LEAF-INDUCED SUBTREES OF LEAF-FIBONACCI TREES

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ABSTRACT. In analogy to a concept of Fibonacci trees, we define the leaf-Fibonacci tree of size $n$ and investigate its number of nonisomorphic leaf-induced subtrees. Denote by $f_0$ the one vertex tree and $f_1$ the tree that consists of a root with two leaves attached to it; the leaf-Fibonacci tree $f_n$ of size $n \geq 2$ is the binary tree whose branches are $f_{n-1}$ and $f_{n-2}$. We derive a nonlinear difference equation for the number $N(f_n)$ of nonisomorphic leaf-induced subtrees (subtrees induced by leaves) of $f_n$, and also prove that $N(f_n)$ is asymptotic to $1.00001887227319\ldots (1.48369689570172\ldots)\phi^n$ ($\phi =$ golden ratio) as $n$ grows to infinity.

1. INTRODUCTION

Fibonacci trees are an alternative approach to a binary search in computer science and information processing [10, p. 417]. The Fibonacci tree of order $n$ is defined as the binary tree whose left branch is the Fibonacci tree of order $n-1$ and right branch is the Fibonacci tree of order $n-2$, while the Fibonacci tree of order 0 or 1 is the tree with only one vertex [10]. We show in Figure 1 the Fibonacci tree of order 5.

![Figure 1. The Fibonacci tree of order 5.](image)

Thus, the Fibonacci tree of order $n$ has precisely $F_{n+1}$ leaves (so $2F_{n+1} - 1$ vertices), where $F_n$ denotes the $n$-th Fibonacci number:

$$F_0 = 0, \quad F_1 = 1, \quad F_n = F_{n-1} + F_{n-2} \quad \text{for} \quad n > 1.$$

Fibonacci trees are also a special case of so-called AVL (“Adel’son-Vel’skii and Landis”—named after the inventors) trees [1]; these trees have the defining property that for every

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internal vertex $v$, the heights (i.e., the greatest distance of a leaf from the root) of the left and right branches of the subtree rooted at $v$ (consisting of $v$ and all its descendants) differ by at most one. According to [1], AVL trees are the first data structure to be invented. Figure 2 shows an AVL tree of height 3. For more information on Fibonacci trees and their uses, we refer to [13, 8, 9, 7].

Figure 2. An AVL tree of height 3.

In analogy to the concept of Fibonacci trees from [10], we define the leaf-Fibonacci tree of size (height) $n$ as follows:

- Denote by $f_0$ the tree with only one vertex and $f_1$ the tree that consists of a root with two leaves attached to it;
- For $n \geq 2$, connect the roots of the trees $f_{n-1}$ and $f_{n-2}$ to a new common vertex to obtain the tree $f_n$.

In other words, the leaf-Fibonacci tree $f_n$ of size $n \geq 2$ is the binary tree whose branches are the leaf-Fibonacci trees $f_{n-1}$ and $f_{n-2}$. Hence, $f_n$ has precisely $F_{n+2}$ leaves, where $F_n$ is the $n$-th Fibonacci number ($F_1 = 1, F_2 = 1, F_3 = 2, F_4 = 3, F_5 = 5, F_6 = 8, F_7 = 13, \ldots$). Figure 3 shows the leaf-Fibonacci tree of size 5.

Figure 3. The leaf-Fibonacci tree of size 5.

In this note, we shall be interested in the number of nonisomorphic subtrees induced by leaves (henceforth, leaf-induced subtrees) of a leaf-Fibonacci tree of size $n$.

Let $T$ be a rooted tree without vertices of outdegree 1 (also known as topological or series-reduced or homeomorphically irreducible trees [3, 2, 5, 12]). Every choice of $k$ leaves
of $T$ induces another topological tree, which is obtained by extracting the minimal subtree of $T$ that contains all the $k$ leaves and suppressing (if any) all vertices of outdegree 1; see Figure 4 for an illustration. Every subtree obtained through this operation is sometimes

![Figure 4. A topological tree (on the left) and the subtree induced by the leaves $\ell_1, \ell_2, \ell_3, \ell_4$ (on the right).](image)

referred to as a leaf-induced subtree [4, 5]. We note the study of subtrees induced by leaves of binary trees finds a noteworthy relevance in phylogenetics—see Semple and Steel’s book [11] which describes the mathematical foundations of phylogenetics.

Two rooted trees are said to be isomorphic if there is a graph isomorphism (preserving adjacency) between them that maps the root of one to the root of the other. It is important to note that the problem of enumerating leaf-induced subtrees becomes trivial if isomorphisms are not taken into account: in fact, it is clear that every topological tree with $n$ leaves has exactly $2^n - 1$ leaf-induced subtrees.

We mention that nonisomorphic leaf-induced subtrees of a topological tree have been studied only very recently: Wagner and the present author [6] obtained exact and asymptotic enumeration results on the number of nonisomorphic leaf-induced subtrees of two classes of $d$-ary trees, namely so-called $d$-ary caterpillars and even $d$-ary trees. In [6], they also derived extremal results for the number of root containing leaf-induced subtrees of a topological tree.

We shall denote the number of nonisomorphic leaf-induced subtrees of the leaf-Fibonacci tree $f_n$ by $N(f_n)$. Our main results are a recurrence relation and an asymptotic formula for $N(f_n)$. As it turns out, the plan to compute $N(f_n)$ will be to consider the number of root containing leaf-induced subtrees of $f_n$.

In [14], Wagner alone studied the number of independent vertex subsets (set of vertices containing no pair of adjacent vertices) of a Fibonacci tree of order $n$ with the notable difference that in his context, the Fibonacci tree of order 0 has no vertices. Wagner
derived a system of recurrence relations for the number of independent vertex subsets of a Fibonacci tree of an arbitrary order \( n \), and also proved that there are positive constants \( A, B > 0 \) such that the number of independent vertex subsets of a Fibonacci tree of order \( n \) is asymptotic to \( A \cdot B^F_n \) as \( n \) grows to infinity. In the present study, we obtain a similar asymptotic formula for the number \( N(f_n) \) of nonisomorphic leaf-induced subtrees of the leaf-Fibonacci tree of size \( n \): we demonstrate—not expectedly—that for some effectively computable constants \( A_1, A_2 > 0 \),
\[
N(f_n) \sim A_1 \cdot A_2^F_n \text{ as } n \to \infty.
\]

2. MAIN RESULTS

We note from the recursive definition of the tree \( f_n \) that \( f_m \) is a leaf-induced subtree of \( f_n \) for every \( m \leq n \). However, not every leaf-induced subtree of \( f_n \) is again a leaf-Fibonacci tree: in fact, by repeatedly removing leaves from \( f_n \), one easily sees that \( f_n \) has leaf-induced subtrees of every number of leaves \( k \) between 1 and \( n \).

As mentioned in the introduction, the plan to compute \( N(f_n) \) will be to consider the number of root containing leaf-induced subtrees of \( f_n \).

**Lemma 1.** All nonisomorphic leaf-induced subtrees with two or more leaves of \( f_n \) can be identified as containing the root of \( f_n \).

**Proof.** The tree \( f_0 \) has only one vertex which is also its leaf and root, so the statement holds vacuously for \( n = 0 \). The statement is trivial for \( n = 1 \) (\( f_1 \) is the only leaf-induced subtree in this case). Let \( n > 1 \) and consider a subset of \( k > 1 \) leaves of \( f_n \). We argue by double induction on \( n \) and \( k \):

- If all \( k \) leaves belong to \( f_{n-1} \) then by the induction hypothesis on \( n \), the induced subtree with \( k \) leaves contains the root of \( f_{n-1} \). Moreover, by the induction hypothesis on \( k \), the tree \( f_{n-1} \) can be identified as containing the root of \( f_n \) (as \( f_{n-1} \) is clearly a leaf-induced subtree of \( f_n \)). Hence, the induced subtree with \( k \) leaves contains the root of \( f_n \).
- If all \( k \) leaves belong to \( f_{n-2} \), then we also deduce by the induction hypothesis that the induced subtree with \( k \) leaves is a root containing leaf-induced subtree of \( f_n \).
- If \( k_1 \) leaves belong to \( f_{n-1} \) and \( k - k_1 \) leaves belong to \( f_{n-2} \), then by the induction hypothesis, the induced subtrees with \( k_1 \) and \( k - k_1 \) leaves are root containing leaf-induced subtrees of \( f_{n-1} \) and \( f_{n-2} \), respectively. Consequently, the root of the induced subtree with \( k \) leaves coincides with the root of \( f_n \).

This completes the induction step as well as the proof of the lemma. \( \square \)

We then obtain the following proposition:

**Proposition 2.** The number \( N(f_n) \) of nonisomorphic leaf-induced subtrees of the leaf-Fibonacci tree \( f_n \) satisfies the following nonlinear recurrence relation:

\[
N(f_n) = 1 + \frac{1}{2} N(f_{n-2}) - \frac{1}{2} N(f_{n-2})^2 + N(f_{n-2}) \cdot N(f_{n-1})
\]
with initial values $N(f_0) = 1, N(f_1) = 2$.

**Proof.** It is obvious that $N(f_0) = 1$ and $N(f_1) = 2$. Let $n > 1$. By Lemma 1, $N(f_n)$ is precisely one more the number of nonisomorphic root containing leaf-induced subtrees of $f_n$ (the subtree with only one vertex has been included). Since all leaf-induced subtrees of the leaf-Fibonacci tree $f_{n-2}$ are again leaf-induced subtrees of $f_{n-1}$, the nonisomorphic root containing leaf-induced subtrees of $f_n$ can be categorised by two types of enumeration:

- Both branches of the induced subtree are leaf-induced subtrees of $f_{n-2}$. The total number of these possibilities is $\binom{1+N(f_{n-2})}{2}$ as the induced subtrees have to be nonisomorphic.
- One of the branches of the induced subtree is a leaf-induced subtree of $f_{n-2}$ while the other branch is a leaf-induced subtree of $f_{n-1}$ but does not belong to the set of leaf-induced subtrees of $f_{n-2}$. The total number of these possibilities is $N(f_{n-2})N(f_{n-1}) - N(f_{n-2})$.

Therefore, we obtain

$$N(f_n) = 1 + \binom{1+N(f_{n-2})}{2} + N(f_{n-2})(N(f_{n-1}) - N(f_{n-2}))$$

$$= 1 + \frac{1}{2}N(f_{n-2}) - \frac{1}{2}N(f_{n-2})^2 + N(f_{n-2}) \cdot N(f_{n-1}),$$

which completes the proof of the proposition. \qed

The sequence $(N(f_n))_{n \geq 0}$ starts as

$N(f_0) = 1, N(f_1) = 2, N(f_2) = 3, N(f_3) = 6, N(f_4) = 16, N(f_5) = 82, N(f_6) = 1193, N(f_7) = 94506, N(f_8) = 112034631, \ldots$

We remark that recursion (1) cannot be solved explicitly. Therefore, finding an asymptotic formula should be in order. In the following theorem, we show—not expectedly—that $N(f_n)$ grows doubly exponentially in $n$.

**Theorem 3.** There are two positive constants $K_1, K_2 > 0$ (both solely depending on the first terms of $(N(f_n))_{n \geq 0}$) such that

$$N(f_n) = (1 + o(1))K_1 \cdot K_2^\left(\frac{1+\sqrt{5}}{2}\right)^n$$

as $n \to \infty$.

**Proof.** For ease of notation, set $A_n := N(f_n)$. Then we have

$$A_n = 1 + \frac{1}{2}A_{n-2} - \frac{1}{2}A_{n-2}^2 + A_{n-2} \cdot A_{n-1}$$

with initial values $A_0 = 1, A_1 = 2$. Since the sequence $(A_n)_{n \geq 0}$ increases with $n$, it is not difficult to note that

$$A_n \geq \frac{1}{2}A_{n-1} \cdot A_{n-2}.$$
for all \( n \geq 2 \). Also, since \( A_n \geq A_2 = 3 \) for all \( n \geq 2 \) and \( 1 + A_1/2 - A_1^2/2 = 0 \), it is not difficult to see that 
\[
A_n \leq A_{n-1} \cdot A_{n-2}
\]
for all \( n \geq 3 \). Thus, we have

\[
\lim_{n \to \infty} \frac{A_{n-1}}{A_n} = 0,
\]

which also implies that the sequence \((A_{n-1}/A_n)_{n \geq 1}\) is bounded for every \( n \geq 1 \). Let us use \( Q_n \) as a shorthand for \( \log(A_n) \) and \( E_n \) as a shorthand for

\[
\log \left( 1 + \frac{1}{2A_{n-1}} - \frac{A_{n-2}}{2A_{n-1}} + \frac{1}{A_{n-1} \cdot A_{n-2}} \right).
\]

With these notations, we have

\[
Q_n = Q_{n-1} + Q_{n-2} + E_n.
\]

By setting \( R_{n-1} := Q_{n-2} \), we obtain the following system (written in matrix form) of two linear difference equations:

\[
\begin{pmatrix}
Q_n \\
R_n
\end{pmatrix} = \begin{pmatrix}
1 & 1 \\
1 & 0
\end{pmatrix} \begin{pmatrix}
Q_{n-1} \\
R_{n-1}
\end{pmatrix} + \begin{pmatrix}
E_n \\
0
\end{pmatrix}.
\]

By iteration on \( n \), one gets

\[
\begin{pmatrix}
Q_n \\
R_n
\end{pmatrix} = \left( \begin{pmatrix}
1 & 1 \\
1 & 0
\end{pmatrix} \right)^{n-1} \begin{pmatrix}
Q_1 \\
Q_0
\end{pmatrix} + \sum_{i=2}^{n} \left( \begin{pmatrix}
1 & 1 \\
1 & 0
\end{pmatrix} \right)^{n-i} \begin{pmatrix}
E_i \\
0
\end{pmatrix}
\]

for all \( n \geq 2 \), as \( R_1 = Q_0 \). The eigenvalue decomposition gives us

\[
\begin{pmatrix}
1 & 1 \\
1 & 0
\end{pmatrix} = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix}
\lambda_1 & \lambda_2 \\
1 & 1
\end{pmatrix} \begin{pmatrix}
\lambda_1 & 0 \\
0 & \lambda_2
\end{pmatrix} \begin{pmatrix}
1 & -\lambda_2 \\
-1 & \lambda_1
\end{pmatrix}
\]

with

\[
\lambda_1 = \frac{1 - \sqrt{5}}{2} \quad \text{and} \quad \lambda_2 = \frac{1 + \sqrt{5}}{2}.
\]

It follows that

\[
\begin{pmatrix}
1 & 1 \\
1 & 0
\end{pmatrix}^m = \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix}
\lambda_1 & \lambda_2 \\
1 & 1
\end{pmatrix} \begin{pmatrix}
\lambda_1^m & 0 \\
0 & \lambda_2^m
\end{pmatrix} \begin{pmatrix}
1 & -\lambda_2 \\
-1 & \lambda_1
\end{pmatrix}
\]

\[
= \frac{1}{\lambda_1 - \lambda_2} \begin{pmatrix}
\lambda_1^{m+1} - \lambda_2^{m+1} & \lambda_1 \cdot \lambda_2^{m+1} - \lambda_1^{m+1} \cdot \lambda_2 \\
\lambda_1^m - \lambda_2^m & \lambda_1 \cdot \lambda_2^m - \lambda_1^m \cdot \lambda_2
\end{pmatrix}
\]

for all integer values of \( m \). Consequently, we have

\[
\begin{pmatrix}
Q_n \\
R_n
\end{pmatrix} = \frac{\log(2)}{\lambda_1 - \lambda_2} \begin{pmatrix}
\lambda_1^n - \lambda_2^n \\
\lambda_1^{n-1} - \lambda_2^{n-1}
\end{pmatrix} + \sum_{i=2}^{n} \frac{E_i}{\lambda_1 - \lambda_2} \begin{pmatrix}
\lambda_1^{n-i} - \lambda_2^{n-i+1} \\
\lambda_1^{n-i} - \lambda_2^{n-i}
\end{pmatrix}
\]
for all \(n \geq 2\) as \(Q_0 = 0\) and \(Q_1 = \log(2)\). Therefore, we obtain

\[ Q_n = \frac{\log(2)}{\lambda_2 - \lambda_1} \left( \lambda_2^n - \lambda_1^n \right) + \frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \left( \lambda_2^{n-i+1} - \lambda_1^{n-i+1} \right) \]

for all \(n \geq 2\). Since the sequence \((E_n)_{n \geq 2}\) is bounded for every \(n \geq 2\) (as \(\lim_{n \to \infty} E_n = 0\) by virtue of (3) and (2)), we derive that

\[
\sum_{i=2}^{n} |E_i| \cdot |\lambda_1|^{n-i+1} \leq \frac{|\lambda_1|^n - |\lambda_1|}{|\lambda_1| - 1} \cdot \sup_{2 \leq m \leq n} |E_m|
\]

for all \(n \geq 2\). This implies that the quantity

\[
\frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \cdot \lambda_1^{n-i+1}
\]

converges to a definite limit as \(n \to \infty\) (note that \(|\lambda_1| < 1\) and \(\sup_{2 \leq m \leq n} |E_m|\) is finite for every \(n \geq 2\)). On the other hand, we have

\[
0 \leq \left| \sum_{i=n+1}^{\infty} E_i \cdot \lambda_2^{n-i+1} \right| \leq \frac{\lambda_2}{\lambda_2 - 1} \cdot \sup_{m \geq n+1} |E_m|
\]

for all \(n \geq 2\) (note that \(\lambda_2 > 1\)), which implies that

\[
\frac{1}{\lambda_2 - \lambda_1} \sum_{i=n+1}^{\infty} E_i \cdot \lambda_2^{n-i+1} = O\left( \sup_{m \geq n+1} |E_m| \right) = o(1)
\]

as \(n \to \infty\). Putting everything together, we arrive at

\[
Q_n = \frac{\lambda_2^n}{\lambda_2 - \lambda_1} \left( \log(2) + \sum_{i=2}^{\infty} E_i \cdot \lambda_2^{i+1} \right) - \frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \cdot \lambda_1^{n-i+1} + O\left( \sup_{m \geq n+1} |E_m| \right) + O(\lambda_1^n)
\]

\[
= \frac{\lambda_2^n}{\lambda_2 - \lambda_1} \left( \log(2) + \sum_{i=2}^{\infty} E_i \cdot \lambda_2^{i+1} \right) - \frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \cdot \lambda_1^{n-i+1} + o(1)
\]

as \(n \to \infty\). We deduce that

\[
A_n = \left( 1 + O\left( \lambda_1^n + \sup_{m \geq n+1} |E_m| \right) \right) \cdot \exp\left( \frac{\lambda_2^n}{\lambda_2 - \lambda_1} \left( \log(2) + \sum_{i=2}^{\infty} E_i \cdot \lambda_2^{i+1} \right) - \frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \cdot \lambda_1^{n-i+1} \right) = (1 + o(1)) \cdot \exp\left( \frac{\lambda_2^n}{\lambda_2 - \lambda_1} \left( \log(2) + \sum_{i=2}^{\infty} E_i \cdot \lambda_2^{i+1} \right) - \frac{1}{\lambda_2 - \lambda_1} \sum_{i=2}^{n} E_i \cdot \lambda_1^{n-i+1} \right)
\]
as \( n \to \infty \). Call \( K_2 \) the quantity
\[
\exp \left( \frac{1}{\lambda_2 - \lambda_1} \left( \log(2) + \sum_{i=2}^{\infty} E_i \cdot \lambda_2^{-i+1} \right) \right),
\]
and \( K_1 \) the quantity
\[
\exp \left( - \frac{1}{\lambda_2 - \lambda_1} \cdot \lim_{n \to \infty} \left( \sum_{i=2}^{n} E_i \cdot \lambda_1^{-i+1} \right) \right).
\]
Thus,
\[
A_n = N(f_n) = (1 + o(1)) K_1 \cdot K_2 = (1 + o(1)) K_1 \cdot K_2^{\left(1 + \sqrt{5} \over 2\right)}
\]
as \( n \to \infty \), where \( K_1 \) and \( K_2 \) can now be written as
\[
K_2 = \exp \left( \frac{1}{\sqrt{5}} \left( \log(2) + \sum_{i=2}^{\infty} \left( \frac{1 + \sqrt{5}}{2} \right)^{-i+1} \right) \right).
\]
\[
K_1 = \exp \left( - \frac{1}{\sqrt{5}} \cdot \lim_{n \to \infty} \left( \sum_{i=2}^{n} \left( \frac{1 - \sqrt{5}}{2} \right)^{n-i+1} \right) \right).
\]
By (numerically) evaluating \( K_1 \) and \( K_2 \), we obtain that the number of nonisomorphic leaf-induced subtrees of the leaf-Fibonacci tree \( f_n \) is asymptotically
\[
1.00001887227319 \cdots (1.48369689570172 \cdots) \left(1 + \sqrt{5} \over 2\right)\]
as \( n \to \infty \). This completes the proof of the theorem.

This asymptotic formula can also be written in terms of the Fibonacci number \( F_n \): the number of leaves of \( f_n \) is given by
\[
|f_n| = F_{n+2} = \frac{1}{\sqrt{5}} \left( \left( \frac{1 + \sqrt{5}}{2} \right)^{2+n} - \left( \frac{1 - \sqrt{5}}{2} \right)^{2+n} \right)
\]
for every \( n \); so we deduce that
\[
\frac{10}{5 + 3\sqrt{5}} \cdot |f_n| \sim \left( \frac{1 + \sqrt{5}}{2} \right)^n
\]
as $n \to \infty$. This implies that
\[
N(f_n) \sim K_1 \cdot K_2^{\frac{10}{5+\sqrt{5}} |f_n|} = 1.00001887227319 \cdots (1.48369689570172 \cdots)^{\frac{5+\sqrt{5}}{2}} |f_n|
\]
as $n \to \infty$.

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