v_{8}\right)$, then $v_{5}$ is idle, while $v_{3}$ and $v_{7}$ are universal. If the MTDS $D$ contains the vertex $v_{4}$, then it


Fig. 3. Caterpillar $T_{36}^{*}$.
does not contain $v_{6}$; otherwise, the set $\varphi(D) \backslash\left\{v_{4}\right\}$ would also be a TDS, which is impossible. If $v_{4}$ is idle, then $T$ is separable by Lemma 2 ; otherwise,

$$
\begin{aligned}
\vartheta(T) & =\vartheta_{+}\left(T, v_{4}\right)+\vartheta_{+}\left(T, v_{6}\right)=\vartheta_{-}\left(T_{6}, v_{6}\right)+\vartheta_{+}\left(T_{5}, v_{7}\right) \\
& \leq \vartheta\left(T_{6}\right)+\vartheta\left(T_{5}\right) \leq f(n-a-4)+f(n-a-3)<f(n) .
\end{aligned}
$$

Assume that $\gamma_{t}\left(T_{8}\right)=\widehat{\gamma}_{t}\left(T_{8}, v_{8}\right)$. We introduce the notation

$$
A_{1}=\vartheta_{+}\left(T_{8}, v_{8}\right), \quad A_{2}=\vartheta\left(T_{8}\right), \quad B_{1}=\widehat{\vartheta}_{+}\left(T_{8}, v_{8}\right), \quad B_{2}=\widehat{\vartheta}\left(T_{8}\right) .
$$

By analogy with the previous case, for any MTDS $D$ the intersection $D \cap\left\{v_{5}, v_{6}, v_{7}, v_{8}\right\}$ coincides with one of the sets $\left\{v_{5}, v_{6}\right\},\left\{v_{6}, v_{7}\right\},\left\{v_{5}, v_{8}\right\}$, or $\left\{v_{7}, v_{8}\right\}$. Recall that $\operatorname{deg}\left(v_{2}\right)=a+1$. Then

$$
\vartheta(T)=(a+1)\left(A_{1}+A_{2}\right)+B_{1}+B_{2} .
$$

Let us remove all leaves adjacent to $v_{2}$ and add $a-1$ new leaves to the vertex $v_{3}$; then we attach the leaf $v_{6}^{\prime}$ to the vertex $v_{6}$. The resulting $n$-vertex 2-caterpillar $T^{\prime}$ satisfies $\vartheta\left(T^{\prime}\right)=$ $(a+1)\left(2 A_{2}+B_{2}\right)$. Since $\gamma_{t}\left(T_{8}\right)=\widehat{\gamma}_{t}\left(T_{8}, v_{8}\right)$, it follows that $A_{2}>0$, whence $\vartheta\left(T^{\prime}\right)>\vartheta(T)$; this contradicts the maximality of $T$.
The proof of Theorem 1 is complete.
Note that the assertion of the theorem does not hold for the class of 3 -caterpillars. Figure 3 shows a 36 -vertex 3 -caterpillar $T_{36}^{*}$ with central vertices $u$ and $v$ that is obtained by attaching four copies of the star $S_{3}$ to each end of the path $P_{4}$. Denote by $M_{k}$ the number of MTDSs of $T_{36}^{*}$ containing $k$ central vertices. Then

$$
\vartheta\left(T_{36}^{*}\right)=M_{2}+M_{1}+M_{0}=3^{8}+2 \cdot 3^{4} \cdot\left(3^{4}-2^{4}\right)+\left(3^{4}-2^{4}\right)^{2}>3^{9}=f(36) .
$$

## 4. CLASS OF ARBITRARY TREES

It is well known that there exist $n$-vertex forests containing at least $(\sqrt{2})^{n}$ minimum dominating sets (for example, the forest $\frac{n}{2} P_{2}$ is suitable for even $n$ ). However, as will be shown in this section, each $n$-vertex tree $T$ contains fewer than $(\sqrt{2})^{n}$ minimum total dominating sets.

Lemma 8. For $n, k \geq 1$, if an $n$-vertex elementary forest $F$ contains at least $k$ connected components, then $(\sqrt{2})^{n} \geq(4 / 3)^{k} \vartheta(F)$.

Proof. Consider the function $g(m)=(\sqrt{2})^{m+1} / m$ defined on the set of positive integers. Since $g(m)$ is monotone increasing as $m \geq 3$, the inequality $g(m) \geq 4 / 3$ holds.

Let $F=S_{m_{1}} \cup S_{m_{2}} \cdots \cup S_{m_{k}}$ (we assume that $m_{1}, m_{2}, \ldots, m_{k}>0$; otherwise $\vartheta(F)=0$ and there is nothing to prove). Then

$$
\frac{(\sqrt{2})^{n}}{\vartheta(F)}=\prod_{i=1}^{k} \frac{(\sqrt{2})^{m_{i}+1}}{m_{i}}=\prod_{i=1}^{k} g\left(m_{i}\right) \geq\left(\frac{4}{3}\right)^{k}
$$

The proof of Lemma 8 is complete.

We say that a maximal $n$-vertex tree is critical if it contains at least $(\sqrt{2})^{n}$ MTDSs and for any $n^{\prime}<n$ every $n^{\prime}$-vertex tree contains fewer than $(\sqrt{2})^{n^{\prime}}$ MTDSs. It is clear from the definition that every critical tree is inseparable. Since all trees of diameter at most 4 are 2-caterpillars, it follows by Theorem 1 and Lemma 8 that they are noncritical. Thus, we assume that each critical tree has a diameter of at least 5 .

Lemma 9. For any critical tree $T$ and any diametrical path $v_{1} v_{2} \ldots v_{k}$, one has $\mathcal{D}\left(v_{4}\right)=3$.
Proof. By Lemma 4, we have $\mathcal{D}\left(v_{3}\right)=0$. Let $\mathcal{D}\left(v_{4}\right) \leq 2$. Then three cases are possible.
CASE OF $\mathcal{D}\left(v_{4}\right)=0$. Recall that $\operatorname{deg}\left(v_{2}\right)=a+1$. Then

$$
\vartheta(T)=\vartheta_{-}\left(T, v_{3}\right)+\vartheta_{+}\left(T, v_{3}\right) \leq a \vartheta\left(T_{4}\right)+\widehat{\vartheta}\left(T_{4}, v_{4}\right)
$$

Note that equality is achieved if $\vartheta_{-}\left(T, v_{3}\right)>0$; otherwise $\vartheta(T)=\widehat{\vartheta}\left(T_{4}, v_{4}\right)$. Let us show that $\gamma_{t}(T)=\gamma_{t}\left(T_{5}\right)+2$. On the one hand, each MTDS $T$ contains at least two vertices in the set $N\left[v_{2}\right]$, whence $\gamma_{t}(T) \geq \gamma_{t}\left(T_{5}\right)+2$. On the other hand, for any MTDS $D_{5}$ of tree $T_{5}$ the set $D_{5} \cup\left\{v_{2}, v_{3}\right\}$ is an MTDS of the tree $T$, whence $\gamma_{t}(T) \leq \gamma_{t}\left(T_{5}\right)+2$. Further, two cases are possible.
CASE OF $\gamma_{t}\left(T_{4}\right)>\gamma_{t}\left(T_{5}\right)$. We have $\gamma_{t}(T)=\gamma_{t}\left(T_{4}\right)+1$. Then the vertex $v_{3}$ is universal in $T$ (otherwise there would be an MTDS of $T$ of cardinality $\gamma_{t}\left(T_{4}\right)+1$ containing the vertices $v_{1}$ and $v_{2}$, which is impossible). If there exists an MTDS $D$ of the tree $T$ containing $v_{5}$, then the set $D \backslash\left\{v_{2}, v_{3}\right\}$ is an MTDS for the tree $T_{4}$, and $\gamma_{t}(T)=\gamma_{t}\left(T_{4}\right)+2$; this is a contradiction. Hence $v_{5}$ is idle in $T$. Note that if the MTDS $D$ of the tree $T$ contains the vertex $v_{4}$, then it does not contain other vertices of $N\left(v_{5}\right)$; otherwise the set $D \backslash\left\{v_{4}\right\}$ also would be a TDS. The vertex $v_{6}$ is not idle in $T$ (otherwise it is separable by Lemma 2), and for each MTDS $D \ni v_{6}$ the set $D \backslash\left\{v_{2}, v_{3}\right\}$ is an MTDS of $T_{5}$. Then $v_{6}$ is not idle in $T_{5}$ and $\partial_{+}\left(T, v_{6}\right) \leq \partial_{+}\left(T_{5}, v_{6}\right)$. Moreover, for any MTDS $D \ni v_{4}$ the set $\left(D \backslash\left\{v_{4}\right\}\right) \cup\left\{v_{6}\right\}$ is also an MTDS, whence $\vartheta_{+}\left(T, v_{4}\right) \leq \vartheta_{+}\left(T, v_{6}\right)$. Consequently,

$$
\vartheta(T) \leq \vartheta_{+}\left(T, v_{4}\right)+\vartheta_{+}\left(T, v_{6}\right) \leq 2 \vartheta_{+}\left(T_{5}, v_{6}\right) \leq 2 \vartheta\left(T_{5}\right)<2(\sqrt{2})^{n-a-3}<(\sqrt{2})^{n}
$$

CASE OF $\gamma_{t}\left(T_{4}\right)=\gamma_{t}\left(T_{5}\right)$. It can readily be seen that

$$
\vartheta\left(T_{4}\right) \leq \vartheta\left(T_{5}\right), \quad \widehat{\vartheta}_{-}\left(T_{4}, v_{4}\right)=\vartheta\left(T_{5}\right)
$$

Let us show that $\widehat{\vartheta}_{+}\left(T_{4}, v_{4}\right) \leq \vartheta\left(T_{5}\right)$. Since the vertex $v_{4}$ is a leaf in the tree $T_{4}$, we have $\gamma_{t}\left(T_{5}\right)=\widehat{\gamma}_{t}\left(T_{4}, v_{4}\right)$. Consider a set $D \subseteq V\left(T_{4}\right)$ of cardinality $\gamma\left(T_{5}\right)$ such that $v_{4} \in D$ and each vertex of $V\left(T_{4}\right) \backslash\left\{v_{4}\right\}$ has a neighbor in $D$. By definition, there exist $\widehat{\vartheta}_{+}\left(T_{4}, v_{4}\right)$ such sets. In this case, $v_{6} \notin D$ (otherwise $D \backslash\left\{v_{4}\right\}$ would be an MTDS of $T_{5}$, which is impossible). Then the set $\left(D \backslash\left\{v_{4}\right\}\right) \cup\left\{v_{6}\right\}$ is an MTDS of $T_{5}$, whence $\widehat{\vartheta}_{+}\left(T_{4}, v_{4}\right) \leq \vartheta\left(T_{5}\right)$. By assumption, $\vartheta\left(T_{5}\right)<(\sqrt{2})^{n-a-3}$. Then

$$
\vartheta(T) \leq a \vartheta\left(T_{4}\right)+\widehat{\vartheta}\left(T_{4}, v_{4}\right) \leq(a+2) \vartheta\left(T_{5}\right)<(a+2)(\sqrt{2})^{n-a-3}<(\sqrt{2})^{n}
$$

CASE of $\mathcal{D}\left(v_{4}\right)=2$. The vertex $v_{4}$ is adjacent to some preleaf $u_{4}$. Then $\operatorname{dist}\left(v_{2}, u_{4}\right)=3$, and the tree $T$ is separable by Lemma 3 .
CASE OF $\mathcal{D}\left(v_{4}\right)=1$. In this case, $v_{4}$ is adjacent to some leaf $v_{4}^{\prime}$ and is not adjacent to preleaves. We assume that the vertex $v_{5}$ is not idle and not universal in $T$ (otherwise $T$ would be separable by Lemmas 2 and 3). There are two cases.
CASE of $\operatorname{deg}\left(v_{4}\right)=3$. Note that if the MTDS of the tree $T$ contains the vertex $v_{5}$, then it can contain any vertex of the neighborhood $N\left(v_{2}\right)$. If, however, the MTDS does not contain $v_{5}$, then it contains the vertex $v_{3}$. Then

$$
\vartheta(T)=\vartheta_{+}\left(T, v_{5}\right)+\vartheta_{-}\left(T, v_{5}\right)=(a+1) \vartheta_{+}\left(T_{4}, v_{5}\right)+\vartheta\left(F_{5}\right) \leq(a+1) \vartheta\left(T_{4}\right)+\vartheta\left(F_{5}\right)
$$

If $\vartheta\left(T_{4}\right) \geq 2 \vartheta\left(F_{5}\right)$, then $\vartheta(T) \leq(a+3 / 2) \vartheta\left(T_{4}\right)<(a+3 / 2)(\sqrt{2})^{n-a-2}$. If, however, $\vartheta\left(T_{4}\right)<2 \vartheta\left(F_{5}\right)$, then $\vartheta(T)<(2 a+3) \vartheta\left(F_{5}\right)<(2 a+3)(\sqrt{2})^{n-a-5}$. One can readily verify that in both cases for all integer $a \geq 1$ one has the inequality $\vartheta(T)<(\sqrt{2})^{n}$.
CASE OF $\operatorname{deg}\left(v_{4}\right) \geq 4$. By $F_{0}$ we denote the forest $T \backslash\left(V\left(T_{5}\right) \cup\left\{v_{4}, v_{4}^{\prime}\right\}\right)$. Set $Q=\vartheta\left(F_{0}\right)$ and $q=\left|V\left(F_{0}\right)\right|$. Note that $F_{0}$ is an elementary forest that consists of at least $\operatorname{deg}\left(v_{4}\right)-2 \geq 2$ connected components. Then by Lemma 8 we have $(\sqrt{2})^{q} / Q \geq 16 / 9$. Since $\vartheta\left(T_{4}\right) \leq(\sqrt{2})^{n-q}$ and $\vartheta\left(F_{5}\right) \leq(\sqrt{2})^{n-q-3}$, we have

$$
\begin{aligned}
\vartheta(T) & =\vartheta_{+}\left(T, v_{5}\right)+\vartheta_{-}\left(T, v_{5}\right) \\
& \leq Q\left(\vartheta\left(T_{4}\right)+\vartheta\left(F_{5}\right)\right) \leq \frac{9}{16}(\sqrt{2})^{q}\left((\sqrt{2})^{n-q}+(\sqrt{2})^{n-q-3}\right)<(\sqrt{2})^{n} .
\end{aligned}
$$

The proof of Lemma 9 is complete.
Lemma 10. For any critical tree $T$ and any of its diametrical paths $v_{1} v_{2} \ldots v_{k}$, one has $\mathcal{D}\left(v_{5}\right) \in\{0,4\}$.

Proof. By Lemmas 4 and $9, \mathcal{D}\left(v_{3}\right)=0$ and $\mathcal{D}\left(v_{4}\right)=3$. Suppose that $\mathcal{D}\left(v_{5}\right) \notin\{0,4\}$. Three cases are possible.
Case of $\mathcal{D}\left(v_{5}\right)=1$. The vertex $v_{5}$ is preleaf. Then $T$ is separable, because $\operatorname{dist}\left(v_{2}, v_{5}\right)=3$; a contradiction.
CASE OF $\mathcal{D}\left(v_{5}\right)=2$. The vertex $v_{5}$ is adjacent to some preleaf vertex $u_{5}$ different from $v_{4}$ and $v_{6}$. Since $\mathcal{D}\left(v_{4}\right)=3$, all neighbors of the vertex $v_{4}$ are adjacent to preleaves. Then, by Lemma 5 , the vertex $v_{4}$ is idle. By Corollary 1 , the tree $T$ is not critical; a contradiction.
CASE OF $\mathcal{D}\left(v_{5}\right)=3$. The vertex $v_{5}$ is adjacent to some vertex $u_{4}$ whose neighbor $u_{3}$ is a preleaf. Note that if $u_{3}$ is not a preterminal vertex, then it is adjacent to some preterminal vertex $u_{2}$ as well as to the leaf $u_{3}^{\prime}$. Then the tree $T$ is not critical by Lemma 4 ; a contradiction. Hence the vertex $u_{3}$ is preterminal, and the vertex $u_{4}$ is $\varphi$-universal in $T$. Then the vertex $v_{4}$ is idle by Lemma 5 , and, by Corollary 1 , the tree $T$ is not critical, a contradiction.
The proof of Lemma 10 is complete.
Theorem 2. For $n \geq 1$, the inequality $\vartheta(T)<(\sqrt{2})^{n}$ holds for any $n$-vertex tree $T$.
Proof. For $n \leq 9$, all $n$-vertex trees are 2-caterpillars, and so they satisfy the condition of the theorem. Suppose that for $n \geq 10$ there exists an $n$-vertex critical tree $T$. Denote by $P=v_{1} v_{2} \ldots v_{k}$ some diametrical path $T$. Then by Lemmas 4,9 , and 10 we have $\mathcal{D}\left(v_{3}\right)=0, \mathcal{D}\left(v_{4}\right)=3$, and $\mathcal{D}\left(v_{5}\right) \in\{0.4\}$. We assume that the vertex $v_{5}$ is adjacent to the vertex $v_{6}$ and also to some vertices $v_{4}^{1}, \ldots, v_{4}^{k}$ (here $\left.v_{4}=v_{4}^{1}\right)$. There are 6 possible cases depending on the value of $\mathcal{D}\left(v_{6}\right)$.
Case of $\mathcal{D}\left(v_{6}\right)=1$. The vertex $v_{6}$ is a preleaf. Then, by Lemma 5 , the vertex $v_{4}$ is idle and, by Corollary 1, the tree $T$ is not critical; a contradiction.
CASE OF $\mathcal{D}\left(v_{6}\right)=2$. The vertex $v_{6}$ is adjacent to some preleaf $u_{5}$. Then, by Lemma 5 , the vertex $v_{5}$ is idle. Denote by $F_{0}$ an elementary forest $T \backslash\left(V\left(T_{6}\right) \cup N\left[v_{5}\right]\right)$. If the vertex $v_{6}$ is not idle in $T_{6}$, then $\gamma_{t}(T)=\gamma_{t}\left(T_{6}\right)+\gamma_{t}\left(F_{0}\right)$. Then the vertex $v_{4}$ is idle in $T$ and $T$ is separable by Lemma 2; a contradiction. If, however, the vertex $v_{6}$ is idle in $T_{6}$, then $\gamma_{t}(T)=\gamma_{t}\left(T_{6}\right)+$ $\gamma_{t}\left(F_{0}\right)+1$. For each $i \in 1, \ldots, k$, from $T$ we delete all edges incident with the vertex $v_{4}^{i}$ except for the edge $v_{4}^{i} v_{5}$. Then the resulting forest $F$ satisfies the equality $\gamma_{t}(F)=\gamma_{t}\left(T_{6}\right)+$ $\gamma_{t}\left(F_{0}\right)+2$, and for any MTDS $D$ of the tree $T$ the set $D \cup\left\{v_{5}\right\}$ is an MTDS of the forest $F$. Thus, $(\sqrt{2})^{n}>\vartheta(F) \geq \vartheta(T)$; a contradiction.
Case of $\mathcal{D}\left(v_{6}\right)=3$. The vertex $v_{6}$ is adjacent to some vertex $u_{5}$ whose neighbor $u_{4}$ is a preleaf. Let us assume that $u_{4}$ is not a preterminal vertex. If there exists a diametrical path $P^{\prime}=u_{1} u_{2} u_{3} u_{4} u_{5} v_{6} \ldots v_{k}$ in $T$, then $\mathcal{D}_{T, P^{\prime}}\left(u_{4}\right)=1$; this contradicts Lemma 9. Otherwise, the vertex $u_{4}$ is adjacent to at least one leaf $u_{4}^{\prime}$ and at least one preterminal vertex. Then, by Lemma 4, the tree $T$ is not critical; a contradiction.


Fig. 4. Structure of tree $T$ in the case of $\mathcal{D}\left(v_{6}\right)=0$.

Thus, the vertex $u_{4}$ is preterminal in $T$. Then the vertex $u_{5}$ is $\varphi$-universal and by Lemma 5 , the vertex $v_{5}$ is idle in $T$. We act by analogy with the previous case. If the vertex $v_{6}$ is not idle in $T_{6}$, then the vertex $v_{4}$ is idle in $T$ and, by Lemma 2, the tree $T$ is separable; a contradiction. Otherwise, for each $i \in 1, \ldots, k$ we remove all edges incident to the vertex $v_{4}^{i}$ except for the edge $v_{4}^{i} v_{5}$. Then for any MTDS $D$ of the tree $T$ the set $D \cup\left\{v_{5}\right\}$ is an MTDS of the resulting forest $F$, whence $(\sqrt{2})^{n}>\vartheta(F) \geq \vartheta(T)$; a contradiction.
CASE OF $\mathcal{D}\left(v_{6}\right)=5$. In this case, there exists some diametrical path $P^{\prime}=u_{1} u_{2} u_{3} u_{4} u_{5} v_{6} \ldots v_{k}$, where $u_{5}$ is different from $v_{5}$ and $v_{7}$. By Lemmas 9 and $10, \mathcal{D}_{T, P^{\prime}}\left(u_{4}\right)=3$ and $\mathcal{D}_{T, P^{\prime}}\left(u_{5}\right) \in\{0,4\}$. Assume that there exists an MTDS $D$ that does not contain $v_{6}$. Then the set

$$
\left(\varphi(D) \backslash\left(N\left(v_{5}\right) \cup N\left(u_{5}\right)\right)\right) \cup\left\{v_{6}\right\}
$$

is also a TDS and is less than $D$ in cardinality; a contradiction. Thus, the vertex $v_{6}$ is universal in $T$. Then the vertex $v_{4}$ is idle by Lemma 5 and, by Corollary 1 , the tree $T$ is not critical; a contradiction.
Case of $\mathcal{D}\left(v_{6}\right)=0$. In this case, $T$ has the structure depicted in Fig. 4. We introduce the notation

$$
A_{1}=\vartheta_{-}\left(T_{7}, v_{7}\right), \quad A_{2}=\vartheta\left(F_{7}\right), \quad B_{1}=\vartheta_{+}\left(T_{7}, v_{7}\right), \quad B_{2}=\widehat{\vartheta}_{+}\left(T_{7}, v_{7}\right) .
$$

Denote by $T_{5}^{\prime}$ the inclusion-maximal subtree $T$ that contains the vertex $v_{5}$ but does not contain the vertices $v_{4}^{1}, \ldots, v_{4}^{k}$. Denote by $F_{0}$ the elementary forest obtained by deleting all vertices of the subtree $T_{6}$ and the neighborhood $N\left[v_{5}\right]$ from the tree $T$. Let $Q=\vartheta\left(F_{0}\right)$ and $q=\left|V\left(F_{0}\right)\right|$. Obviously, $\gamma_{t}(T)=\gamma_{t}\left(T_{5}^{\prime}\right)+\gamma_{t}\left(F_{0}\right)$. Then each MTDS of the tree $T$ contains exactly two vertices of the set $N\left[v_{5}\right] \cup N\left[v_{6}\right]$, which are either adjacent or at a distance of 3 from each other. Note that if $A_{1} \geq A_{2}$, then the pair $\left\{v_{4}^{i}, v_{5}\right\}$ cannot be included in the MTDS. Similarly, if $B_{1} \geq B_{2}$, then the pair $\left\{v_{5}, v_{6}\right\}$ cannot be included in the MTDS. Then

$$
\vartheta(T) \leq Q\left(k \cdot \min \left(A_{1}, A_{2}\right)+A_{2}+k \cdot \min \left(B_{1}, B_{2}\right)+B_{2}\right) .
$$

Since $\vartheta\left(T_{5}^{\prime}\right)=\left(A_{2}+B_{2}\right)<(\sqrt{2})^{n-q-k}$, we have $\left(A_{2}+B_{2}\right)(\sqrt{2})^{q+k}<(\sqrt{2})^{n}$. Then it suffices to prove that

$$
\left(A_{2}+B_{2}\right)(\sqrt{2})^{q+k}>Q(k+1)\left(A_{2}+B_{2}\right) .
$$

Since $\mathcal{D}\left(v_{4}\right)=3$, it follows that the forest $F$ contains at least two connected components and $(\sqrt{2})^{q} / Q \geq(4 / 3)^{2}$. On the other hand, $(\sqrt{2})^{k} /(k+1) \geq 2 / 3$, whence we obtain the desired inequality.
Case of $\mathcal{D}\left(v_{6}\right)=4$. In this case, $T$ has the structure shown in Fig. 5. If there exists some diametrical path $P^{\prime}=u_{1} u_{2} u_{3} u_{4} u_{5} v_{6} v_{7} \ldots v_{s}$, where the vertex $u_{5}$ differs from $v_{5}$, then we apply the arguments from the case of $\mathcal{D}\left(v_{6}\right)=5$. Otherwise, the vertex $v_{6}$ is adjacent to some vertices $u_{5}^{1}, \ldots, u_{5}^{m}$ (where $m \geq 1$ ) all of whose neighbors except for the vertex $v_{6}$ have degree 2 and are adjacent to some terminal vertices. Let us introduce the notation $A_{1}, A_{2}, B_{1}, B_{2}, Q, q$ by analogy with the previous case. Denote by $F_{0}^{\prime}$ the elementary forest obtained by removing all vertices of the subtree $T_{7}$ and the neighborhood $N\left[v_{6}\right]$ from the tree $T_{6}$. Let $W=\vartheta\left(F_{0}^{\prime}\right)$ and $w=\left|V\left(F_{0}^{\prime}\right)\right|$. Each MTDS of the tree $T$ contains exactly two vertices of the set $N\left[v_{5}\right] \cup N\left[v_{6}\right]$ that are either adjacent or at a distance of 3 from each other. Then

$$
\vartheta(T) \leq Q W\left(k(m+1) \min \left(A_{1}, A_{2}\right)+m A_{2}+A_{2}+k \cdot \min \left(B_{1}, B_{2}\right)+B_{2}\right) .
$$



Fig. 5. Structure of tree $T$ in the case of $\mathcal{D}\left(v_{6}\right)=4$.

Denote by $T_{5}^{\prime \prime}$ the inclusion-maximal subtree of the tree $T_{5}$ that contains the vertices $v_{5}$ and $v_{6}$ and does not contain the vertices $v_{4}^{1}, \ldots, v_{4}^{k}$ and $u_{5}^{1}, \ldots, u_{5}^{m}$. Then

$$
\vartheta\left(T_{5}^{\prime \prime}\right)=\vartheta_{+}\left(T_{5}^{\prime \prime}, v_{5}\right)+\vartheta_{+}\left(T_{5}^{\prime \prime}, v_{7}\right)=A_{2}+B_{2}<(\sqrt{2})^{n-q-w-k-m}
$$

Let us show that

$$
\left(A_{2}+B_{2}\right)(\sqrt{2})^{q+w+k+m}>Q W\left((k+1) m A_{2}+(m+1) A_{2}+k B_{2}+B_{2}\right)
$$

We assume that $A_{2} \leq B_{2}$. Then it suffices to prove the inequality

$$
(\sqrt{2})^{q+w+k+m}>Q W(k+1)(m+1)
$$

By Lemma 9, the forest $F \cup F^{\prime}$ contains at least three connected components. Then

$$
\frac{(\sqrt{2})^{q+w+k+m}}{Q W(k+1)(l+1)}=\frac{(\sqrt{2})^{q+w}}{Q W} \frac{(\sqrt{2})^{k+m}}{(k+1)(m+1)} \geq\left(\frac{4}{3}\right)^{3}\left(\frac{2}{3}\right)^{2}>1
$$

Thus, $\vartheta(T)<(\sqrt{2})^{n}$.
The proof of Theorem 2 is complete.

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