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# The average order of a subtree of a tree 

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## A R T I C L E I N F O

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#### Abstract

Let $T$ be a tree all of whose internal vertices have degree at least three. In 1983 Jamison conjectured in JCT B that the average order of a subtree of $T$ is at least half the order of $T$. In this paper a proof is provided. In addition, it is proved that the average order of a subtree of $T$ is at most three quarters the order of $T$. Several open questions are stated.


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## 1. Introduction

The order of a tree is the number of its vertices. The following notation will be used throughout the paper. For a tree $T$, its order is denoted $n:=n(T)$ and the number of leaves $n^{\prime}:=n^{\prime}(T)$. This paper concerns the average order of a subtree of a tree $T$. If $T$ has $N$ subtrees (not including the empty tree) of orders $n_{1}, n_{2}, \ldots, n_{N}$, then let

$$
\mu_{T}:=\frac{1}{N} \sum_{i=1}^{N} n_{i}
$$

denote the average order of subtrees of $T$. If $T$ has order $n$, call

$$
D_{T}:=\frac{\mu_{T}}{n}
$$

the density of $T$. The density allows us to compare average subtree order of trees of different sizes. The density is also the probability that a vertex chosen at random from $T$ will belong to a randomly chosen subtree of $T$. In [1] Jamison conjectured that if $T$ is a tree whose internal vertices have degree at least three, then the average order of a subtree is at least half the order of $T$. In other words, for

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Fig. 1. Star $S_{n}$.


Fig. 2. Caterpillar $C_{j}$ with $j+2$ leaves.
such a tree, $D_{T} \geqslant \frac{1}{2}$. The bound given below is the main result of this paper. The proof of the lower bound appears in Section 2 and the proof of the upper bound in Section 3.

Theorem 1. If $T$ is a tree all of whose internal vertices have degree at least three, then

$$
\frac{1}{2} \leqslant D_{T}<\frac{3}{4}
$$

Both bounds are best possible in the sense that there exists an infinite sequence $\left\{S_{n}\right\}$ of trees such that $\lim _{n \rightarrow \infty} D_{S_{n}}=1 / 2$ and a sequence $\left\{C_{j}\right\}$ of trees such that $\lim _{j \rightarrow \infty} D_{C_{j}}=3 / 4$. The sequence $S_{n}$ of stars of order $n$, shown in Fig. 1, is an example in the first case. The sequence $\left\{C_{j}\right\}$ of caterpillars with $j+2$ leaves shown in Fig. 2 is an example in the second case. In fact, the exact formula for the density

$$
D_{C_{j}}=\frac{27 j 2^{j-1}-3 \cdot 2^{j+2}+4 j+16}{(2 j+2)\left(9 \cdot 2^{j}-j-6\right)}
$$

can be derived using the recursions in Lemma 1 . (The somewhat complicated derivation involves solving recurrences giving the parameters of $C_{j+1}$ in terms of the parameters of $C_{j}$. The recurrences are obtained by taking the root in Lemma 1 as a vertex of degree 3 at one of the two ends of the caterpillar.)

This paper concerns exclusively those trees whose internal vertices have degree at least 3 . They are also referred to as homeomorphically irreducible trees and series reduced trees. Let this family of trees be denoted $\mathcal{T}_{3}$. It is known [1] that, for trees in general (no restriction on the degrees), the tree of order $n$ that minimizes the average order is the path $P_{n}$, in which case $\mu_{P_{n}}=(n+2) / 3$. Therefore, for trees in general, $D_{T} \geqslant 1 / 3$, and this is best possible. Examples appear in [1] of sequences $\left\{T_{j}\right\}$ of trees such that $D_{T_{j}} \rightarrow 1$ as $j \rightarrow \infty$. So, in the general case, the trivial upper bound $D_{T} \leqslant 1$ is best possible.

Concerning trees whose internal vertices have degree at least 3 , several questions remain open. The first question concerns the upper bound of $3 / 4$ on the density. Consider the ratio $\operatorname{diam}(T) / n^{\prime}(T)$ of the diameter to the number of leaves of a tree $T$ in $\mathcal{T}_{3}$. The ratio $\operatorname{diam}(T) / n^{\prime}(T)$ is close to 1 if and only if both $n^{\prime}(T) / n(T)$ is close to $1 / 2$ and $\operatorname{diam}(T) / n(T)$ is close to $1 / 2$. Moreover, $n^{\prime}(T) / n(T)$ is close to $1 / 2$ if and only if the average degree of an internal vertex is close to 3 , and $\operatorname{diam}(T) / n(T)$ is close to $1 / 2$ if and only if $T$ is "stretched out." This motivates the following question.

Question 1. Is it the case that a sequence $\left\{T_{j}\right\}$ of distinct trees in $\mathcal{T}_{3}$ satisfies

$$
\lim _{j \rightarrow \infty} D_{T_{j}}=\frac{3}{4}
$$

if and only if $\operatorname{diam}\left(T_{j}\right) / n^{\prime}\left(T_{j}\right) \rightarrow 1$ ?


Fig. 3. Joining $k$ copies of $C_{h}$.


Fig. 4. Complete $k$-ary tree of height $h(k=4$ and $h=3)$.
The next two questions concern the lower bound of $1 / 2$ on the density.
Question 2. For a sequence $\left\{T_{j}\right\}$ of distinct trees in $\mathcal{T}_{3}$, what are necessary and sufficient conditions for $D_{T_{j}} \rightarrow 1 / 2$ ?

Consider the following two conditions on a sequence $\left\{T_{j}\right\}$ of distinct trees in $\mathcal{T}_{3}$.

1. Bounded diameter. There is a number $B$ such that $\operatorname{diam}(T) \leqslant B$ for all $T \in\left\{T_{j}\right\}$.
2. Unbounded degree. For any number $B$ there is a $T \in\left\{T_{j}\right\}$ and a vertex $v$ of $T$ such that $\operatorname{deg}(v) \geqslant B$.

Clearly the bounded diameter condition implies the unbounded degree condition. However, even the bounded diameter condition is not a sufficient condition for $D_{T_{j}} \rightarrow 1 / 2$ as $j \rightarrow \infty$. An example is as follows. Fix integer $h$, and let $C_{h}$ be the caterpillar defined above, with $v_{0}$ an arbitrarily chosen vertex of $C_{h}$. Using $k$ disjoint copies of $C_{h}$, let $T_{k}$ be the tree formed by joining the $k$ copies of the vertex $v_{0}$ in the caterpillars to an isolated vertex $v$. See Fig. 3. It can be shown using Lemma 1 that, for $h$ sufficiently large, $D_{T_{k}} \nrightarrow 1 / 2$ as $k \rightarrow \infty$. But clearly $\left\{T_{k}\right\}$ has bounded diameter.

There are certainly sequences $\left\{T_{j}\right\}$ of bounded diameter for which $D_{T_{j}} \rightarrow 1 / 2$ as $j \rightarrow \infty$. For example, let $h$ be fixed and let $T_{k}$ be the complete $k$-ary tree of height $h$ (see Fig. 4) or simply consider the sequence $\left\{S_{j}\right\}$ of stars on $j$ vertices. Then calculation using Lemma 1 shows that $D_{T_{k}} \rightarrow 1 / 2$ as $k \rightarrow \infty$. This motivates the following question.

Question 3. For a sequence $\left\{T_{j}\right\}$ of trees in $\mathcal{T}_{3}$, is either the bounded diameter or the unbounded degree condition a necessary condition for $D_{T_{j}} \rightarrow 1 / 2$ ?

Moon and Meir [2] determined the average density over all trees of order $n$ to be $1-e^{-1} \approx .6321$ as $n \rightarrow \infty$.

Question 4. What is the limit of the average density over all trees in $\mathcal{T}_{3}$ of order $n$ as $n \rightarrow \infty$ ?

## 2. Proof of the lower bound

A tree with no internal vertices of degree 2 satisfies the first of the following inequalities, and if there is at most one internal node of degree 2 , then the second

$$
\begin{equation*}
2 n^{\prime} \geqslant n+2, \quad 2 n^{\prime} \geqslant n+1 . \tag{1}
\end{equation*}
$$

A root of a tree is a designated vertex, its children the adjacent vertices.
(*) It is assumed throughout this section that each internal vertex, with the possible exception of the root, has degree at least 3. The root is assumed to have degree at least 2.

For a tree rooted at vertex $v$, the number of subtrees containing the root, and the number not containing the root, are denoted $N(v)$ and $\bar{N}(v)$, respectively. Each subset $L$ of leaves of a tree rooted at $v$ determines a unique subtree containing $v$, i.e., the subtree whose vertices are those with a descendant in $L$. Thus there is an injection from the set of subsets of leaves into the set of rooted subtrees, giving $N(v) \geqslant 2^{n^{\prime}}$. Clearly, if the tree is not a star rooted at the center, then the inequality is strict

$$
\begin{equation*}
N(v)>2^{n^{\prime}} \tag{2}
\end{equation*}
$$

The average order of a subtree containing the root, and not containing the root, are denoted $\mu(v)$ and $\bar{\mu}(v)$, respectively. The following formula relates the parameters of the unrooted tree to those of the rooted tree

$$
\mu_{T}=\frac{\mu(v) N(v)+\bar{\mu}(v) \bar{N}(v)}{N(v)+\bar{N}(v)}
$$

Letting $D(v)=\mu(v) / n$ and $\bar{D}(v)=\bar{\mu}(v) / n$ denote the densities for subtrees containing and not containing the root, respectively, the above equation becomes

$$
\begin{equation*}
D_{T}=\frac{D(v) N(v)+\bar{D}(v) \bar{N}(v)}{N(v)+\bar{N}(v)} \tag{3}
\end{equation*}
$$

If $v_{1}, v_{2}, \ldots, v_{k}$ are the children of the root $v$, let $T_{1}, T_{2}, \ldots, T_{k}$ denote the connected components of $T-v$, considered as trees rooted at $v_{1}, v_{2}, \ldots, v_{k}$, respectively. Let $N_{i}, \bar{N}_{i}, \mu_{i}, \bar{\mu}_{i}$ denote the number of subtrees of $T_{i}$ containing the root $v_{i}$, not containing the root, the average order of those containing the root, and not containing the root, respectively.

Lemma 1. The following recursive formulas are valid for a rooted tree:

$$
\begin{array}{ll}
N(v)=\prod_{i=1}^{k}\left(N_{i}+1\right), & \mu(v)=1+\sum_{i=1}^{k} \mu_{i} \frac{N_{i}}{N_{i}+1}, \\
\bar{N}(v)=\sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right), & \bar{\mu}(v)=\frac{\sum_{i=1}^{k}\left(\mu_{i} N_{i}+\bar{\mu}_{i} \bar{N}_{i}\right)}{\sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right)} .
\end{array}
$$

Proof. The recursion for $\bar{N}(v)$ is clear. The recursion for $N(v)$ comes from the fact that there is an obvious bijection between the set of subtrees rooted at $v$ and the set of $k$-element subsets $\left\{t_{1}, t_{2}, \ldots, t_{k}\right\}$ where $t_{i}$ is a rooted subtree of $T_{i}$ - including the empty tree.

Concerning the recursion for $\mu(v)$, let $S$ be the sum of the orders of all rooted subtrees of $T$. As explained above, each rooted subtree $t_{i}$ of $T_{i}$ is contained in exactly $\prod_{j \neq i}\left(N_{j}+1\right)$ rooted subtrees of $T$. The subtree $t_{i}$ therefore contributes $n\left(t_{i}\right) \prod_{j \neq i}\left(N_{j}+1\right)$ toward the sum $S$. Hence all the subtrees of $T_{i}$ combined contribute $\mu_{i} N_{i} \prod_{j \neq i}\left(N_{j}+1\right)$. Summing over all subtrees $T_{1}, T_{2}, \ldots, T_{k}$ gives

$$
S=\sum_{i=1}^{k} \mu_{i} N_{i} \prod_{j \neq i}\left(N_{j}+1\right)+N(v)
$$

the term $N(v)$ being the contribution from the root $v$. Hence, using the recursion for $N(v)$,

$$
\mu(v)=\frac{\sum_{i=1}^{k} \mu_{i} N_{i} \prod_{j \neq i}\left(N_{j}+1\right)+N(v)}{N(v)}=1+\sum_{i=1}^{k} \mu_{i} \frac{N_{i}}{N_{i}+1}
$$



Fig. 5. Figure $a$ (on the left) and $b$ (on the right).

The recursion for $\bar{\mu}(v)$ is clear by splitting the subtrees of the $T_{i}$ into those that contain and do not contain their root, respectively.

Lemma 2. If $T$ is a tree rooted at vertex $v$, then $N(v)>\bar{N}(v)$.

Proof. It is easy to verify by induction that, for any positive integers $N_{i}$, it is the case that $\prod_{i=1}^{k}\left(N_{i}+1\right) \geqslant 2 \sum_{i=1}^{k} N_{i}$ if $k \geqslant 2$. The first case $k=2$ is equivalent to $\left(N_{1}-1\right)\left(N_{2}-1\right) \geqslant 0$. The induction step from $k-1$ to $k$ is equivalent to $N_{k} \geqslant 2$.

The statement of the lemma is again proved by induction, on the order of $T$. It is trivially true for the tree of order 1 (a single vertex). Applying this inequality above, the induction hypothesis, and Lemma 1 to any tree $T$ satisfying our assumption (*) gives

$$
N(v)=\prod_{i=1}^{k}\left(N_{i}+1\right) \geqslant 2 \sum_{i=1}^{k} N_{i}>\sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right)=\bar{N}(v) .
$$

Lemma 3. If $T$ is a tree rooted at vertex $v$ then, except for the graph in Fig. 5b, we have

$$
D(v) \geqslant \frac{1}{2}\left(1+\frac{1}{n^{\prime}+1}\right)
$$

Proof. Let $T_{1}, \ldots, T_{k}$ be the subtrees as defined earlier. Let $k_{1}$ be the number of such subtrees of order $1, k_{2}$ the number isomorphic to the rooted tree in Fig. 5a, and $k_{3}$ the number isomorphic to the rooted tree in Fig. 5b. Let $T_{1}, \ldots, T_{k^{\prime}}$ be the remaining subtrees. The proof proceeds by induction on the order of the tree $T$. It is easy to check that the statement is true for the rooted tree of order 1 and the rooted tree of order 3. (The rooted tree of order 2 is not relevant because the root is assumed to have at least 2 children.) Applying the induction hypothesis to the recursion for $\mu(v)$ in Lemma 1 yields the following. The induction hypothesis can be used in the second inequality below because each tree $T_{i}, i=1,2 \ldots, k^{\prime}$, is not the tree in Fig. 5b. Inequality (2) implies $N_{i} \geqslant 2^{n_{i}^{\prime}}+1 \geqslant 2 n_{i}^{\prime}+2$ for subtrees $T_{i}$ with $n_{i}^{\prime} \geqslant 3$, which is also used

$$
\begin{aligned}
\mu(v) & =1+\sum_{i=1}^{k} \mu_{i} \frac{N_{i}}{N_{i}+1}=1+\frac{1}{2} k_{1}+\frac{8}{5} k_{2}+\frac{31}{11} k_{3}+\sum_{i=1}^{k^{\prime}} \mu_{i} \frac{N_{i}}{N_{i}+1} \\
& \geqslant 1+\frac{1}{2} k_{1}+\frac{8}{5} k_{2}+\frac{31}{11} k_{3}+\frac{1}{2} \sum_{i=1}^{k^{\prime}}\left(1+\frac{1}{n_{i}^{\prime}+1}\right) n_{i} \frac{N_{i}}{N_{i}+1} \\
& \geqslant 1+\frac{1}{2} k_{1}+\frac{8}{5} k_{2}+\frac{31}{11} k_{3}+\frac{1}{2} \sum_{i=1}^{k^{\prime}}\left(1+\frac{1}{n_{i}^{\prime}+1}\right)\left(\frac{2 n_{i}^{\prime}+2}{2 n_{i}^{\prime}+3}\right) n_{i} \\
& \geqslant 1+\frac{1}{2} k_{1}+\frac{8}{5} k_{2}+\frac{31}{11} k_{3}+\sum_{i=1}^{k^{\prime}} \frac{n_{i}^{\prime}+2}{2 n_{i}^{\prime}+3} n_{i} .
\end{aligned}
$$

To prove that $\mu(v) \geqslant \frac{1}{2}\left(1+\frac{1}{n^{\prime}+1}\right) n$ it now suffices to prove

$$
\begin{aligned}
1 & +\frac{1}{2} k_{1}+\frac{8}{5} k_{2}+\frac{31}{11} k_{3}+\sum_{i=1}^{k^{\prime}} \frac{n_{i}^{\prime}+2}{2 n_{i}^{\prime}+3} n_{i} \\
& \geqslant \frac{1}{2}\left(1+k_{1}+3 k_{2}+5 k_{3}+\sum_{i=1}^{k^{\prime}} n_{i}+\frac{1+k_{1}+3 k_{2}+5 k_{3}+\sum_{i=1}^{k^{\prime}} n_{i}}{1+k_{1}+2 k_{2}+3 k_{3}+\sum_{i=1}^{k^{\prime}} n_{i}^{\prime}}\right),
\end{aligned}
$$

which simplifies to

$$
\begin{equation*}
1+\frac{1}{5} k_{2}+\frac{7}{11} k_{3}+\sum_{i=1}^{k^{\prime}} \frac{n_{i}}{2 n_{i}^{\prime}+3} \geqslant \frac{1+k_{1}+3 k_{2}+5 k_{3}+\sum_{i=1}^{k^{\prime}} n_{i}}{1+k_{1}+2 k_{2}+3 k_{3}+\sum_{i=1}^{k^{\prime}} n_{i}^{\prime}} . \tag{4}
\end{equation*}
$$

To prove the inequality above, first consider the case $k^{\prime}=0$. In this case it is sufficient to show that

$$
f\left(k_{1}, k_{2}, k_{3}\right):=\left(1+\frac{1}{5} k_{2}+\frac{7}{11} k_{3}\right)\left(1+k_{1}+2 k_{2}+3 k_{3}\right)-\left(1+k_{1}+3 k_{2}+5 k_{3}\right) \geqslant 0 .
$$

Since we are assuming throughout this section that the root has degree at least 2 , we have $k_{1}+k_{2}+k_{3} \geqslant 2$. It is easy to check that $f\left(k_{1}, k_{2}, k_{3}\right) \geqslant 0$ for all values where $k_{1}+k_{2}+k_{3}=2$. Taking partial derivatives reveals that $f\left(k_{1}, k_{2}, k_{3}\right)$ is non-decreasing with respect to $k_{1}$ for all $k_{1}, k_{2}, k_{3} \geqslant 0$ and non-decreasing with respect to both $k_{2}$ and $k_{3}$ if either $k_{2} \geqslant 1$ or $k_{3} \geqslant 1$. This implies that $f\left(k_{1}, k_{2}, k_{3}\right) \geqslant 0$ for all values where $k_{1}+k_{2}+k_{3} \geqslant 2$.

Next consider the case $k^{\prime}>0$. From the paragraph above, either $f\left(k_{1}, k_{2}, k_{3}\right) \geqslant 0$ or $k_{1}=k_{3}=0$, $k_{2}=1$. In either case, a little elementary algebra shows that inequality (4) holds if

$$
1+\sum_{i=1}^{k^{\prime}} \frac{n_{i}}{2 n_{i}^{\prime}+3} \geqslant \frac{1+\sum_{i=1}^{k^{\prime}} n_{i}}{1+\sum_{i=1}^{k^{\prime}} n_{i}^{\prime}} .
$$

Since $n_{i} \geqslant n_{i}^{\prime}+1$, we have $\frac{n_{i}}{2 n_{i}^{+}+3}>\frac{1}{3}$. Also, since $2 n_{i}^{\prime} \geqslant n_{i}+1$ from inequality ( 1 ), we have $2>\frac{1+\sum_{i=1}^{k^{\prime}} n_{i}}{1+\sum_{i=1}^{k_{i}^{\prime}} n_{i}^{\prime}}$. Therefore, if $k^{\prime} \geqslant 3$, then

$$
1+\sum_{i=1}^{k^{\prime}} \frac{n_{i}}{2 n_{i}^{\prime}+3}>1+3(1 / 3)=2>\frac{1+\sum_{i=1}^{k^{\prime}} n_{i}}{1+\sum_{i=1}^{k^{\prime}} n_{i}^{\prime}} .
$$

This only leaves the case $k^{\prime} \leqslant 2$, in which case we need to show

$$
1+\frac{n_{1}}{2 n_{1}^{\prime}+3} \geqslant \frac{1+n_{1}}{1+n_{1}^{\prime}} \quad \text { and } \quad 1+\frac{n_{1}}{2 n_{1}^{\prime}+3}+\frac{n_{2}}{2 n_{2}^{\prime}+3} \geqslant \frac{1+n_{1}+n_{2}}{1+n_{1}^{\prime}+n_{2}^{\prime}} .
$$

The case $k^{\prime}=1$ (on the left) simplifies to $n_{1}^{\prime}\left(2 n_{1}^{\prime}+3\right) \geqslant n_{1}\left(n_{1}^{\prime}+2\right)$, which in turn follows from the fact that $2 n_{1}^{\prime} \geqslant n_{1}+1$ from inequality (1). Although algebraically tedious, the case $k^{\prime}=2$ can similarly be verified using the fact that $2 n_{i}^{\prime} \geqslant n_{i}+1$.

In the tree $T$, let $v_{0}$ be a vertex that maximizes $N(v)$, i.e., $N\left(v_{0}\right) \geqslant N(v)$ for all vertices $v$. Call $v_{0}$ a maximizing vertex.

Lemma 4. If $T$ is a tree rooted at a maximizing vertex $v_{0}$, then

$$
N_{1} \leqslant \prod_{i \neq 1}\left(N_{i}+1\right) .
$$

Proof. Let $v_{1}, v_{2}, \ldots, v_{k}$ be the children of the root $v_{0}$. Let $v_{0}, u_{1}, u_{2}, \ldots, u_{s}$ be the vertices adjacent to $v_{1}$, and let $N\left(u_{i}\right)$ denote the number of subtrees of $T-v_{1}$ rooted at $u_{i}$. Let $N_{0}$ denote the number of subtrees of $T-v_{1}$ rooted at $v_{0}$. By the recursions for $N\left(v_{0}\right)$ in Lemma 1 ,

$$
\begin{aligned}
& N\left(v_{0}\right)=\left(N_{1}+1\right) \prod_{i \neq 1}\left(N_{i}+1\right)=N_{1} \prod_{i \neq 1}\left(N_{i}+1\right)+\prod_{i \neq 1}\left(N_{i}+1\right), \\
& N\left(v_{1}\right)=\left(N_{0}+1\right) \prod_{i=1}^{s}\left(N\left(u_{i}\right)+1\right)=\left(1+\prod_{i \neq 1}\left(N_{i}+1\right)\right) N_{1}=N_{1} \prod_{i \neq 1}\left(N_{i}+1\right)+N_{1} .
\end{aligned}
$$

The result now follows from the assumption that $N\left(v_{0}\right) \geqslant N\left(v_{1}\right)$.
Lemma 5. If $T$ is a tree rooted at a maximizing vertex $v_{0}$ with $\operatorname{deg}\left(v_{0}\right) \geqslant 3$, then

$$
\prod_{i=1}^{k}\left(N_{i}+1\right)>\frac{4}{9}\left(\sum_{i=1}^{k} N_{i}\right)^{2}
$$

Proof. Order the children of $v_{0}$ so that $N_{1} \geqslant N_{2} \geqslant \cdots \geqslant N_{k}$. Consider

$$
f\left(N_{1}\right)=\frac{\prod_{i=1}^{k}\left(N_{i}+1\right)}{\left(\sum_{i=1}^{k} N_{i}\right)^{2}}
$$

as a function of variable $N_{1}$ (the other $N_{i}$ considered as constants). Taking the derivative reveals that the function is increasing if $N_{1} \leqslant\left(\sum_{i \neq 1} N_{i}\right)-2$ and decreasing if $N_{1} \geqslant\left(\sum_{i \neq 1} N_{i}\right)-2$. By the shape of the graph of $f\left(N_{1}\right)$ and by Lemma 4, the function $f$ can attain a minimum only if $N_{1}=N_{2}$ or $N_{1}=\prod_{i \neq 1}\left(N_{i}+1\right)$. It can be checked that $f\left(N_{2}\right) \geqslant f\left(\prod_{i \neq 1}\left(N_{i}+1\right)\right)$, so the minimum is attained for $N_{1}=\prod_{i \neq 1}\left(N_{i}+1\right)$. (The inequality is easy to check when $k=2$. For $k \geqslant 3$, let $P=\prod_{i=3}^{k} N_{i}$ and $S=\sum_{i=3}^{k} N_{i}$, and express the inequality in terms of $P, S$, and $q:=N_{2}$, regarding these variable as real numbers. Holding $P$ fixed, it follows from some algebra that the inequality is true if it is true when all the factors of $P$ and summands of $S$ are equal to $q$, i.e., $P=q^{r}, S=r q$, where $r$ is not necessarily an integer. Once this substitution is made, additional algebra suffices to verify the inequality.) Therefore

$$
\frac{\prod_{i=1}^{k}\left(N_{i}+1\right)}{\left(\sum_{i=1}^{k} N_{i}\right)^{2}}=f\left(N_{1}\right) \geqslant f\left(\prod_{i \neq 1}\left(N_{i}+1\right)\right)=\frac{\left(\prod_{i \neq 1}\left(N_{i}+1\right)\right)\left(\prod_{i \neq 1}\left(N_{i}+1\right)+1\right)}{\left(\sum_{i \neq 1} N_{i}+\prod_{i \neq 1}\left(N_{i}+1\right)\right)^{2}} .
$$

Letting $a=\prod_{i \neq 1}\left(N_{i}+1\right)$ and $b=\sum_{i \neq 1} N_{i}$, it is sufficient to show that

$$
\frac{a(a+1)}{(a+b)^{2}}>\frac{4}{9}
$$

By the inequality used in the proof of Lemma 2 we have, in the case $\operatorname{deg}\left(v_{0}\right) \geqslant 3$,

$$
\frac{b}{a}=\frac{\sum_{i \neq 1} N_{i}}{\prod_{i \neq 1}\left(N_{i}+1\right)} \leqslant \frac{1}{2} .
$$

Therefore

$$
\frac{a(a+1)}{(a+b)^{2}} \geqslant \frac{a(a+1)}{(a+a / 2)^{2}}=\frac{4}{9}\left(1+\frac{1}{a}\right)>\frac{4}{9} .
$$

Lemma 6. If $T$ is a tree rooted at a maximizing vertex $v_{0}$ with $\operatorname{deg}\left(v_{0}\right) \geqslant 3$, then

$$
N\left(v_{0}\right)>\frac{1}{9} \bar{N}\left(v_{0}\right)^{2} .
$$



Fig. 6. The exceptions.

Proof. Using Lemmas 1, 2, and 5, we have

$$
\begin{aligned}
N\left(v_{0}\right) & =\prod_{i=1}^{k}\left(N_{i}+1\right)>\frac{4}{9}\left(\sum_{i=1}^{k} N_{i}\right)^{2}=\frac{1}{9}\left(\sum_{i=1}^{k}\left(N_{i}+N_{i}\right)\right)^{2} \\
& >\frac{1}{9}\left(\sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right)\right)^{2}=\frac{1}{9} \bar{N}\left(v_{0}\right)^{2} .
\end{aligned}
$$

Lemma 7. For a tree $T$ all of whose internal vertices have degree at least three and a maximizing vertex $v_{0}$, we have $D_{T}>\frac{1}{2}$ if any one of the following conditions hold.
(a) $N\left(v_{0}\right) \geqslant n^{\prime} \bar{N}\left(v_{0}\right)$;
(b) $\bar{N}\left(v_{0}\right) \geqslant 9 n^{\prime}$;
(c) $N\left(v_{0}\right) \geqslant 9 n^{\prime 2}$.

Proof. By formula (3), $D_{T}>\frac{1}{2}$ if and only if

$$
\left(2 D\left(v_{0}\right)-1\right) N\left(v_{0}\right)>\left(1-2 \bar{D}\left(v_{0}\right)\right) \bar{N}\left(v_{0}\right)
$$

Clearly $\bar{D}\left(v_{0}\right) \geqslant 1 / n$. This and Lemma 3 imply that the above inequality holds if

$$
N\left(v_{0}\right)>\left(n^{\prime}+1\right)\left(1-\frac{2}{n}\right) \bar{N}\left(v_{0}\right) .
$$

Inequality (1), namely $2 n^{\prime} \geqslant n+2$, implies that this is the case if

$$
\begin{equation*}
N\left(v_{0}\right) \geqslant n^{\prime} \bar{N}\left(v_{0}\right) \tag{5}
\end{equation*}
$$

which is condition (a) in the statement of the lemma. It is routine to check that a leaf of $T$ cannot be the maximizing vertex. Hence $v_{0}$ has degree at least 3 and by applying Lemma 6 , the above inequality holds if $\bar{N}\left(v_{0}\right) \geqslant 9 n^{\prime}$, which is statement (b) of the lemma. If, on the other hand, $\bar{N}\left(v_{0}\right)<9 n^{\prime}$, then condition (a) holds if $N\left(v_{0}\right) \geqslant 9 n^{\prime 2}$, which is condition (c) in the statement of the lemma.

Proof of the lower bound in Theorem 1. By (2) we have $N\left(v_{0}\right) \geqslant 2^{n^{\prime}} \geqslant 9 n^{\prime 2}$ for $n^{\prime} \geqslant 10$. Therefore, by condition (c) in Lemma 7, it is sufficient to verify conditions (a), (b) or (c) for all trees with 9 or fewer leaves. There are relatively few such trees. Moreover, as we systematically constructed the trees according to the number subtrees of order one in $T-v_{0}$, many possibilities could be quickly eliminated by using Lemmas 2 and 4 . Only the star $S_{4}$ and the 8 in Fig. 6 failed to satisfy any of the conditions of Lemma 7. The density of each of these was computed and found to be at least $\frac{1}{2}$.

## 3. Proof of the upper bound

Again, it is assumed throughout this section that the degrees of all internal vertices of rooted trees are at least 3 , except possibly the root.

Proof of the upper bound in Theorem 1. It will be shown that, for any tree $T$ rooted at vertex $v$, all of whose internal vertices have degree at least three,
(i) $D(v)<\frac{3}{4}$ and
(ii) $\bar{D}(v)<\frac{3}{4}$.

The upper bound then follows immediately from Eq. (3). Statements (i) and (ii) are proved in the next two lemmas.

Lemma 8. If $T$ is a tree rooted at $v$ with $\operatorname{deg}(v) \geqslant 2$, then

$$
D(v) \leqslant \frac{3}{4}\left(1-\frac{1}{3 n}\right)
$$

Proof. Let $T_{1}, \ldots, T_{k}$ be the subtrees as defined earlier. Let $k_{1}$ be the number of such subtrees of order 1 , and let $T_{1}, \ldots, T_{k^{\prime}}$ be the remaining subtrees. The proof proceeds by induction on the order of the tree $T$. It is easy to check that the statement is true for th rooted tree of order 3. Consider any tree satisfying assumption (*). Applying the induction hypothesis to the recursion for $\mu(v)$ in Lemma 1 yields the following

$$
\begin{aligned}
\mu(v) & =1+\sum_{i=1}^{k} \mu_{i} \frac{N_{i}}{N_{i}+1}=1+\frac{1}{2} k_{1}+\sum_{i=1}^{k^{\prime}} \mu_{i} \frac{N_{i}}{N_{i}+1} \\
& \leqslant 1+\frac{1}{2} k_{1}+\frac{3}{4} \sum_{i=1}^{k^{\prime}}\left(1-\frac{1}{3 n_{i}}\right) n_{i} \frac{N_{i}}{N_{i}+1} \\
& \leqslant 1+\frac{1}{2} k_{1}+\frac{3}{4} \sum_{i=1}^{k^{\prime}}\left(1-\frac{1}{3 n_{i}}\right) n_{i} \\
& =1+\frac{1}{2} k_{1}+\frac{3}{4} \sum_{i=1}^{k^{\prime}} n_{i}-\frac{k^{\prime}}{4} .
\end{aligned}
$$

To prove that $\mu(v) \leqslant \frac{3}{4}\left(1-\frac{1}{3 n}\right) n=\frac{3}{4}\left(1+k_{1}+\sum_{i=1}^{k^{\prime}} n_{i}\right)-\frac{1}{4}$ it now suffices to prove

$$
1+\frac{1}{2} k_{1}+\frac{3}{4} \sum_{i=1}^{k^{\prime}} n_{i}-\frac{k^{\prime}}{4} \leqslant \frac{3}{4}\left(1+k_{1}+\sum_{i=1}^{k^{\prime}} n_{i}\right)-\frac{1}{4}
$$

which simplifies to $2 \leqslant k_{1}+k^{\prime}$, which is true because $k_{1}+k^{\prime}=\operatorname{deg}(v) \geqslant 2$.

Lemma 9. If $T$ is a tree rooted at $v$ with $\operatorname{deg}(v) \geqslant 2$, then

$$
\bar{D}(v)<\frac{3}{4}
$$

Proof. Let $T_{1}, \ldots, T_{k}$ be the subtrees as previously defined. Let $k_{1}$ be the number of such subtrees of order 1 , and let $T_{1}, \ldots, T_{k^{\prime}}$ be the remaining subtrees. The proof proceeds by induction on the order of the tree $T$. It is easy to check that the statement is true for the rooted tree of order 3. Applying Lemma 8 and the induction hypothesis to the recursion for $\bar{\mu}(v)$ in Lemma 1 yields

$$
\bar{\mu}(v)=\frac{\sum_{i=1}^{k}\left(\mu_{i} N_{i}+\bar{\mu}_{i} \bar{N}_{i}\right)}{\sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right)} \Longrightarrow
$$

$$
\begin{aligned}
\bar{D}(v) & =\frac{\sum_{i=1}^{k}\left(D_{i} n_{i} N_{i}+\bar{D}_{i} n_{i} \bar{N}_{i}\right)}{n \sum_{i=1}^{k}\left(N_{i}+\bar{N}_{i}\right)}=\frac{k_{1}+\sum_{i=1}^{k^{\prime}}\left(D_{i} n_{i} N_{i}+\bar{D}_{i} n_{i} \bar{N}_{i}\right)}{\left(1+k_{1}+\sum_{i=1}^{k^{\prime}} n_{i}\right)\left(k_{1}+\sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right)\right)} \\
& <\frac{k_{1}+\frac{3}{4} \sum_{i=1}^{k^{\prime}} n_{i}\left(N_{i}+\bar{N}_{i}\right)}{\left(k_{1}+\sum_{i=1}^{k^{\prime}} n_{i}\right)\left(k_{1}+\sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right)\right)} .
\end{aligned}
$$

To prove that $\bar{D}(v)<3 / 4$ it now suffices to prove

$$
\frac{3}{4}\left(\left(k_{1}+\sum_{i=1}^{k^{\prime}} n_{i}\right)\left(k_{1}+\sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right)\right)-\sum_{i=1}^{k^{\prime}} n_{i}\left(N_{i}+\bar{N}_{i}\right)\right) \geqslant k_{1} .
$$

## Because

$$
\sum_{i=1}^{k^{\prime}} n_{i} \sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right) \geqslant \sum_{i=1}^{k^{\prime}} n_{i}\left(N_{i}+\bar{N}_{i}\right)
$$

it suffices to prove

$$
\frac{3}{4} k_{1}\left(k_{1}+\sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right)\right) \geqslant k_{1}
$$

which is true because

$$
\frac{3}{4} k_{1}\left(k_{1}+\sum_{i=1}^{k^{\prime}}\left(N_{i}+\bar{N}_{i}\right)\right) \geqslant \frac{3}{4} k_{1}\left(k_{1}+k^{\prime}\right)=\frac{3}{4} k_{1} \operatorname{deg}(v) \geqslant \frac{3}{2} k_{1} .
$$

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