Graphs, Partitions and Fibonacci Numbers. ⋆

Dedicated to Professor Helmut Prodinger on the occasion of his 50th birthday

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Abstract

The Fibonacci number of a graph is the number of independent vertex subsets. In this paper, we investigate trees with large Fibonacci number. In particular, we show that all trees with n edges and Fibonacci number $> 2^{n-1} + 5$ have diameter ≤ 4 and determine the order of these trees with respect to their Fibonacci numbers. Furthermore, it is shown that the average Fibonacci number of a star-like tree (i.e. diameter ≤ 4) is asymptotically $A \cdot 2^n \cdot \exp(B\sqrt{n}) \cdot n^{3/4}$ for constants A, B as $n \to \infty$. This is proved by using a natural correspondence between partitions of integers and star-like trees.

Key words: Star-like tree, partition, Fibonacci number, independent set

1 Introduction

Let $G = (V(G), E(G))$ denote a graph with vertex set $V(G)$ and edge set $E(G)$. All graphs considered here are finite and simple. In general we will use

⋆ The work was supported by Austrian Science Fund project no. S-8307-MAT.

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Preprint submitted to Discrete Applied Mathematics *27 October 2006*

the terminology introduced in [5]. We will write $G \setminus \{v_1, v_2, \ldots\}$ for the graph which results from deleting the vertices $v_1, v_2, \ldots \in V(G)$ and all edges incident with them, and we will write $G \setminus \{e_1, e_2, \ldots\}$ for the graph $(V(G), E(G) \setminus \{e_1, e_2, \ldots\})$, where $e_1, e_2, \ldots \in E(G)$.

For a graph G, its Fibonacci number – simply denoted by $F(G)$ – is defined as the number of subsets of $V(G)$ in which no two vertices are adjacent in G, i.e. in graph-theoretical terminology, the number of independent sets of G, including the empty set. The concept of the Fibonacci number for a graph was introduced in [28] and discussed in several papers [17,18]. Paper [17] investigated the Fibonacci number of binary trees (and more generally, t-ary and simple generated trees) including asymptotic results for $n = |E(G)| \to \infty$. In [28] it was observed that the star S_n with n edges has maximal Fibonacci

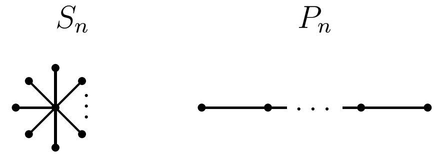

Fig. 1. The star and the path.

number among all trees with n edges and $F(S_n) = 2^n + 1$. Furthermore it was shown that the path P_n with n edges is the tree with minimal Fibonacci number among all trees with n edges and $F(P_n) = f_{n+3}$, where $f_0 = 0$, $f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$ for $n > 1$ denotes the sequence of Fibonacci numbers.

A related, but far more difficult problem is the question of finding the maximum number of maximal independent sets in a graph, which was settled by Moon and Moser [25] and independently by Erdős. In a series of papers, analogous results were determined for special types of graphs, including trees, forests and connected graphs (cf. [11,12,29,34]).

For the number of independent sets, bounds for several classes of graphs were given. For instance, Alameddine [1] considered maximal outerplanar graphs, Dutton et al. [9] gave bounds involving the maximum number of independent edges, and Liu [23] studied certain classes of connected graphs.

A concept that is highly related to the Fibonacci number is the independence polynomial (cf. [6,16]), a polynomial whose k-th coefficient is the number of independent subsets of size k. It is obvious that the Fibonacci number is exactly the value at 1.

A mathematical application for the number of independent subsets is given in group theory: a subset S of an additive group is called sum-free if it contains no elements x, y, z such that $x + y = z$ (cf. [7,30]). The question of bounding the number of sum-free sets is connected to the number of independent sets in the corresponding Cayley graphs. In fact, from a theorem of Alon [2] (every

k-regular graph on n vertices has at most $2^{(1/2+\epsilon(k))n}$ independent subsets, where $\epsilon(k)$ tends to 0 as $k \to \infty$), it follows that there are $2^{(1/2+o(1))n}$ sum-free subsets of $\{1, 2, \ldots, n\}$. Alon's result was generalized to hypergraphs in a recent paper of Ordentlich and Roth [26].

It is of particular interest to determine the number of independent sets of a grid graph, which is of importance in statistical physics (cf. [4]). It is known that the Fibonacci number of a (n, m)-grid graph grows with α^{mn}, where $\alpha = 1.503048082$ is the so-called hard square entropy constant. The bound for this constant was successively improved by Weber [33], Engel [10] and Calkin and Wilf [8].

There is yet another application for the concept of the Fibonacci number of a graph in theoretical chemistry. For a molecular graph, this number was extensively studied in the monograph [24] and in various subsequent papers [19,32]. There the chemical use of the Fibonacci number $F(G)$ is demonstrated and the number is called σ-index or Merrifield-Simmons index and it is denoted by $\sigma(G)$.

The σ-index is introduced as a map from the set of chemical compounds represented by graphs to the set of real numbers. Experimental results show that the σ-index (and various similar index functions) is closely correlated with some physicochemical characteristics. Of recent interest in combinatorial chemistry are the corresponding inverse problems: given the value of the σ-index, one wants to design chemical compounds (given as graphs or trees) having that index value. The inverse problem has applications in the design of combinatorial libraries for drug discovery.

In [19] the authors established an algorithm for computing the σ-index of a given tree. Furthermore they investigated the inverse problem for the σ-index (and related index functions) and they also established a polynomial time algorithm for constructing a tree with given σ-index (provided that such a tree exists). In fact, it is not known whether there exists a tree with given σ-index s for all but finitely many positive integers s, even though the remark after Definition 4 suggests this. However, it is known that every positive integer is the number of independent subsets of a bipartite graph (cf. Linek [22]).

For a more detailed study of the properties of the Merrifield-Simmons index we refer to the monograph [24].

In the present paper we are interested in trees with n edges and large Fibonacci numbers. We already know the maximal tree with respect to its Fibonacci number; it is the star S_n. In the main result of the paper we will determine all trees T with n edges satisfying

$$2^{n-1} + 5 = F(CS_n) \leq F(T) \leq F(S_n) = 2^n + 1, \tag{1}$$

where CS_n denotes the "Christmas star" with n edges: it consists of a star with arbitrarily many rays and a "tail" of four edges connected to the center of the star (thus, its diameter is 5). CS_{11} is shown in Figure 2. Similar results, obtained by somewhat different methods, are due to Lin and Lin [21] and Wang et al. [20].

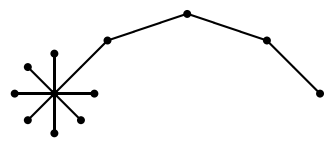

Fig. 2. The "Christmas star" CS_{11}.

It will be shown that the trees which satisfy inequality (1) belong to a family of trees (which we call "star-like") that corresponds to partitions of n into positive integers. We also include an asymptotic result (for $n \to \infty$) concerning the average Fibonacci number of these star-like trees. For the basic properties concerning partitions we refer to [3]. In particular, the famous Hardy-Ramanujan-Rademacher theorem ([3, Theorem 5.1]) plays an important role in our proofs.

Theorem 0

$$p(n) \sim \frac{\exp\left(\pi\sqrt{2n/3}\right)}{4\sqrt{3}n},$$

where

$$p(n) = |\{(c_1, \ldots, c_d) \,:\, c_1 \geq \ldots \geq c_d,\ c_1 + \cdots + c_d = n, c_i \geq 1, d \in \mathbb{N}\}|$$

denotes the number of partitions of n into positive numbers.

In Section 2 we introduce the basic concepts and prove some auxiliary results concerning graphs and partitions. Section 3 contains a proof of the main theorem. The proof depends on ordering star-like trees by their Fibonacci numbers. Section 4 is devoted to the asymptotic results and in the final Section 5 we mention some open problems.

2 Notation and preliminary results

In this paper we will only consider trees T. As in the introduction, the Fibonacci number of T is denoted by $F(T)$.

Definition 1 A tree is called *star-like* if it has diameter ≤ 4.

Definition 2 Let $(c_1, \ldots, c_d)$ be a partition of n. The star-like tree assigned to this partition is the tree which is constructed in the following way (cf. Figure 3):

- let $S_1, \ldots, S_d$ be stars with $c_1 - 1, \ldots, c_d - 1$ edges respectively, and let $v_1, \ldots, v_d$ be their centers.
- add a vertex v to the union $S_1 \cup \ldots \cup S_d$ and connect v to $v_1, \ldots, v_d$.

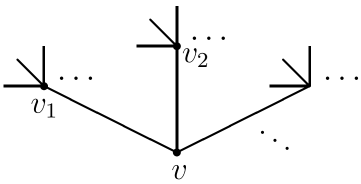

Fig. 3. A star-like tree.

Then $v_1, \ldots, v_d$ have degree $c_1, \ldots, c_d$ respectively, and the resulting graph has exactly $d + (c_1 - 1) + \ldots + (c_d - 1) = c_1 + \ldots + c_d = n$ edges. The tree itself is denoted by $S(c_1, \ldots, c_d)$, its Fibonacci number by $f(c_1, \ldots, c_d)$.

Proposition 1 Every star-like tree T is of the form $S(c_1, \ldots, c_d)$ for some partition of n; this partition is unique if the tree has diameter 4. Otherwise, there are exactly two different partitions, except in the case of the tree $S(\frac{n+1}{2}, 1, \ldots, 1)$ if n is odd.

Proof: First, let the diameter of T be equal to 4. Choose any diameter v_0, v_1, v_2, v_3, v_4. Then the distance from v_2 to any other vertex w must be ≤ 2 (otherwise, there would be a path of length ≥ 5 from v_0 to w or from v_4 to w). Therefore, all components of $T \setminus \{v_2\}$ are stars, and their midpoints are connected to v_2. It follows that the tree has the desired form, where v_2 is the unique midpoint (from every other point, there are paths of length ≥ 3).

If the diameter is 3, then we see (analogously) that T must be a double-star, i.e. the union of two stars whose centers are connected by an edge. Then there are two possibilities for the midpoint yielding the two possible representations $S(k, \underbrace{1, \ldots, 1}_{l-1})$ and $S(l, \underbrace{1, \ldots, 1}_{k-1})$, where k and l are the degrees of the two center-vertices. These representations coincide if and only if $k = l = \frac{n+1}{2}$.

Finally, the star with n edges (which has diameter 2) has the two representations $S(1, \ldots, 1)$ and $S(n)$. Thus, the claim is proved. $\square$

Definition 3 Let $c_1, \ldots, c_{d-1}$ be integers with $c_i \geq 0$. Then the tree which is made up from a path $v_0, v_1, \ldots, v_d$ of length d by attaching c_i new edges to v_i ($1 \leq i \leq d - 1$, see Figure 4) is called a $(c_1, \ldots, c_{d-1})$-*star chain*, denoted by $C(c_1, \ldots, c_{d-1})$. It has $n = c_1 + \ldots + c_{d-1} + d$ edges. $C(c_1, \ldots, c_{d-1})$ is also known as a *caterpillar tree* (see [15]).

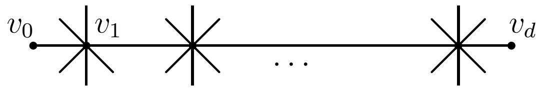

Fig. 4. A star chain.

Definition 4 Let $\mathcal{T}(n)$ be the set of all trees with n edges. We define relations $\succ$ and $\overset{!}{\succ}$ on $\mathcal{T}(n)$ by

$$T_1 \succ T_2 :\Longleftrightarrow F(T_1) > F(T_2)$$

$$T_1 \overset{!}{\succ} T_2 :\Longleftrightarrow T_1 \succ T_2 \wedge (\nexists T \in \mathcal{T}(n) : \ F(T_1) > F(T) > F(T_2))$$

Remark: $\succ$ is not a total order on $\mathcal{T}(n)$; e.g., the following two trees from $\mathcal{T}(7)$ both have Fibonacci number 60:

Fig. 5. Two trees with Fibonacci number 60.

Indeed, there are even arbitrarily large sets of trees with both equally many edges and equal Fibonacci number. This is an immediate consequence of the fact that $|\mathcal{T}(n)| \sim \beta \alpha^n n^{-5/2}$ (where $\alpha = 2.955765\ldots$, see [14,27]), which grows faster than the maximal Fibonacci number $2^n + 1$ (by Lemma 3).

Lemma 2 (cf. [13,20]) Let G be an arbitrary graph.

- If $G = G_1 \cup G_2 \ldots \cup G_k$ is the union of disjoint graphs, we have

$$F(G) = \prod_{i=1}^{k} F(G_i).$$

- If $v \in V(G)$, we have

$$F(G) = F(G \setminus \{v\}) + F(G \setminus (\{v\} \cup N(v))),$$

  where $N(v)$ denotes the neighborhood of v.

In particular, let T be a tree and $v \in V(T)$, and let $T_1, \ldots, T_k$ be the components of $T \setminus \{v\}$. Furthermore, define $v_i := N(v) \cap T_i$. Combining the two formulas, we obtain

$$F(T) = \prod_{i=1}^{k} F(T_i) + \prod_{i=1}^{k} F(T_i \setminus \{v_i\}).$$

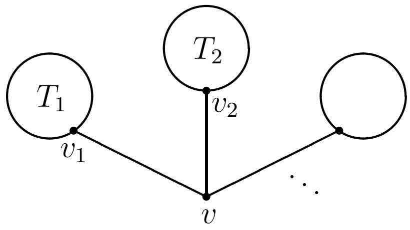

Fig. 6. Illustration of Lemma 2.

Proof: The first claim is obvious from the fact that an independent subset in G is the union of independent subsets in the components G_i; this correspondence is bijective. For the second claim, note that the first summand gives the number of independent subsets not containing v, whereas the second summand gives the number of independent subsets containing v. □

The following result is due to Prodinger and Tichy [28], for completeness we include a proof here. In [19] this result was rediscovered and extended to arbitrary graphs.

Lemma 3 For a given number of edges n, the tree T which maximizes $F(T)$ is the star S_n with n rays; $F(S_n) = 2^n + 1$.

Proof: by induction on n. For $n = 0$, there is nothing to prove. Now, assume that the result holds for n, and let T be a tree with $n+1$ edges. Furthermore, let v be a leaf of T, and let v_1 be the unique neighbor of v. Then $F(T) = F(T \setminus \{v\}) + F(T \setminus \{v, v_1\})$ by the preceding lemma.

By the induction hypothesis, we know that $F(T \setminus \{v\}) \leq F(S_n) = 2^n + 1$, with equality if and only if $T \setminus \{v_1\} \simeq S_n$. The graph $T \setminus \{v, v_1\}$ contains n vertices, so $F(T \setminus \{v, v_1\}) \leq 2^n$ (the total number of possible vertex subsets), with equality if and only if $T \setminus \{v, v_1\}$ is a graph without edges. This happens only if $T \setminus \{v\} \simeq S_n$, where v_1 is the center of the star. It follows immediately that $F(T)$ is maximal for $T \simeq S_{n+1}$, and that $F(S_{n+1}) = 2^n + 1 + 2^n = 2^{n+1} + 1$. □

Lemma 4 (replacement lemma) Let T be a tree, $e = (v, v_1) \in E(T)$ an edge, and let T_1 be the component of $T \setminus \{e\}$ which contains v_1. Now we apply the following transformation: replace all the edges of T_1 by edges incident with v; in other words, T_1 is replaced by a star with center v. If the resulting tree is denoted by T', the inequality $F(T') \geq F(T)$ holds.

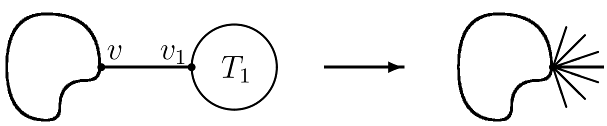

Fig. 7. Illustration of Lemma 4.

Proof: We apply Lemma 2 to v: let $T_2, \ldots, T_k$ be the components of $T \setminus \{v\}$ other than T_1, and let m be the number of vertices of T_1. It is obvious that $F(T_i \setminus \{v_i\}) < F(T_i)$ $(2 \leq i \leq k)$. Thus,

$$\prod_{i=2}^{k} F(T_i) \geq \prod_{i=2}^{k} F(T_i \setminus \{v_i\})$$

with equality if and only if $k = 1$ (in this case, we have two empty products of value 1). By Lemma 3, we know that $F(T_1) \leq 2^{m-1} + 1$ and $F(T_1 \setminus \{v_1\}) \leq 2^{m-1}$, with equality if and only if T_1 is a star with center v_1. Now applying Lemma 2 to v yields

$$F(T) = \prod_{i=1}^{k} F(T_i) + \prod_{i=1}^{k} F(T_i \setminus \{v_i\})$$

and

$$F(T') = 2^m \prod_{i=2}^{k} F(T_i) + \prod_{i=2}^{k} F(T_i \setminus \{v_i\})$$

Using the inequalities from above, we obtain

$$(2^m - F(T_1)) \prod_{i=2}^{k} F(T_i) \geq (F(T_1 \setminus \{v_1\}) - 1) \prod_{i=2}^{k} F(T_i \setminus \{v_i\})$$

with equality if either $m = 1$ (in this case, both sides are 0) or $T_i \simeq S_m$ is a star with center v_1 and $k = 1$ – note that in both cases, $T' \simeq T$. From this inequality and the formulas for $F(T')$ and $F(T)$, it follows easily that $F(T') \geq F(T)$, with equality in the aforementioned cases. □

Theorem 5 *For a given number n of edges and given diameter D, the tree T with maximal Fibonacci number $F(T)$ is the $(n-D, \underbrace{0, \ldots, 0}_{D-2})$-star chain, i.e. the tree in Figure 8 with Fibonacci number $2^{n-D+1} f_{D+1} + f_D$ (where $f_0 = 0$, $f_1 = 1$, $f_{n+1} = f_n + f_{n-1}$).*

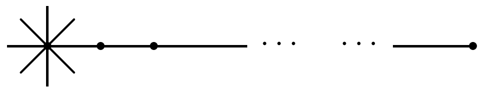

Fig. 8. Tree with maximal Fibonacci number, given the diameter.

Remark: Note that $2^{n-D+1} f_{D+1} + f_D > 2^{n-D} f_{D+2} + f_{D+1}$ (which is equivalent to $2^{n-D} f_{D-1} > f_{D-1}$, an obvious inequality). This means that the maximal Fibonacci number, given the number of edges n and the diameter D, is a decreasing function in D.

Proof: by induction on n. For $n \leq 2$, the assertion is trivial. Now let $n \geq 3$. First, we prove that the tree T of maximal Fibonacci number must be a star chain.

Let $v_0, v_1, \ldots, v_D$ be a diameter. Then vertices v_0 and v_D must be leaves. By Lemma 4, the Fibonacci number increases if we replace all components of $T \setminus \{v_i\}$ which contain none of the other v_j ($0 \leq j \leq D$) by single edges incident with v_i. We apply this transformation for all i ($1 \leq i \leq D-1$). Note that the diameter remains unchanged; the resulting tree is a star chain, i.e. $T \simeq C(c_1, \ldots, c_{D-1})$, where $c_i = \deg v_i - 2$ (cf. Figure 4).

We set $R_1 := T \setminus \{v_0\}$ and $R_2 := R_1 \setminus (\{v_1\} \cup (N(v_1) \setminus \{v_2\}))$. In other words, R_2 is the tree which results if we "cut off" v_0, v_1 and the vertices adjacent to v_1 (except v_2). Then we have, by Lemma 2 applied to v_0,

$$F(T) = F(R_1) + 2^{c_1} F(R_2).$$

We consider two cases:

(1) $c_1 \geq 1$. Then R_1 has diameter D, and thus (by the induction hypothesis), $F(R_1)$ is maximal if and only if $R_1 \simeq C(n-1-D, \underbrace{0, \ldots, 0}_{D-2})$. Furthermore, R_2 contains the simple path $P = \{v_2, \ldots, v_D\}$. Therefore,

$$F(R_2) \leq F(P) \cdot 2^{|R_2 \setminus P|} = F(P) \cdot 2^{c_2 + \ldots + c_{D-1}} = F_{D+1} \cdot 2^{n-c_1-D}$$

with equality if and only if $R_2 = P$. However, this means that

$$F(T) \leq F(C(n-1-D, \underbrace{0, \ldots, 0}_{D-2})) + 2^{n-D} f_{D+1}$$

with equality if and only if $c_2 = c_3 = \ldots = c_{D-1} = 0$, i.e. $T \simeq C(n-D, \underbrace{0, \ldots, 0}_{D-2})$.

(2) $c_1 = 0$. Then R_1 has diameter $D-1$, and R_2 has diameter $D-2$ or $D-1$. By the induction hypothesis, $F(R_1)$ is maximal if and only if $R_1 \simeq C(n-D, \underbrace{0, \ldots, 0}_{D-3})$, i.e. either $c_2 = n-D,\ c_3 = \ldots = c_{D-1} = 0$ or $c_{D-1} = n-D,\ c_2 = \ldots = c_{D-2} = 0$.

Analogously, by the induction hypothesis, $F(R_2)$ is maximal if either $R_2 \simeq C(n-1-D, \underbrace{0, \ldots, 0}_{D-3})$ (diameter $D-1$) or $R_2 \simeq C(n-D, \underbrace{0, \ldots, 0}_{D-4})$ (diameter $D-2$). But since we know that the function $2^{n-D+1} f_{D+1} + f_D$ is decreasing in D, $F(R_2)$ is maximal if and only if R_2 has diameter $D-2$, and $c_3 = n-D,\ c_2 = c_4 = \ldots = c_{D-1} = 0$ or $c_{D-1} = n-D,\ c_2 = \ldots = c_{D-2} = 0$. As in Case 1, it follows that $F(T)$ is maximal if and only if

$$c_2 = \ldots = c_{D-2} = 0 \text{ and } c_{D-1} = n - D, \text{ i.e. } T \simeq C(n-D, \underbrace{0, \ldots, 0}_{D-2}).$$

Finally, the induction step for the formula for $F(T)$ is easily done as follows (with R_1, R_2 as in Case 1):

$$\begin{aligned} F(T) &= F(R_1) + 2^{c_1} F(R_2) \\ &= F(C(n-1-D, 0, \ldots, 0)) + 2^{n-D} F(P) \\ &= 2^{n-D} f_{D+1} + f_D + 2^{n-D} f_{D+1} \\ &= 2^{n-D+1} f_{D+1} + f_D. \end{aligned}$$

□

Corollary 6 The non-star-like tree of maximal Fibonacci number is the "Christmas star" $CS_n \simeq C(n-5, 0, \ldots, 0)$ with a diameter of 5 and $F(CS_n) = 2^{n-1}+5$ (Figure 2).

Now, we see that all trees with a Fibonacci number larger than $2^{n-1} + 5$ are star-like, so we only have to consider star-like trees in the following. We start with an explicit formula for the star-like tree corresponding to a partition $(c_1, \ldots, c_d)$.

Lemma 7

$$f(c_1, \ldots, c_d) = F(S(c_1, \ldots, c_d)) = \prod_{i=1}^{d} (2^{c_i - 1} + 1) + 2^{n-d}.$$

Proof: This follows trivially from Lemma 2 using the fact that the star S_{c_i-1} has Fibonacci number $2^{c_i-1} + 1$. □

Lemma 8 If a partition contains a, b with $a \geq b+2$, the corresponding Fibonacci number (i.e. the Fibonacci number of the corresponding star-like tree) decreases when a, b are replaced by $a-1, b+1$.

Proof: As the length of the partition remains unchanged, the term 2^{n-d} in Lemma 7 stays the same. Thus, it suffices to prove that $(2^{a-1}+1)(2^{b-1}+1) > (2^{a-2}+1)(2^b+1)$:

$$\begin{aligned} & (2^{a-1}+1)(2^{b-1}+1) > (2^{a-2}+1)(2^b+1) \\ \Leftrightarrow\ & 2^{a-1} + 2^{b-1} > 2^{a-2} + 2^b \\ \Leftrightarrow\ & 2^{a-2} > 2^{b-1}, \end{aligned}$$

which is correct by the assumption that $a \geq b+2$. □

Corollary 9 If the partition length d is fixed, the corresponding Fibonacci number is maximal for the partition $(n-d+1, 1, \ldots, 1)$ and minimal for the partition $(k+1, \ldots, k+1, k, \ldots, k)$ with $k = \lfloor \frac{n}{d} \rfloor$.

The second-largest Fibonacci number is obtained for the partition $(n-d, 2, 1, \ldots, 1)$ (if $1 < d \leq n-2$), the third-largest for $(n-d-1, 3, 1, \ldots, 1)$ (if $1 < d \leq n-4$) or $(2, 2, 2, 1, \ldots, 1)$ (if $d = n-3$).

Proof: If a partition of fixed length d is different from $(n-d+1, 1, \ldots, 1)$, the partition contains $a \geq b \geq 2$. If we replace them by $a+1, b-1$, the Fibonacci number increases by Lemma 8. Analogously, if the partition is different from $(k+1, \ldots, k+1, k, \ldots, k)$, we can find parts $a \geq b+2$ and apply Lemma 8. This proves the statements for maximum and minimum.

For $d \geq n-1$ or $d = 1$, the partition is uniquely determined by its length. Thus there is no second-largest Fibonacci number in this case. Now, a partition different from $(n-d+1, 1, \ldots, 1)$ and $(n-d, 2, 1, \ldots, 1)$ must contain either two parts $a \geq b \geq 3$ or three parts $c \geq a \geq b \geq 2$. In both cases, we replace a, b by $a+1, b-1$. Then we obtain a partition different from $(n-d+1, 1, \ldots, 1)$, and the Fibonacci number increases (by Lemma 8). This proves the second part.

If $d \geq n-2$ or $d = 1$, there are no further partitions. If $d = n-3$, there is only one partition remaining, namely $(2, 2, 2, 1, \ldots, 1)$. Thus it is also the partition giving the third-largest Fibonacci number. Eventually, if $1 < d \leq n-4$, and a partition is different from $(n-d+1, 1, \ldots, 1)$, $(n-d, 2, 1, \ldots, 1)$, and $(n-d-1, 3, 1, \ldots, 1)$, it contains either two parts $a \geq b \geq 4$ or three parts $c \geq a \geq b \geq 2$ with $c \geq 3$ or four parts $c_1 = c_2 = a = b = 2$ (as $d \leq n-4$, the partition cannot be $(2, 2, 2, 1, \ldots, 1)$). Again, we can replace a, b by $a+1, b-1$ to increase the Fibonacci number, and we obtain partitions different from $(n-d+1, 1, \ldots, 1)$ and $(n-d, 2, 1, \ldots, 1)$ (either two parts ≥ 3 or three parts ≥ 2 remain). It follows that the third-largest Fibonacci number occurs for the partition $(n-d-1, 3, 1, \ldots, 1)$. □

Lemma 10 Let the number of edges be $n \geq 8$. If a star-like tree is not of the form $S(n-d+1, 1, \ldots, 1)$, $S(n-d, 2, 1, \ldots, 1)$, or $S(n-k, k)$, it has Fibonacci number $< 2^{n-1}$.

Proof: By Corollary 9, it suffices to prove the claim for the trees $S(n-d-1, 3, 1, \ldots, 1)$, $(3 \leq d \leq n-4)$ and $S(2, 2, 2, 1, \ldots, 1)$:

$$
\begin{aligned}
f(n-d-1,3,1,\ldots,1) &\overset{\text{Lemma 7}}{=} (2^{n-d-2}+1)\cdot 5\cdot 2^{d-2}+2^{n-d}\\
&= \frac{5}{16}\cdot 2^n + 5\cdot 2^{d-2}+2^{n-d}\\
&\le \frac{5}{16}\cdot 2^n + 10 + \frac{1}{8}\cdot 2^n\\
&= \frac{7}{16}\cdot 2^n + 10 < 2^{n-1} \text{ (as } n\ge 8)
\end{aligned}
$$

and

$$
\begin{aligned}
f(2,2,2,1,\ldots,1) &\overset{\text{Lemma 7}}{=} 3^3\cdot 2^{n-6}+8\\
&= \frac{27}{64}\cdot 2^n + 8 < 2^{n-1} \text{ (as } n\ge 8).
\end{aligned}
$$

The inequality $5\cdot 2^{d-2}+2^{n-d}\le 10+\frac{1}{8}\cdot 2^n$ can be verified by the observation that the function $2^{d-2}+2^{n-d}$ is convex in d and has thus its maximum at one of the interval borders. Since $5\cdot 2^{n-6}+16\le 10+2^{n-3}$ for $n\ge 7$, we have the stated inequality. In the following, analogous arguments will be used several times. □

Lemma 11 We have

$$
\begin{aligned}
f(n-d+1,1,\ldots,1) &= 2^{n-1}+2^{d-1}+2^{n-d},\\
f(n-d,2,1,\ldots,1) &= \frac{3}{8}\cdot 2^n + \frac{3}{4}\cdot 2^d + 2^{n-d},\\
f(n-k,k) &= 2^{n-1}+2^{k-1}+2^{n-k-1}+1.
\end{aligned}
$$

Proof: All these formulas follow trivially from Lemma 7. □

3 Main results

Theorem 12 (Main Theorem) *For $n\ge 9$, we have*

$$
\begin{aligned}
&S_n = S(1,\ldots,1) \overset{!}{\succ} S(2,1,\ldots,1) \overset{!}{\succ} S(3,1,\ldots,1) \overset{!}{\succ} S(n-2,2) \overset{!}{\succ} S(4,1,\ldots,1)\\
&\overset{!}{\succ} S(n-3,3) \overset{!}{\succ} S(2,2,1,\ldots,1) \overset{!}{\succ} S(5,1,\ldots,1) \overset{!}{\succ} S(n-4,4) \overset{!}{\succ} S(6,1,\ldots,1)\\
&\overset{!}{\succ} S(n-5,5) \overset{!}{\succ} \ldots \overset{!}{\succ}\\
&\begin{cases}
S(\frac{n}{2},1,\ldots,1) \overset{!}{\succ} S(\frac{n+2}{2},\frac{n-2}{2}) \overset{!}{\succ} S(\frac{n}{2},\frac{n}{2}) \overset{!}{\succ} S(n-3,2,1) \overset{!}{\succ} CS_n & n \text{ even}\\
S(\frac{n-1}{2},1,\ldots,1) \overset{!}{\succ} S(\frac{n+3}{2},\frac{n-3}{2}) \overset{!}{\succ} S(\frac{n+1}{2},1,\ldots,1) \overset{!}{\succ} S(\frac{n+1}{2},\frac{n-1}{2}) & \\
\quad \overset{!}{\succ} S(n-3,2,1) \overset{!}{\succ} CS_n & n \text{ odd.}
\end{cases}
\end{aligned}
$$

Proof: By Theorem 5, all $T \succ CS_n$ must have diameter ≤ 4. Thus we know from Lemma 10 that we only have to consider trees of the forms given there. We already know their Fibonacci numbers from Lemma 11.

By the argument mentioned in the proof of Lemma 10,

$$\begin{aligned} f(n-d,2,1,\ldots,1) &= \frac{3}{8}\cdot 2^n + \frac{3}{4}\cdot 2^d + 2^{n-d} \\ &\leq \max\left(\frac{3}{8}\cdot 2^n + 12 + 2^{n-4}, \frac{3}{8}\cdot 2^n + 3\cdot 2^{n-5} + 8\right) \\ &= \frac{3}{8}\cdot 2^n + 3\cdot 2^{n-5} + 8 < 2^{n-1} \text{ (as } n \geq 9) \end{aligned}$$

for all $4 \leq d \leq n-3$, so we need not care about all trees of the form $S(n-d,2,1,\ldots,1)$ with $4 \leq d \leq n-3$. It is only necessary to determine the order of the remaining trees. We do this in several steps:

- $f(n-d+1,1,\ldots,1) > f(d,n-d)$ $(n-2 \geq d \geq n/2)$ is equivalent to

$$2^{n-1} + 2^{d-1} + 2^{n-d} > 2^{n-1} + 2^{d-1} + 2^{n-d-1} + 1 \;\Leftrightarrow\; 2^{n-d-1} > 1,$$

  which is obviously true for $d \leq n-2$.
- $f(n-d,d) > f(n-d+2,1,\ldots,1)$ $(n-2 \geq d \geq (n+3)/2)$ is equivalent to

$$2^{n-1} + 2^{d-1} + 2^{n-d-1} + 1 > 2^{n-1} + 2^{d-2} + 2^{n-d+1} \;\Leftrightarrow\; 2^{d-2} + 1 > 3\cdot 2^{n-d-1},$$

  which also holds within the given range of d.
- $f(1,\ldots,1) > f(2,1,\ldots,1) > f(3,1,\ldots,1)$ is equivalent to

$$2^n + 1 > 3\cdot 2^{n-2} + 2 > 5\cdot 2^{n-3} + 4,$$

  which is also obvious.
- $f(n-3,3) > f(2,2,1,\ldots,1) > f(5,1,\ldots,1)$ is equivalent to another simple inequality:

$$\frac{9}{16}\cdot 2^n + 5 > \frac{9}{16}\cdot 2^n + 4 > \frac{17}{32}\cdot 2^n + 16,$$

  which holds true for $n \geq 9$.
- $f(\frac{n+2}{2},\frac{n-2}{2}) > f(\frac{n}{2},\frac{n}{2})$ (n even) follows immediately from Lemma 8.
- $f(\frac{n}{2},\frac{n}{2}) > f(n-3,2,1) > F(CS_n)$ (n even) is equivalent to the obvious inequality

$$2^{n-1} + 2^{n/2} + 1 > 2^{n-1} + 6 > 2^{n-1} + 5.$$

- Finally, $f(\frac{n+1}{2},\frac{n-1}{2}) > f(n-3,2,1) > F(CS_n)$ (n odd) is equivalent to

$$2^{n-1} + 3\cdot 2^{(n-3)/2} + 1 > 2^{n-1} + 6 > 2^{n-1} + 5,$$

  which is obvious, too.

All these put together yield the theorem. Note that the sequence of trees of the form $S(k,1,\dots,1)$ ends with $(\lfloor\frac{n+1}{2}\rfloor,1,\dots,1)$, as the trees $S(k,1,\dots,1)$ and $S(n-k+1,1,\dots,1)$ are isomorphic. $\square$

Theorem 13 *The star-like tree with n edges and minimal Fibonacci number is $S(3,\dots,3)$, $S(3,\dots,3,2)$ or $S(3,\dots,3,2,2)$ (depending on the residue class of n modulo 3), if $n \geq 25$.*

Proof: By Corollary 9, the partition of minimal Fibonacci number has the form $(k+1,\dots,k+1,k,\dots,k)$. First we prove the following statement:

If an even element $2l$ in the partition is replaced by l times 2 ($l \geq 2$), the Fibonacci number decreases; similarly, if an odd element $2l+1$ in the partition is replaced by $l-1$ times 2 and one 3 ($l \geq 2$), the Fibonacci number decreases.

This is proved as follows: as the length of the permutation grows, the term 2^{n-d} in the formula of Lemma 7 decreases. Therefore, it suffices to prove that the remaining term doesn't increase, i.e. $2^{2l-1}+1 \geq 3^l$ and $2^{2l}+1 \geq 5\cdot 3^{l-1}$. Both follow easily by induction on l.

Thus we know that the minimal Fibonacci number occurs for a partition which only contains 1's, 2's and 3's. More specifically, it must be a partition of the form $(3,\dots,3,2,\dots,2)$ or $(2,\dots,2,1,\dots,1)$. By Lemma 7, we have

$$f(\underbrace{3,\dots,3}_{k},\underbrace{2,\dots,2}_{(n-3k)/2}) = 5^k 3^{(n-3k)/2} + 2^{(n+k)/2} \text{ and } f(\underbrace{2,\dots,2}_{k},\underbrace{1,\dots,1}_{n-2k}) = 3^k 2^{n-2k} + 2^k.$$

Both are decreasing in k, for $k \leq n/3$ and $k \leq n/2$ respectively:

$$\begin{aligned}
&5^{k-2}3^{(n-3k+6)/2} + 2^{(n+k-2)/2} \geq 5^k 3^{(n-3k)/2} + 2^{(n+k)/2} \\
\Leftrightarrow\ & 3^{n/2}\left((25/27)^{(k-2)/2} - (25/27)^{k/2}\right) \geq 2^{(n+k-2)/2} \\
\Leftrightarrow\ & (2/25)\cdot 3^{n/2}\cdot(25/27)^{k/2} \geq 2^{(n+k-2)/2} \\
\Leftrightarrow\ & (4/25)\cdot(3/2)^{n/2} \geq (54/25)^{k/2},
\end{aligned}$$

which is true for $k \leq n/3$ and $n \geq 25$:

$$\begin{aligned}
(4/25)\cdot(3/2)^{n/2} &= (4/25)\cdot(54/25)^{n/6}\cdot(5/4)^{n/3} \geq (4/25)\cdot(54/25)^{n/6}\cdot(5/4)^{25/3} \\
&> (54/25)^{n/6} \geq (54/25)^{k/2}.
\end{aligned}$$

Note that we only need to consider k and $k-2$, since k must have the same parity as n. On the other hand,

$$\begin{aligned} & 3^{k-1}2^{n-2k+2} + 2^{k-1} \geq 3^k 2^{n-2k} + 2^k \\ \Leftrightarrow\ & 2^n \left((3/4)^{k-1} - (3/4)^k \right) \geq 2^{k-1} \\ \Leftrightarrow\ & (2/3) \cdot 2^n \geq (8/3)^k \\ \Leftrightarrow\ & (2/3) \cdot (3/2)^{n/2} \cdot (8/3)^{n/2} \geq (8/3)^k, \end{aligned}$$

which is obviously true for all $k \leq n/2$ and $n \geq 2$.

Thus the minimum is attained for the maximal value of k in both cases, i.e. $k = \frac{n-r}{3}$ (where $r = 0, 4, 2$ for $n \equiv 0, 1, 2 \mod 3$) and $k = \lfloor n/2 \rfloor$ respectively. To complete the proof, we only need the following observations:

$$f(\underbrace{2, \ldots, 2}_{(n-1)/2}, 1) > f(\underbrace{2, \ldots, 2}_{(n-3)/2}, 3) \ (n \text{ odd}),$$

$$f(\underbrace{2, \ldots, 2}_{n/2}) > f(\underbrace{2, \ldots, 2}_{(n-6)/2}, 3, 3) \ (n \text{ even}).$$

The first is equivalent to

$$\begin{aligned} & 2 \cdot 3^{(n-1)/2} + 2^{(n-1)/2} > 5 \cdot 3^{(n-3)/2} + 2^{(n+1)/2} \\ \Leftrightarrow\ & 3^{(n-3)/2} > 2^{(n-1)/2}, \end{aligned}$$

which holds for $n \geq 7$. The second is equivalent to

$$\begin{aligned} & 3^{n/2} + 2^{n/2} > 5^2 \cdot 3^{(n-6)/2} + 2^{(n+2)/2} \\ \Leftrightarrow\ & 3^{(n-6)/2} > 2^{(n-2)/2}, \end{aligned}$$

which holds for $n \geq 13$. This completes the proof. □

4 Asymptotic results

Theorem 14 *There are $p(n) - \lfloor \frac{n}{2} \rfloor$ nonisomorphic star-like trees with n edges, where $p(n) \sim \frac{\exp(\pi\sqrt{2n/3})}{4\sqrt{3}n}$ is the number of partitions of n.*

Proof: By Proposition 1, each partition corresponds to exactly one star-like tree and vice versa. The only exceptions are partitions of the form $(k, 1, \ldots, 1)$. Two different partitions represent the same tree if and only if they are of the form $(k, 1, \ldots, 1)$ and $(l, 1, \ldots, 1)$ $(k, l \geq 1,\ k \neq l)$ with $k + l = n + 1$. There are exactly $\lfloor \frac{n}{2} \rfloor$ pairs (k, l) with $1 \leq k < l$ and $k + l = n + 1$. This already proves the claim. $\square$

Theorem 15 *The average Fibonacci number of a star-like tree with n edges is asymptotically ($n \to \infty$) $A \cdot 2^n \cdot \exp(B\sqrt{n}) \cdot n^{3/4}$, where*

$$A = \left(\frac{\pi^4}{27} - \frac{2\pi^2}{9}(\log 2)^2\right)^{-1/4} \prod_{j=1}^{\infty}(1 - 2^{-j})^{-1} = 2.739149898\ldots$$

and

$$B = \sqrt{\pi^2/3 - 2(\log 2)^2} - \sqrt{2\pi^2/3} = -1.039005919\ldots.$$

Proof: The proof is rather lengthy and technical, so we only give the main ideas here. All details can be found in [31]. Note first that there is an almost 1-1-correspondence between partitions and star-like trees. Therefore, we only have to determine

$$s(n) := \sum_{c} \left(\prod_{i=1}^{d} (2^{c_i - 1} + 1) + 2^{n-d} \right),$$

where the sum ranges over all partitions $c = (c_1, \ldots, c_d)$ of n. Now, it is easy to see that the generating function for this sum is given by

$$\prod_{j=1}^{\infty}(1 - (2^{j-1} + 1)x^j)^{-1} + \prod_{j=1}^{\infty}(1 - 2^{j-1}x^j)^{-1}.$$

If we replace x by $z/2$, we obtain a generating function for $2^{-n}s(n)$:

$$\prod_{j=1}^{\infty}\left(1 - \left(\frac{1}{2} + 2^{-j}\right)z^j\right)^{-1} + \prod_{j=1}^{\infty}\left(1 - \frac{1}{2}z^j\right)^{-1}.$$

It turns out that only the first summand gives an asymptotically relevant contribution. We write $G(z) := \prod_{j=1}^{\infty}(1 - (\frac{1}{2} + 2^{-j})z^j)^{-1}$ und $F(z) := \prod_{j=1}^{\infty}(1 - \frac{1}{2}z^j)^{-1}$. Both functions are holomorphic on every compact disk of radius < 1 around 0. Applying Cauchy's residue theorem, we obtain

$$2^{-n}s(n) = \frac{1}{2\pi i}\left(\int_{\mathcal{C}_1} z^{-n-1}G(z)\,dz + \int_{\mathcal{C}_2} z^{-n-1}F(z)\,dz \right)$$

for appropriate curves $\mathcal{C}_1$, $\mathcal{C}_2$ around 0. Now, both integrals are estimated by means of the saddle point method. We set

$$z^{-n}G(z) = \exp g(z),$$

i.e. $g(z) = -\sum_{j=1}^{\infty} \log(1 - (1/2 + 2^{-j})z^j) - n \log z$, and use the Euler-Maclaurin summation formula to obtain

$$g'(e^{-\beta}) = e^{\beta}\left(\frac{b^2}{\beta^2} + \frac{1}{\beta} + O(1) - n\right),$$

where $b^2 = \frac{\pi^2}{12} - \frac{(\log 2)^2}{2}$, so $\beta = \frac{b}{\sqrt{n}} + \frac{1}{2n} + O(n^{-3/2})$ for the saddle point $z = e^{-\beta}$. Using the Euler-Maclaurin formula again yields

$$\begin{aligned} g(e^{-\beta}) &= 2b\sqrt{n} + \log \frac{\sqrt{n}}{2\sqrt{2}ab} + O(n^{-1/2}), \\ g''(e^{-\beta}) &= \frac{2}{b} n^{3/2} + O(n), \\ g'''(e^{-\beta}) &= O(n^2). \end{aligned}$$

Here, $a = \prod_{j=1}^{\infty}(1-2^{-j})$. Now, a routine application of the saddle point method (we integrate along the circle $\mathcal{C}_1 = \{z = e^{-\beta+it} : t \in [0, 2\pi)\}$) gives us

$$\frac{1}{2\pi i} \int_{\mathcal{C}_1} z^{-n-1} G(z)\, dz \sim \frac{1}{4a\sqrt{2\pi b}} e^{2b\sqrt{n}} n^{-1/4}$$

and analogously

$$\frac{1}{2\pi i} \int_{\mathcal{C}_2} z^{-n-1} F(z)\, dz \sim \sqrt{\frac{b}{8\pi}} e^{2b\sqrt{n}} n^{-3/4}.$$

Altogether, we have

$$s(n) \sim 2^n \frac{1}{4a\sqrt{2\pi b}} e^{2b\sqrt{n}} n^{-1/4},$$

which proves the theorem together with the Hardy-Ramanujan-Rademacher formula (Theorem 0). □

5 Open Problems and Acknowledgment

5.1 Problems

The following open questions seem to be very natural:

- Can one find a result analogous to Theorem 5 for the minimum? Theorem 13 provides such a result for diameter 4, and for diameter 2 and 3, we can see the minimum from Theorem 12.
- Can one find the maximal Fibonacci number under other restrictions such as bounding the degree of the edges, bounding the number of leaves, etc.?
- Can one compute the exact asymptotics of the average Fibonacci number of trees?

5.2 Acknowledgment

The second author is very grateful to Arnold Knopfmacher and Helmut Prodinger for inviting him to The John Knopfmacher Centre for Applicable Analysis and Number Theory at the University of the Witwatersrand in Johannesburg. This has been the starting point for the work on the present paper. The authors also want to thank two anonymous referees for their valuable suggestions.

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