Extremal results on average subtree density of series-reduced trees

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Abstract

Vince and Wang [6] showed that the average subtree density of a series-reduced tree is between $\frac{1}{2}$ and $\frac{3}{4}$, answering a conjecture of Jamison [4]. They ask under what conditions a sequence of such trees may have average subtree density tending to either bound; we answer these questions by giving simple necessary and sufficient conditions in each case.

1 Introduction

In this paper we consider the average order over all subtrees of a fixed tree $T$. We call this quantity $\mu(T)$, and the average subtree density $D(T) = \frac{\mu(T)}{n(T)}$ where $n(T)$ is the number of vertices of $T$. Equivalently, we may think of $\mu(T)$ as the sum over vertices of $T$ of the proportion of subtrees which contain that vertex, and $D(T)$ as the average over vertices of $T$ of the proportion of subtrees which contain that vertex; we shall frequently use these alternative definitions.

These invariants were introduced by Jamison [4], who studied the extremal problem, showing that the tree of order $n$ which minimises the average order of a subtree is the path $P_n$, for which $\mu(P_n) = \frac{n+2}{3}$, but that there exist trees with $D(T)$ arbitrarily close to 1. Meir and Moon [5] gave asymptotic results on the average value of $D(T)$ over all trees of order $n$.

We shall focus our attention on trees whose internal vertices all have degree at least three; we write $T_3$ for the set of trees with at least one internal vertex and all internal vertices having degree at least three (so we exclude the one- and two-vertex trees which would otherwise vacuously satisfy the condition). Such trees are sometimes referred to as series-reduced trees or homeomorphically irreducible trees [1], and have been studied in other contexts (e.g. [2]). (As usual, we refer to vertices of degree at least 2 as “internal vertices” of a tree, and other vertices as “leaves”.)

For trees $T \in T_3$, Jamison [4] conjectured that $D(T) \geq \frac{1}{2}$; this, along with the upper bound $D(T) < \frac{3}{4}$, was proved by Vince and Wang [6], who also asked

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questions about under what conditions a sequence of distinct trees in $T_3$ can have density tending to either limit. We shall give a simpler proof of their upper bound, as well as answering their questions by giving exact necessary and sufficient conditions for a sequence of trees in $T_3$ to have density tending to $\frac{1}{2}$ or $\frac{3}{4}$.

2 The upper bound

For a given tree $T$, the subgraphs of $T$ which are also trees must all be induced subgraphs. Write $S(T)$ for the set of subsets of $V(T)$ which induce a subgraph which is a tree. We require each subtree to have at least one vertex, so that $\emptyset \notin S(T)$ but $\{v\} \in S(T)$ for every $v \in V$.

First we make a simple observation which immediately gives us the upper bound $D(T) < \frac{3}{4}$ for $T \in T_3$.

Lemma 1. If $v$ is a leaf of a tree $T$ with at least four vertices, less than half of the subtrees of $T$ contain $v$.

Proof. Write $u$ for the neighbour of $v$. For every $S \in S(T)$ with $v \in S$ and $S \neq \{v\}$ write $S' = S - v$; then $S' \in S(T)$, and $u \in S'$. Conversely, if $u \in R$, $v \notin R$ and $R \in S(T)$ then $R = S'$ for some $S \in S(T)$ containing $v$. Thus there is a one-to-one correspondence between subtrees containing $v$ (other than singleton $v$) and subtrees containing $u$ but not $v$. Since there are at least two subtrees which contain neither $u$ nor $v$ (namely any other single vertex), there are more subtrees which do not contain $v$ than subtrees which do.

Any tree (other than the single-vertex tree) has at least two leaves; if $T \in T_3$ then we can say more, giving us our desired result.

Lemma 2. If $T \in T_3$ has $n$ vertices then $\mu(T) < \frac{3n^2 - 2}{n}$.

Proof. Since $T$ has $n - 1$ edges, $\sum d(v) = 2n - 2$. If $T$ has $l$ leaves then each of the $n - l$ internal vertices has degree at least 3, so $2n - 2 \geq l + 3(n - l)$, i.e. $l \geq \frac{n^2 - 2}{2}$. Recall that $\mu(T)$ is the sum over vertices of the proportion of subtrees containing that vertex. By definition, $T$ has at least four vertices, so we may apply Lemma 1 to get $\mu(T) < \frac{1}{2} + (n - l) \leq \frac{3n^2 - 2}{n}$.

We shall frequently recall the observation above that if a tree in $T_3$ has $n$ vertices and $l$ leaves then $l \geq \frac{n^2 - 2}{2}$.

Vince and Wang [6] ask under what conditions a sequence of distinct trees in $T_3$ can have densities tending to $\frac{1}{2}$. They consider the conditions of bounded diameter and of unbounded degree, observing that neither is sufficient. In fact the bounded diameter condition (which would imply unbounded degree) is not necessary either. Using Lemma 1 we can see that a sufficient condition is that the proportion of leaves tends to 1, since if $T$ has $n$ vertices and at least $(1 - \varepsilon)n$ leaves then $\mu(T) < \varepsilon n + \frac{1}{2}(1 - \varepsilon)n$ and so $D(T) < \frac{1}{2}(1 + \varepsilon)$. We can certainly construct sequences of trees for which the diameter is unbounded but the proportion of
leaves tends to 1, such as the tree formed by connecting \( n \) stars of order \( n \) by a path. We might hope that this condition on the proportion of leaves is also necessary; in the next section we shall show that this is so.

Vince and Wang [6] also give a sequence of trees in \( T_3 \) with density tending to \( \frac{3}{4} \) and go on to ask about necessary and sufficient conditions for a sequence of distinct trees in \( T_3 \) to have density tending to \( \frac{3}{4} \). They suggest that suitable conditions might be that both the proportion of leaves tends to \( \frac{1}{2} \) (the minimum possible limit for trees in \( T_3 \)) and the ratio of the diameter to the number of vertices tends to \( \frac{1}{2} \) (the maximum possible limit for trees in \( T_3 \)). From Lemma 1 it is clear that the first condition is necessary. The second is not, however, as we shall see.

3 Twigs and improved upper bounds

Define a vertex \( v \) of a tree to be a twig if \( d(v) \geq 2 \) but at least \( d(v) - 1 \) of its neighbours are leaves. An equivalent definition is that the twigs of \( T \) are the leaves of the tree \( T' \) formed by deleting all the leaves of \( T \). In this section we aim to show that trees for which \( D(T) \) is close to \( \frac{3}{4} \) must have few twigs.

We have already defined \( S(T) \) for a given tree \( T \). Let \( S'(T) \) be obtained from \( S(T) \) by adding \( \emptyset \) but removing \( \{v\} \) for every leaf \( v \) (other singleton sets remain). \( \mu(T) \) is the average order of a subset of \( V(T) \) in \( S(T) \). Here we shall find it more convenient to consider \( \mu'(T) \), the average order of a subset in \( S'(T) \), and so we wish to establish an inequality between the two.

**Lemma 3.** For any tree \( T \) with at least four vertices, \( \mu(T) \leq \mu'(T) \), with equality only for the path on four vertices, \( P_4 \).

**Proof.** Suppose that \( T \) has \( n \) vertices and \( l \) leaves. Consider the subsets of \( V(T) \) in \( S(T) \cap S'(T) \), that is to say the nonempty subsets which induce subtrees which are not single leaves of \( T \). Let the number of such subsets be \( A \) and the total of their orders be \( \mu(T) = \frac{A + l}{a+1} \), \( \mu'(T) = \frac{A}{a+1} \). Firstly, we claim that \( \mu'(T) \geq 2 \): since the \( a \) subtrees in \( S(T) \cap S'(T) \) comprise \( n - l \) of order 1, one of order \( n \), \( l \) of order \( n - 1 \) obtained by removing a leaf from \( T \), and \( a - n - 1 \) others, each of order at least 2,

\[
A \geq 2(a - n - 1) + (n - l) + n + l(n - 1) = 2a + (n - 2)l - 2 \geq 2a + 2.
\]

The last line follows since \( n \geq 4 \) and \( l \geq 2 \); equality therefore occurs only when \( n = 4 \) and \( l = 2 \), i.e. \( T = P_4 \).
Now, since \( l \geq 2 \), \( \frac{1}{l-1} \leq 2 \leq \mu'(T) \) (with equality only if \( T = P_4 \)). So
\[
\mu(T) = \frac{A + l}{a + l} = \frac{a + 1}{a + l} \frac{A}{a + 1} + \frac{l - 1}{l + a} \frac{l}{l - 1}
\leq \frac{a + 1}{a + l} \mu'(T) + \frac{l - 1}{l + a} \mu'(T)
= \mu'(T),
\]
as required, again with equality only if \( T = P_4 \).

**Lemma 4.** If \( T \in \mathcal{T}_3 \) has \( n \geq 4 \) vertices and \( t \) twigs then \( \mu(T) < \frac{3n}{2} - \frac{2t}{5} \).

**Proof.** We shall instead show that \( \mu'(T) < \frac{3n}{2} - \frac{2t}{5} \); by the previous lemma, this is sufficient. \( \mu'(T) \) is the average number of vertices belonging to a subset in \( S'(T) \); equivalently, it is the sum over all vertices of the proportion of subsets in \( S'(T) \) which contain that vertex.

If \( w \) is any leaf not adjacent to a twig then removing \( w \) from any set in \( S'(T) \) containing it gives another set in \( S'(T) \), and all sets obtained in this way are distinct, so \( w \) is in at most half of the sets in \( S'(T) \). Certainly any vertex which is neither a twig nor a leaf is in at most all sets in \( S'(T) \).

Suppose \( T \) has \( l_1 \) leaves which are adjacent to twigs and \( l_2 \) leaves not adjacent to twigs. Consider the tree \( T' \) obtained from \( T \) by removing the \( l_1 \) leaves adjacent to twigs of \( T \). Each vertex which was a twig in \( T \) is now a leaf in \( T' \) and any other internal vertex of \( T \) has the same degree in \( T' \), so either \( T' \in \mathcal{T}_3 \) or \( T' \) is the one-vertex tree or \( T' \) is the two-vertex tree. Recall that any tree in \( \mathcal{T}_3 \) with \( k \) vertices has at least \( 4k^2 \) leaves. \( T' \) has \( n - l_1 \) vertices and \( l_2 + t \) leaves, so if \( T' \in \mathcal{T}_3 \) then \( l_2 + t \geq \frac{n - l_1 + 2}{2} \), i.e. \( l_2 \geq \frac{n - l_1 - 2t + 2}{2} \). If \( T' \) is the one-vertex tree then \( l_1 = n - 1 \), \( t = 1 \) and \( l_2 = 0 \), so \( l_2 = \frac{n - l_1 - 2t + 2}{2} \). If \( T' \) is the two-vertex tree then \( l_1 = n - 2 \), \( t = 2 \) and \( l_2 = 0 \), so \( l_2 = \frac{n - l_1 - 2t + 2}{2} \). In each case \( l_2 \geq \frac{n - l_1 - 2t + 2}{2} \).

For any twig, \( v \), with \( a \) adjacent leaves, we define an equivalence relation on \( S'(T) \) by saying two sets are equivalent if they differ only on \( v \) and adjacent leaves. Since any set in \( S'(T) \) which contains a leaf adjacent to \( v \) must also contain \( v \), each equivalence class consists either of a single set which does not contain \( v \), or of \( 2^a + 1 \) sets, one not containing \( v \) and the remainder containing \( v \) and any subset of adjacent leaves. Thus the proportion of sets in \( S'(T) \) which contain \( v \) is at most \( \frac{2^a}{2^{a+1}} \), and the proportion which contain any given leaf adjacent to \( v \) is at most \( \frac{2^{a-1}}{2^{a+1}} \). Note that, since \( d(v) \geq 3 \), \( a \geq 2 \).

Let the twigs of \( T \) be \( v_1, v_2, \ldots, v_t \), with \( a_1, a_2, \ldots, a_t \) leaves respectively, so that \( l_1 = \sum a_i \geq 2t \). The sum, as \( u \) ranges over all twigs and leaves adjacent to twigs, of the proportion of sets in \( S'(T) \) which contain \( u \) is therefore
\[
\sum_{i=1}^{t} \frac{2^a_i + a_i2^{a_i-1}}{2^{a_i} + 1} \leq \sum_{i=1}^{t} \frac{28a_i + 16}{45} = \frac{28l_1 + 16t}{45},
\]
where the first inequality is the result of Lemma 5 following. We shall now combine all these bounds to bound $\mu'_T$.

\[
\mu'(T) = \sum_{v \in V(T)} \frac{|\{S \in S'(T) : v \in S\}|}{|S'(T)|}
\leq (n - t - l_1 - l_2) + \frac{l_2}{2} + \frac{28l_1 + 16t}{45}
\]

\[
= n - \frac{29t}{45} - \frac{17l_1}{45} - \frac{l_2}{2}
\leq n - \frac{29t}{45} - \frac{17l_1}{45} - \frac{n - l_1 - 2t + 1}{4}
\]

\[
= \frac{3n}{4} - \frac{13t}{90} - \frac{23l_1}{180} - \frac{1}{4}
\leq \frac{3n}{4} - \frac{2t}{5} - \frac{1}{4},
\]

where the final inequality follows from the observation that $l_1 \geq 2t$.

Lemma 5. If $a \geq 2$ is an integer then $\frac{2a^a + a^{a-1}}{2^{a+1}} \leq \frac{28a + 16}{45}$.

Proof. Since

\[
\frac{28a + 16}{45} - \frac{2a^a + a^{a-1}}{2^{a+1}} = \frac{11a2^a + 56a + 32 - 58 \times 2^a}{90(2^a + 1)},
\]

it is sufficient to show that

\[
11a2^a + 56a + 32 \geq 58 \times 2^a.
\]

If $a \geq 6$ then $11a2^a \geq 58 \times 2^a$, so it only remains to check for $a = 2, 3, 4, 5$. For $a = 2$ and $a = 3$ the LHS and RHS are equal; for $a = 4$ and $a = 5$ the LHS is greater.

If $T$ has $n$ vertices and at least $\varepsilon n$ twigs, then, $D(T) = \frac{1}{n} \mu(T) < \frac{3}{4} - \frac{2}{5} \varepsilon$, and so for a sequence of trees to have average subtree density tending to $\frac{3}{4}$ it is necessary for the proportion of twigs to tend to 0. In the previous section we showed that it is also necessary for the proportion of leaves to tend to $\frac{1}{2}$. We might hope that it is necessary and sufficient for both the proportion of leaves to tend to $\frac{1}{2}$ and the proportion of twigs to tend to 0; we shall later show that this is the case.

4 Rooted approximations

In this section we will consider trees with a designated vertex, the root. We shall compare the average order of a subtree to the average order of a subtree containing the root. For trees in $\mathcal{T}_3$, we shall show that for a suitably chosen root these two quantities differ by at most a constant.
Let $\mathcal{T}_3^*$ be the set of rooted trees such that the root has degree at least two and every other internal vertex has degree at least three, together with the single-vertex rooted tree. The motivation for this definition is that any tree in $\mathcal{T}_3^*$, when rooted at any internal vertex, is in $\mathcal{T}_3^*$, and that the definition of $\mathcal{T}_3^*$ permits induction in the following manner. For any $T \in \mathcal{T}_3^*$ other than the single-vertex tree, we may delete the root to leave two or more components. We may consider each component as a new tree; it must contain exactly one neighbour of the deleted root and, if rooted at that vertex, is in $\mathcal{T}_3^*$. In some cases we shall prove results for all rooted trees using a similar inductive process.

For a tree $T$ with a vertex $v$ write $\alpha(T, v)$ for the number of subtrees containing $v$ and $\overline{\alpha}(T, v)$ for the number not containing $v$; likewise, write $\lambda(T, v)$ for the average order of subtrees containing and not containing $v$ respectively. (Recall that, by definition, all subtrees are non-empty.) Similarly define $\alpha(T, e)$, etc., when $e$ is an edge. We start by observing that we may calculate $\lambda(T, v)$ in terms of the parameters of the components of $T - v$. This observation also appears in the papers of Jamison [4] and Vince and Wang [6].

**Lemma 6.** Let $T$ be a rooted tree with root $v$. If $v$ has $d$ neighbours $v_1, v_2, \ldots, v_d$, let $T_i$ for $1 \leq i \leq d$ be the component of $T - v$ containing $v_i$. Then

$$\lambda(T, v) = 1 + \sum_{i=1}^{d} \frac{\lambda(T_i, v_i)\alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1}.$$  

*Proof.* If $S$ is chosen uniformly from all subtrees of $T$ which contain $v$, the average number of vertices in $S$ is the sum of the average number of vertices in each $S \cap T_i$, plus one (for $v$ itself, which is not in any $T_i$). For each $i$, consider the equivalence relation where two subtrees $S_1, S_2$ are equivalent if they differ only on vertices of $T_i$; since each subtree contains $v$, each equivalence class contains $\alpha(T_i, v_i) + 1$ subtrees, one with empty intersection with $T_i$, and the others having intersections corresponding to the subtrees of $T_i$ containing $v_i$. The sum of the orders of these intersections is therefore $\alpha(T_i, v_i)\lambda(T_i, v_i)$, so the average intersection over each equivalence class, and hence the overall average intersection with $T_i$, is $\frac{\lambda(T_i, v_i)\alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1}$. Summing over $i$ gives the desired result. \[\square\]

We shall need the following bound, which appears in the paper of Vince and Wang [6]; we include their proof for completeness.

**Lemma 7 ([6]).** If $T \in \mathcal{T}_3^*$ with root $v$ then $\alpha(T, v) \geq \overline{\alpha}(T, v)$.

*Proof.* We use induction on the order of $T$. For the one-vertex tree the result is trivial; otherwise $v$ has at least two neighbours, $v_1, v_2, \ldots, v_d$, and $T - v$ has corresponding components $T_1, T_2, \ldots, T_d$. Then

$$\alpha(T, v) = \prod_{i=1}^{d} (\alpha(T_i, v_i) + 1),$$
since a subtree containing $v$ consists of $v$ together with either a subtree containing $v_i$ or no vertices from each $T_i$. Also
\[
\bar{\alpha}(T, v) = \sum_{i=1}^{d} (\alpha(T_i, v_i) + \bar{\alpha}(T_i, v_i)),
\]
since each subtree not containing $v$ is a subtree of one of the $T_i$.

We claim that, for any positive integers $a_1, a_2, \ldots, a_d$, with $d \geq 2$,
\[
\prod_{i=1}^{d} (a_i + 1) \geq 2 \sum_{i=1}^{d} a_i.
\]
We prove this by induction on $d$. For $d = 2$,
\[
(a_1 + 1)(a_2 + 1) - 2(a_1 + a_2) = (a_1 - 1)(a_2 - 1) \geq 0;
\]
for $d \geq 3$,
\[
\prod_{i=1}^{d} (a_i + 1) = (a_d + 1) \prod_{i=1}^{d-1} (a_i + 1)
\]
\[
\geq 2(a_d + 1) \sum_{i=1}^{d-1} a_i
\]
\[
\geq 2a_d + 2 \sum_{i=1}^{d-1} a_i,
\]
as required.

Hence, using the induction hypothesis for $T_i$,
\[
\alpha(T, v) = \prod_{i=1}^{d} (\alpha(T_i, v_i) + 1)
\]
\[
\geq 2 \sum_{i=1}^{d} \alpha(T_i, v_i)
\]
\[
\geq \sum_{i=1}^{d} (\alpha(T_i, v_i) + \bar{\alpha}(T_i, v_i))
\]
\[
= \bar{\alpha}(T, v),
\]
as required.

We shall also need a lower bound on $\alpha(T, v)$.

**Lemma 8.** Let $T$ be any rooted tree with root $v$, $n$ vertices and $l$ leaves, not counting the root as a leaf. Then $\alpha(T, v) \geq n - l - 1 + 2^l$.

**Proof.** For each vertex $w$, consider the subtree $S_w$ consisting of a path from $v$ to $w$ (the single-vertex path if $v = w$). Each such subtree is distinct (since if $v \neq w$ then $w$ is the unique leaf of $S_w$ other than $v$) and contains $v$, so $\alpha(T, v) \geq n$.

In addition, if $l > 1$, consider the subtrees consisting of all vertices other than the leaves (including the root, which we do not count as a leaf) together with any set of at least two leaves. All such subtrees are distinct and are not paths ending at the root, so not equal to $S_w$ for any $w$. There are $2^l - l - 1$ such subtrees, so $\alpha(T, v) \geq n - l - 1 + 2^l \geq n$. 

7
This bound is best possible for any \( l < n \), as seen by considering the tree consisting of a vertex adjacent to \( l \) leaves and connected to the root by a path of length \( n - l - 1 \) (by which we mean that this vertex is itself the root when \( n - l - 1 = 0 \)).

Since the root is not counted among the leaves, even if it has degree 1, \( n - l - 1 \geq 0 \) and so we shall sometimes use the weaker bound \( \alpha(T, v) \geq 2^l \).

Now we shall use these bounds to show that, for any \( T \in \mathcal{T}_3 \) with at least 30 vertices, we may approximate \( \mu(T) \) by \( \lambda(T, v) \) for some suitable choice of \( v \).

**Lemma 9.** If \( T \in \mathcal{T}_3 \) is a tree with \( n \geq 30 \) vertices then either there is an edge \( e \) for which \( 2\alpha(T, e) \geq n\alpha(T, e) \) or there is an internal vertex \( v \) for which \( 2\alpha(T, v) \geq n\alpha(T, v) \).

**Proof.** Pick any edge \( e = \{v_1, v_2\} \). Let \( T_1, T_2 \) be the components of \( T - e \) containing \( v_1, v_2 \) respectively. Then each subtree not containing \( e \) is a subtree of one component of \( T - e \), and each subtree containing \( e \) is the union of a subtree of \( T_1 \) containing \( v_1 \) and a subtree of \( T_2 \) containing \( v_2 \), so

\[
\begin{align*}
\alpha(T, e) &= \alpha(T, v_1)\alpha(T, v_2), \\
\bar{\alpha}(T, e) &= \bar{\alpha}(T, v_1) + \bar{\alpha}(T, v_2) + \alpha(T, v_1) + \alpha(T, v_2).
\end{align*}
\]

Without loss of generality we may assume \( \alpha(T, v_1) \geq \alpha(T, v_2) \), so, using Lemma 7 \( \bar{\alpha}(T, e) \leq 4\alpha(T, v_1) \) and so \( 2\alpha(T, e) \geq \frac{1}{2}\alpha(T, v_2)\bar{\alpha}(T, e) \). If \( T_2 \) has \( k \) leaves then \( \alpha(T_2, v_2) \geq 2^k \), so \( e \) suffices if the number of leaves on each side is at least \( \log_2 n + 1 \).

If no such \( e \) exists then we must have a central vertex \( v \) with each component of \( T - v \) having fewer than \( \log_2 n + 1 \) leaves. (Since \( T \) has at least \( \frac{n+2}{2} \) leaves, and this is much more than \( \log_2 n + 1 \) for \( n \geq 30 \), certainly such a \( v \) is an internal vertex.) Let \( w \) be the neighbour maximising \( \alpha(T_w, w) \) (where \( T_w \) is the component of \( T - v \) containing \( w \)); suppose \( T_w \) has \( k \) leaves and \( T \) has \( l \). Now

\[
\begin{align*}
\alpha(T, v) &\geq \alpha(T, vw) \\
&\geq 2^{l-k}\alpha(T_w, w), \\
\bar{\alpha}(T, v) &= \sum_{u \in \Gamma(v)} (\alpha(T_u, u) + \bar{\alpha}(T_u, u)) \\
&\leq \sum_{u \in \Gamma(v)} 2\alpha(T_u, u) \\
&\leq 2n\alpha(T_w, w),
\end{align*}
\]

and \( l \geq \frac{n+2}{2} > \log_2 n + 1 \), so

\[
\frac{\alpha(T, v)}{\bar{\alpha}(T, v)} > \frac{2^{2^l - \log_2 n}}{2n} = \frac{2^{2^l}}{2n^2}.
\]

So we are done if \( 2^{2^l} \geq n^3 \), i.e. if \( n \geq 6 \log_2 n \), which holds if \( n \geq 30 \). \( \square \)
This result immediately gives us the desired approximation.

**Corollary 10.** If \( T \in T_3 \) has \( n \geq 30 \) vertices then there is some internal \( v \) with \( |\mu(T) - \lambda(T, v)| < 2 \).

**Proof.** Since

\[
\mu(T) = \frac{\alpha(T, v)\lambda(T, v) + \bar{\alpha}(T, v)\bar{\lambda}(T, v)}{\alpha(T, v) + \bar{\alpha}(T, v)}
\]

and \( 0 < \lambda(T, v), \bar{\lambda}(T, v) < n \), it is sufficient to find an internal \( v \) such that

\[
2\alpha(T, v) \geq n\bar{\alpha}(T, v).
\]

Either we are immediately done by Lemma 9 or we have an edge satisfying the same relation; in the latter case at least one vertex on that edge is internal, and will suffice since if \( e = vw \) then \( \alpha(T, v) \geq \alpha(T, e) \) and \( \bar{\alpha}(T, e) \geq \bar{\alpha}(T, v) \).

\[ \square \]

## 5 Ranking vertices and lower bounds

In order to show that we require the proportion of leaves to tend to 1 if the average subtree density is to tend to \( \frac{1}{2} \) we need a better lower bound for trees which have many internal vertices. The following bound may be deduced from our subsequent stronger result, but we shall prove this weaker version first to give the basic idea.

**Lemma 11.** If \( T \in T^*_3 \) has root \( v \) and \( n \) vertices of which \( k \) are not leaves then \( \lambda(T, v) \geq \frac{n+1}{2} + \frac{k-1}{10} \).

**Proof.** Again, we prove this by induction on \( n \); it is trivial for \( n = 1 \). If \( n > 1 \), let \( v \) have \( l \) neighbours which are leaves, and \( m \) which are not. Let \( v_1, \ldots, v_m \) be these neighbours and \( v_{m+1}, \ldots, v_{m+l} \) be the leaves. Let \( T_i \) be the component of \( T - v \) containing \( v_i \), and write \( n_i, k_i \) for the number of vertices and the number of vertices which are not leaves respectively. Now \( \sum_{i=1}^m n_i = n - l - 1 \), \( \sum_{i=1}^m k_i = k - 1 \), and

\[
\lambda(T, v) = 1 + \sum_{i=1}^{m+l} \frac{\lambda(T_i, v_i)\alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1}
\]

\[
= 1 + \frac{l}{2} + \sum_{i=1}^m \frac{\lambda(T_i, v_i)\alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1}
\]

\[
\geq 1 + \frac{l}{2} + \sum_{i=1}^m \frac{(n_i + 1 + \frac{k_i-1}{2})\alpha(T_i, v_i)}{2(\alpha(T_i, v_i) + 1)}.
\]

by the induction hypothesis. Note that, for \( 1 \leq i \leq m \), since \( T_i \) is not a single vertex but \( T_i \in T^*_3 \), \( n_i \geq 3 \). Also any tree in \( T^*_3 \) with \( n_i \) vertices has at least

9
\(\frac{n+1}{2}\) leaves. Since the set of all non-leaf vertices together with any subset of leaves forms a subtree of \(T_i\) containing \(v_i\), \(\alpha(T_i, v_i) \geq \frac{n+1}{2} \geq \frac{11n_i-1}{8}\), where the second inequality is easily checked to hold for \(n_i \geq 3\). Finally, since \(T_i\) has at least \(\frac{n_i+1}{2}\) leaves, \(k_i \leq \frac{n_i-1}{2}\) and so \(\frac{11n_i-1}{8} \geq \frac{5}{4}k_i\). Thus

\[
\lambda(T, v) \geq 1 + \frac{l}{2} + \sum_{i=1}^{m} \left(\frac{n_i+1 + k_i-1}{2} \alpha(T_i, v_i)\right) \\
\geq 1 + \frac{l}{2} + \sum_{i=1}^{m} \left(\frac{n_i+1 + k_i-1}{2} \left(\frac{5n_i+k_i}{4}\right)\right) \\
= 1 + \frac{l}{2} + \sum_{i=1}^{m} \frac{n_i + k_i}{2} \\
= \frac{n+1}{2} + \frac{k - 1}{10}
\]

as required.

This result is best possible for \(n \geq 3k+1\), attained by the tree whose root has \(n - 3k\) children which are leaves and \(k\) other children, each having two children. If \(T \in T_3\) then we have shown that \(\lambda(T, v) \geq \frac{n+1}{2} + \frac{k-1}{10}\) for any internal vertex \(v\), since if \(T\) is rooted at \(v\) it is in \(T_3^*\).

We may immediately conclude our desired result.

**Theorem 12.** A sequence of distinct trees in \(T_3\) has average subtree density tending to \(\frac{1}{2}\) if and only if the proportion of leaves tends to 1.

**Proof.** Write \((T_i)_{i \geq 0}\) for our sequence and let \(T_i\) have \(n_i\) vertices and \(n_i\xi_i\) leaves. Since there are only finitely many trees of each order, \(n_i \to \infty\) and for \(i\) sufficiently large there exists an internal vertex \(v_i\) such that \(|\mu(T_i) - \lambda(T_i, v_i)| < 2\). Then \(|D(T_i) - \frac{3}{5} \lambda(T_i, v_i)| \to 0\), and

\[
\frac{3}{5} - \frac{1}{10}\xi_i < \lambda(T_i, v_i) < 1 - \frac{1}{2}\xi_i,
\]

so \(D(T_i) \to \frac{1}{2}\) if and only if \(\xi_i \to 1\).

For density tending to \(\frac{3}{4}\), we need to divide the vertices into more classes. We shall consider only rooted trees for this purpose.

For a rooted tree \(T \in T_3^*\) with root \(v\), we regard each vertex \(w \neq v\) as having one parent, the neighbour of \(w\) on the path from \(v\) to \(w\), and \(d(w) - 1\) children, the other neighbours of \(w\). Thus each child of a vertex is a neighbour which is further from the root. We shall inductively define the rank of a vertex other than the root: a vertex with no children (i.e. a leaf) has rank zero; the rank of each other vertex is one more than the maximum rank of its children. An equivalent explicit definition is that the rank is the maximum length of a path starting at that vertex which does not include its parent. We shall leave the rank of the root undefined.
We wish to find a lower bound on $\lambda(T, v)$ in terms of the ranks of the vertices. Write $m_j(T, v)$ for the number of vertices of rank $j$ when $T$ is rooted at $v$ (for any $T$, $m_j(T, v) = 0$ for all sufficiently large $j$, certainly for any $j$ exceeding the diameter of $T$). Note that since each vertex of rank $j+1$ has at least one child of rank $j$, and these are all distinct, $m_{j+1}(T, v) \leq m_j(T, v)$.

**Theorem 13.** If $T \in T^*_3$ has root $v$ and $n$ vertices then

$$\lambda(T, v) \geq 1 + \sum_{j \geq 0} c_j m_j(T, v),$$

where the values of $c_j$ for $j \geq 0$ are given by

$$c_j = 1 - \frac{1 + \frac{j}{2} + \sum_{i=0}^{j-1} c_i}{2^{j+1} + j};$$

note that when $j = 0$ the sum in the above expression is empty and so $c_0 = \frac{1}{2}$.

**Proof.** First, we need some bounds on the $c_j$. We claim by induction that

$$c_j \leq 1 - \frac{1 + j}{2^{j+1} + j} \leq 1$$

and that

$$c_j \geq 1 - \frac{1 + \frac{3j}{2}}{2^{j+1} + j} \geq \frac{1}{2}.$$  

We shall only use $\frac{1}{2} \leq c_j \leq 1$ (which is certainly true for $j=0$) in our induction step: if this is true for every $0 \leq j < k$ then

$$c_k \leq 1 - \frac{1 + k}{2^{k+1} + k} \leq 1$$

and

$$c_k \geq 1 - \frac{1 + \frac{3k}{2}}{2^{k+1} + k},$$

as required. It only remains to check that

$$1 - \frac{1 + \frac{3k}{2}}{2^{k+1} + k} \geq \frac{1}{2}$$

for every $k \geq 0$; this is true since $2^k \geq k+1$ so $2^{k+1} + k \geq 3k + 2$. Thus, by induction, the bounds above hold for every $k \geq 0$.

Now we claim that these bounds imply that $c_j \to 1$ as $j \to \infty$ and that $c_{j+1} \geq c_j$ for every $j$. The first statement is a trivial consequence of the lower bound. To prove the other, note that

$$\frac{1 - c_j}{1 - c_{j+1}} \leq \frac{\left( \frac{j+1}{2^{j+1} + j} \right) \left( \frac{2^{j+2} + j + 1}{2^{j+1} + j + 1} \right)}{4j2^j + 4 \times 2^j + j^2 + 2j + 1} \leq \frac{3j2^j + 5 \times 2^j + \frac{3}{2}j^2 + \frac{5}{2}j}{2^{j+1} + j + 1}.$$
Since
\[
(4j^2 + 4 \times 2^j + j^2 + 2j + 1) - (3j^2 + 5 \times 2^j + \frac{3}{2}j^2 + \frac{5}{2}j) \\
= 2^j(j - 1) + 1 - \frac{1}{2}j^2 - \frac{1}{2}j \\
\geq (j + 1)(j - 1) + 1 - j^2 = 0,
\]
it follows that \(1 - c_j \geq 1 - c_{j+1}\), i.e. \(c_j \leq c_{j+1}\).

We are now ready to prove the main result, which we shall do by induction on \(n\); it is trivial for \(n = 1\) (when \(m_j(T, v) = 0\) for every \(j\)). If \(n > 1\), let \(v\) have \(d\) neighbours \(v_1, \ldots, v_d\) of ranks \(r_1, \ldots, r_d\); let \(T_i\) be the component of \(T - v\) containing \(v_i\), and write \(n_i\) and \(m_j(T_i, v_i)\) for the number of vertices and the number of vertices of rank \(j\) respectively. Note that for each vertex in \(T_i\) other than the root, the rank of that vertex in \(T_i\) is equal to its rank in \(T\). Therefore, the difference \(m_j(T, v) - \sum_{i=1}^{d} m_j(T_i, v_i)\) is the number of the \(v_i\) which have rank \(j\) in \(T_i\), and so
\[
\sum_{j \geq 0} c_j m_j(T, v) = \sum_{i=1}^{d} \left( c_{r_i} + \sum_{j \geq 0} c_j m_j(T_i, v_i) \right).
\]
Also,
\[
\lambda(T, v) = 1 + \sum_{i=1}^{d} \frac{\lambda(T_i, v_i) \alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1} \geq 1 + \sum_{i=1}^{d} \frac{1 + \sum_{j \geq 0} c_j m_j(T_i, v_i) \alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1},
\]
by the induction hypothesis, and so it is sufficient to prove that for every \(i\)
\[
\frac{1 + \sum_{j \geq 0} c_j m_j(T_i, v_i) \alpha(T_i, v_i)}{\alpha(T_i, v_i) + 1} \geq \sum_{j \geq 0} c_j m_j(T_i, v_i) + c_{r_i},
\]
or equivalently
\[
1 - c_{r_i} \geq \frac{1 + \sum_{j \geq 0} c_j m_j(T_i, v_i)}{\alpha(T_i, v_i) + 1}.
\]
If \(r_i = 0\) then the root has no children and \(m_j(T_i, v_i) = 0\) for each \(j\); also \(\alpha(T_i, v_i) = 1\) so this is true (and the two sides are equal). If \(r_i = 1\) then all the children of the root are leaves; if it has \(l\) children then \(l \geq 2\) and so
\[
\frac{1 + \sum_{j \geq 0} c_j m_j(T_i, v_i)}{\alpha(T_i, v_i) + 1} = \frac{1 + \frac{l}{2}}{1 + 2^l} \leq \frac{2}{5} = 1 - c_1,
\]
as required.

From here onwards, then, we shall assume \( r_i > 1 \). In that case the root is not a leaf and since \( T_i \in \mathcal{T}_3^r \) it has at least \( \frac{a_i + 1}{2} \) leaves; it also contains the root and at least one vertex of rank \( j \) for every \( 1 \leq j < r_i \). By Lemma \[3\] then,

\[
\alpha(T_i, v_i) \geq 2^{\frac{a_i + 1}{2}} + r_i - 1.
\]

We now turn to bound \( \sum_{j \geq 0} c_j m_j(T_i, v_i) \). Recall that, for each \( j, c_j + 1 \geq c_j \) but \( m_{j+1}(T_i, v_i) \leq m_j(T_i, v_i) \). Also note that, since \( v_i \) has rank \( r_i \) in \( T \), \( m_j(T_i, v_i) \geq 1 \) for each \( j < r_i \) but \( m_j(T_i, v_i) = 0 \) for each \( j \geq r_i \).

\[
(r_i - 1) \sum_{j=1}^{r_i-1} c_j m_j(T_i, v_i) \leq \left( \sum_{j=1}^{r_i-1} c_j \right) \left( \sum_{j=1}^{r_i-1} m_j(T_i, v_i) \right)
\]

by Chebyshov’s sum inequality (see, e.g., \[3\]). Using the fact that

\[
\sum_{j=0}^{r_i-1} m_j(T_i, v_i) = n_i - 1,
\]

and writing \( l_i = m_0(T_i, v_i) \), we get

\[
\sum_{j=0}^{r_i-1} c_j m_j(T_i, v_i) \leq c_0 l_i + \left( \frac{c_1 + c_2 + \cdots + c_{r_i-1}}{r_i - 1} \right) (n_i - l_i - 1).
\]

Since \( c_0 = \frac{1}{2} \leq c_i \), the right-hand side is a decreasing function of \( l_i \). Remembering that \( l_i \geq \frac{n_i + 1}{2} \), then,

\[
\sum_{j \geq 0} c_j m_j(T_i, v_i) \leq \frac{1}{2} \left( \frac{n_i + 1}{2} \right) + \left( \frac{c_1 + c_2 + \cdots + c_{r_i-1}}{r_i - 1} \right) \left( \frac{n_i - 3}{2} \right),
\]

and, combining our two bounds,

\[
\frac{1 + \sum_{j \geq 0} c_j m_j(T_i, v_i)}{\alpha(T_i, v_i) + 1} \leq \frac{1 + \frac{1}{2} \left( \frac{n_i + 1}{2} \right) + \left( \frac{c_1 + c_2 + \cdots + c_{r_i-1}}{r_i - 1} \right) \left( \frac{n_i - 3}{2} \right)}{2^{\frac{a_i + 1}{2}} + r_i}.
\]

Recall that \( T_i \) has at most \( \frac{a_i + 1}{2} \) vertices which are not leaves, which include the root and at least one vertex of rank \( j \) for each \( 1 \leq j < r_i \). Thus \( n_i \geq 2r_i + 1 \).

Fix \( r \geq 2 \) and write

\[
\begin{align*}
  f_r(k) &= 1 + \frac{1}{2} \left( \frac{k + 1}{2} \right) + \left( \frac{c_1 + c_2 + \cdots + c_r}{r - 1} \right) \left( \frac{k - 3}{2} \right) ,
  g_r(k) &= 2^{\frac{a_i + 1}{2}} + r.
\end{align*}
\]

If \( k \geq 2r + 1 \geq 5 \), since \( 1 \geq c_j \geq \frac{1}{2} \) for each \( j \), \( f_r(k) \geq \frac{k}{2} \) and \( f_r(k + 1) - f_r(k) \leq \frac{3}{2} \), so

\[
\frac{f_r(k + 1) - f_r(k)}{f_r(k)} \leq \frac{3}{2r} \leq \frac{3}{10},
\]

\[13\]
also, $2^{k+1} \geq 2^{r+1} \geq 4r$ and so

$$\frac{g_r(k+1) - g_r(k)}{g_r(k)} = \frac{(\sqrt{2} - 1)2^{k+1}}{2^{k+1} + r} \geq \frac{(\sqrt{2} - 1)}{1 + \frac{r}{2}} > \frac{8}{25}.$$  

Consequently, $\frac{f_r(k+1)}{f_r(k)} < \frac{g_r(k+1)}{g_r(k)}$ and so $\frac{f_r(k)}{g_r(k)}$ is a decreasing function of $k$ and maximised at $k = 2r + 1$ (given the requirement that $k \geq 2r + 1$). Therefore,

$$1 + \sum_{j \geq 0} c_j m_j(T_i, v_i) \leq \frac{1}{\alpha(T_i, v_i) + 1} \leq \frac{1 + \frac{1}{2} \left(\frac{2^{k+1}}{r_i} + \frac{\sum \epsilon_j}{r_i - 1}\right) \left(\frac{2^{k+1}}{r_i}\right)}{2^{k+1} + r_i} \leq \frac{1 + \frac{1}{2} (r_i + 1) + \left(\frac{c_0 + c_1 + \cdots + c_{r_i - 1}}{r_i - 1}\right) (r_i - 1)}{2^{r_i + 1} + r_i} = \frac{1 + \frac{r_i}{2} + c_0 + c_1 + c_2 + \cdots + c_{r_i - 1}}{2^{r_i + 1} + r_i} = 1 - c_{r_i},$$

as required.

The sequence $(c_j)_{j \geq 0}$ begins $\frac{1}{2}, \frac{3}{2}, \frac{6}{2}, 1471, 4819, 7078, \ldots$, but we shall only need that it is increasing and tends to one. We may combine the above bound with that of Lemma 4 to obtain necessary and sufficient conditions for a sequence of trees in $\mathcal{T}_3$ to have density tending to $\frac{3}{4}$.

**Theorem 14.** A sequence of distinct trees in $\mathcal{T}_3$ has average subtree density tending to $\frac{3}{4}$ if and only if the proportion of leaves tends to $\frac{1}{2}$ and the proportion of twigs tends to $0$.

**Proof.** Write $(T_i)_{i \geq 0}$ for our sequence and let $T_i$ have $n_i$ vertices, $n_i \xi_i$ leaves and $n_i \varepsilon_i$ twigs. We know that $\xi_i > \frac{1}{2}$ for every $i$, since the number of leaves is at least $\frac{\left(\frac{1}{2}\right)^k}{k+1}$. By Lemmas 3 and 4, we have the two upper bounds $\mu(T_i) < n_i - \frac{1}{2} n_i \xi_i$ and $\mu(T_i) \leq \frac{3}{4}n_i - \frac{1}{4} n_i \xi_i$, so $D(T_i) < 1 - \frac{1}{4} \xi_i$ and $D(T_i) < \frac{3}{4} - \frac{1}{4} \xi_i$. If $\xi_i \neq \frac{1}{2}$, then for some $\delta > 0$, $\xi_i > \frac{1}{2} + \delta$, and so $D(T_i) < \frac{3}{4} - \frac{1}{4} \delta$, for infinitely many $i$; if $\xi_i \neq \frac{1}{2}$ then similarly there is some $\delta > 0$ for which $D(T_i) < \frac{3}{4} - \frac{1}{4} \delta$ for infinitely many $i$.

Conversely, suppose $\xi_i \to \frac{1}{2}$ and $\xi_i \to 0$. Since there are only finitely many trees of each order, $n_i \to \infty$ and for $i$ sufficiently large there exists $v_i$ such that $|\mu(T_i) - \lambda(T_i, v_i)| < 2$; again $|D(T_i) - \frac{1}{n_i} \lambda(T_i, v_i)| \to 0$.

Consider $T_i$ rooted at $v_i$. There are at most $n_i \xi_i$ vertices of rank zero and $n_i \varepsilon_i$ of rank one. In fact, since each vertex of rank $j + 1$ has a child of rank $j$, and these are distinct, there are at most $n_i \varepsilon_i$ vertices of rank $j$ for every $j \geq 1$.

For any $\delta > 0$ we may find $k$ such that $c_{k+1} > 1 - \delta$. Then, using the same
notation as before,
\[
\lambda(T_i, v_i) \geq 1 + \sum_{j \geq 0} c_j m_j(T_i, v_i)
\]
\[
\geq \frac{1}{2} \left( \sum_{j=0}^{k} m_j(T_i, v_i) \right) + c_{k+1} \left( 1 + \sum_{j \geq k+1} m_j(T_i, v_i) \right)
\]
\[
= \frac{1}{2} \left( \sum_{j=0}^{k} m_j(T_i, v_i) \right) + c_{k+1} \left( n_i - \sum_{j=0}^{k} m_j(T_i, v_i) \right)
\]
\[
> \frac{1}{2} n_i (\xi_i + k \varepsilon_i) + (1 - \delta)n_i(1 - \xi_i - k \varepsilon_i)
\]

For \( i \) sufficiently large, \( \frac{1}{2} < \xi_i + k \varepsilon_i < \frac{1}{2}(1 + \delta) \), so
\[
\frac{\lambda(T_i, v_i)}{n_i} > \frac{1}{4} + \frac{1}{2}(1 - \delta)^2 > \frac{3}{4} - \delta.
\]

Since \( \frac{1}{n_i} \lambda(T_i, v_i) < \frac{3}{4} + \frac{2}{n_i}, \frac{1}{n_i} \lambda(T_i, v_i) \to \frac{3}{4} \), and so \( D(T_i) \to \frac{3}{4} \).

\[\square\]

6 Final Remarks

Theorems 12 and 14 give a complete classification of sequences of series-reduced trees with average subtree density tending to either extremal value. We remarked earlier that it is not necessary for the ratio of the diameter to the number of vertices to tend to \( \frac{1}{2} \) in order for the average subtree density to tend to \( \frac{3}{4} \); we conclude by giving a sequence with average subtree density tending to \( \frac{3}{4} \) for which the ratio of the diameter to the number of vertices tends to 0.

For \( k \geq 3 \) and \( r \geq 1 \), we define the starfish \( S_{Fk,r} \) with \( k \) arms and radius \( r \) as follows: take \( k \) paths of length \( r \) (i.e. having \( r + 1 \) vertices) with a shared end-vertex but otherwise disjoint. Now to each vertex of degree two attach an additional leaf.

\( S_{Fk,r} \) has \( 2k(r - 1) + 1 \) vertices, \( kr \) leaves and \( k \) twigs; its diameter is \( 2r \).

It follows from Theorem 12 that a sequence \( (S_{Fk_i,r_i})_{i \geq 0} \) of starfish has average subtree density tending to \( \frac{3}{4} \) provided \( r_i \to \infty \); if also \( k_i \to \infty \) then the ratio of the diameter to the number of vertices tends to 0.

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