The Number of Huffman Codes, Compact Trees, and Sums of Unit Fractions

Christian Elsholtz, Clemens Heuberger, and Helmut Prodinger

Abstract—**The number of "nonequivalent" compact Huffman codes of length r over an alphabet of size t has been studied frequently. Equivalently, the number of "nonequivalent" complete t-ary trees has been examined. We first survey the literature, unifying several independent approaches to the problem. Then, improving on earlier work, we prove a very precise asymptotic result on the counting function, consisting of two main terms and an error term.**

Index Terms—**Algorithm design and analysis, codes, equations, sequences, tree graphs.**

I. Introduction

In this paper, we study a combinatorial object that has appeared in the literature in several equivalent forms, such as compact Huffman codes, canonical rooted trees, and level sequences. In this paper, we have the following two aims: we first give a thorough survey of the existing literature, thus unifying these approaches (Sections II and III).

Second, we count these compact Huffman codes (respectively, canonical rooted trees, level sequences) with an accuracy that goes much beyond what was previously known. In particular, the best previously available asymptotic approximation for the number of binary trees would allow to approximate the number of objects with giving the first 39% of the bits, whereas our new asymptotic formula with two main terms achieves an approximation which gives about 80% of the leading bits. In the case of t-ary trees, we achieve comparable results. Here, the previous literature only contained an asymptotic result, but no explicit error term. Moreover, we have implemented an exact generating function and can compute exact values of these sequences for large examples.

Section IV contains the statement of the main result, indicated previously, and the following sections contain the proof.

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II. Several Equivalent Definitions

In this section, we list a number of equivalent ways of defining our main object. This reflects that the same type of question has been studied from various points of view, independent of the corresponding results expressed in a different mathematical language.

A. Coding Theory

Let a source emit words $w_1,\dots,w_r$ with probabilities $p_1,\dots,p_r$, respectively. Here, $0 \le p_i \le 1$ and $\sum_{i=1}^r p_i = 1$. For each word w_i, we assign a codeword $c_i = c_i(w_i)$ of length l_i, over an alphabet of size t. Given the word probabilities p_i Huffman [22] constructed a code with minimum average word length $\bar{l} = \sum_{i=1}^r p_i l_i$. These Huffman codes are prefix free, and can therefore be decoded instantaneously. Moreover, these codes can be found efficiently.

A code is called *compact* if it satisfies the Kraft equality

$$\sum_{i=1}^{r} \frac{1}{t^{l_i}} = 1. \qquad \text{(II.1)}$$

Let l_r be the maximum word length. When multiplying the equation by t^{l_r}, we observe that in a compact code, the number of codewords of length l_r is divisible by t. Also, if there are two distinct codewords starting with the same prefix $a_1 \dots a_q$ but then continuing differently, $a_1\dots a_q b_1\dots$ and $a_1\dots a_q b_2\dots$, then all t possible symbols must occur at position $q+1$. In other words, if a sequence branches, it branches into all t possible directions. This is the reason why it is possible to model the situation by means of a rooted t-ary tree, which we do in the following. It is possible to arrive from a given Huffman code at a solution of (II.1), and vice versa, to arrive from a solution to this equation at an admissible Huffman code. All Huffman codes with the same set of word lengths are considered as "equivalent" codes.

This motivates the following two equivalent definitions. The first is based on Kraft's equality, and stresses the number theoretic properties and was at the origin of Boyd's [6] work.

Definition 1 (Number Theoretic Definition): Let $f_t(r)$ denote the number of solutions of the equation

$$\sum_{i=1}^{r} \frac{1}{t^{x_i}} = 1$$

where the x_i are nonnegative integers and $0 \le x_1 \le \cdots \le x_r$.

For more information on other counting functions related to representations of one as a sum of unit fractions, see [8] and [11].

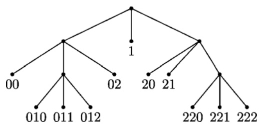


Fig. 1. Rooted tree corresponding to the code $\{00, 010, 011, 012, 02, 1, 20, 21, 220, 221, 222\}$.

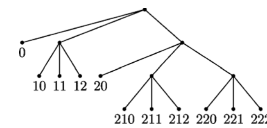


Fig. 2. Canonical tree corresponding to $\{0, 10, 11, 12, 20, 210, 211, 212, 220, 221, 222\}$.

Collecting the number of words of the same length (corresponding to x_i in the last definition), one arrives at the following definition.

Definition 2 (Huffman Sequences): Let $t \geq 2$ and $r \geq 1$ be positive integers. Let $f_t(r)$ denote the number of sequences of nonnegative integers

$$(a_0, a_1, \ldots, a_l), \quad l \geq 0,\ a_l > 0$$
$$\sum_{i=0}^{l} a_i = r, \quad \sum_{i=0}^{l} \frac{a_i}{t^i} = 1.$$

The name "Huffman sequence" comes from the observation that there is a bijection between distinct Huffman sequences and nonequivalent compact Huffman codes, and that every Huffman code can actually be obtained from a given probability vector by applying the Huffman algorithm. To see the latter, let us just remark that the Huffman sequence $(a_0, a_1, \ldots, a_l)$ with $\sum_{i=0}^{l} a_i = r$ can be obtained if we take as probability vector $(p_1, \ldots, p_r)$, the p's being the r values of $\frac{1}{t^i}$, each with frequency a_i. As observed previously, a_l is divisible by t. Hence, the first step of the Huffman algorithm combines t times the least probability t^{-l} to one new probability t^{-l+1}. This reduces the problem to a smaller one, and inductively we can assume that the statement is true for all smaller instances. For some further comments, see Hankerson *et al.* [20, Exercise 4.3.6, p. 85], and also in a quite general setup in Hoffman *et al.* [21, p. 116].

B. Rooted Trees

Let us look at a small example. Let $t = 3$. Let the code consist of the codewords

$$00, 010, 011, 012, 02, 1, 20, 21, 220, 221, 222.$$

The code can be nicely represented by the tree in Fig. 1. This motivates that counting the number of nonequivalent Huffman codes is equivalent to counting certain rooted trees.

A rooted tree is a connected cycle-free graph, with one vertex being distinguished (root). (We will draw it on the top, all other vertices below). We say the tree is t-ary, if all those vertices, which are not the root, are either a leaf, which is an end of a path from the root, or have one predecessor and t children. All nonleaves are called inner vertices. Note that the root is also an internal vertex unless for the trivial tree of order one. In other words, for the trees we consider, the root has degree t, and all other vertices either have degree 1 (leaf) or have degree $t + 1$.

Definition 3 (Canonical Rooted Tree): A rooted tree is called canonical if its corresponding prefix code has the property that the lexicographic ordering of its words corresponds to a nondecreasing ordering of the word lengths.

Let us say that two rooted t-ary trees are equivalent, if their number of leaves at distance i from the root is the same, for all i. Let $f_t(r)$ denote the number of equivalence classes of t-ary rooted trees with exactly r leaves.

Note that each equivalence class contains exactly one canonical tree. Also, if the tree has a_i leaves at distance i from the root, then $\sum_i \frac{a_i}{t^i} = 1$. This follows inductively, since a leaf at distance i from the root, i.e., which contributes a weight $\frac{1}{t^i}$, can be split into t children at distance $i + 1$, of weight $\frac{1}{t^{i+1}}$ each. The number of "inner" vertices is $n = \frac{r-1}{t-1}$.

As such a rooted t-ary tree corresponds to a compact code, we also call these trees "compact trees."

Using Definition 3, one would, for example, replace the code

$$\{00, 010, 011, 012, 02, 1, 20, 21, 220, 221, 222\}$$

by the following equivalent code:

$$\{0, 10, 11, 12, 20, 210, 211, 212, 220, 221, 222\}.$$

The corresponding canonical rooted tree is in Fig. 2. In our usual way of drawing these diagrams, a canonical tree therefore has the longer paths as far to the right-hand side as possible.

C. Bounded Degree Sequences and Proper Words

The number a_i of codewords of length i, or leaves at level i is of course bounded above by t^i. But there is no absolute bound on $\frac{a_i}{a_{i-1}}$. For a given $(a_1, a_2, \ldots)$, let us study another sequence instead, namely $b_1 = 1$, $b_i = tb_{i-1} - a_{i-1}$, see Komlos *et al.* [26] and Flajolet and Prodinger [15]. The problem of counting these sequences is equivalent to the earlier counting problem. For these sequences, the ratios $\frac{b_i}{b_{i-1}}$ are bounded, which is why one may call these sequences "bounded degree sequences." Flajolet and Prodinger [15] used this definition when they counted level number sequences of trees.

Definition 4 (Bounded Degree): Let $t \geq 2, r \geq 2$ be integers. Let $f_t(r)$ denote the number of sequences

$$(b_1, \ldots, b_l), \quad l \geq 1, \quad b_1 = 1$$
$$1 \leq b_i \leq tb_{i-1}\ (i = 2, \ldots, l), \quad \sum_{i=1}^{l} b_i = \frac{r-1}{t-1}.$$

For convenience, we will later also use

$$g_t(n) = f_t(1 + n(t-1)).$$

Again, one can think of $n = \frac{r-1}{t-1}$ as the number of inner vertices, in the language of rooted trees. A bijection between the last two definitions is as follows: Given a canonical tree, we set b_i to be the number of internal vertices at height $i - 1$. Observe that the b_i internal vertices guarantee that there are at most tb_i vertices of any type (internal vertices or leaves) on the next level.

A similar definition is due to Even and Lempel [13].

Definition 5 (Proper Words): Let $t \geq 2$ and $n \geq 1$ be integers. A word $u_1, \ldots, u_m$ over the alphabet $\{0, 1\}$ is said to be a proper word, if it can be written in the form $u_1, \ldots, u_m = 0^{c_0}10^{c_1}1\ldots0^{c_{l-1}}10^{c_l}$ such that $c_0 = 0$ and $0 \leq c_{i+1} \leq tc_i + t - 1$ holds for all $0 \leq i \leq l-1$. Note that the sequence c_i describes the lengths of the runs of consecutive zeros. We note also that from the representation as a word of length n, we immediately get $\sum_{i=0}^{l} c_i = m - l$.

To see that Definition 5 is equivalent to Definition 4, we simply note that the relations $b_{i+1} = c_i + 1$ and $m + 1 = n = \frac{r-1}{t-1}$ induce a bijection between the objects counted in the two definitions. Even and Lempel [13] also give a combinatorial interpretation of this bijection (for $t = 2$, but the generalization is straightforward): essentially, for each 1 in a proper word, they replace a leaf of maximum height by an internal vertex with t leaves as successors; for each 0, they replace a leaf of second-most height by an internal vertex with t leaves as successors.

We briefly mention some further approaches that investigate equivalent sequences. Working on a different problem, Minc [29] reduced it to the study of a binary bounded degree sequence, see Definition 4 above. Let A be a free commutative entropic cyclic groupoid. The number of elements of A of a given degree turns out to satisfy the aforementioned relation. (For a full description, we must refer to [29]). The condition in Definition 4 looks like a special partition function. Andrews [2] expanded on Minc's work, in particular studying generating functions.

A related problem, on lambda algebras Λ_p, has been related to these sequences, see [38].

There are a number of publications that use bounded degree sequences: Brown and Gitler (see [7, Lemma 2.2]) used them in connection with certain lattices related to Steenrod algebras. Carlsson (see [10, Proposition 4]) used bounded degree sequences in his work on the solution of a conjecture of Segal. Other examples are papers by Bousfeld *et al.* (see [5, Sec. 5.3 and 5.5]) and Mahowald (see [28, Section V]) on Adams spectral sequences. However, it seems, in this work, the bounded degree sequences are used as a tool, not as an object of independent study.

D. Example

As an example for these various definitions, let us compute $f_2(5) = 3$ in the different forms. Using Definition 1

$$
\begin{aligned}
1 &= \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \frac{1}{16} \\
&= \frac{1}{2} + \frac{1}{8} + \frac{1}{8} + \frac{1}{8} + \frac{1}{8} \\
&= \frac{1}{4} + \frac{1}{4} + \frac{1}{4} + \frac{1}{8} + \frac{1}{8}
\end{aligned}
$$

is a complete list of all solutions.

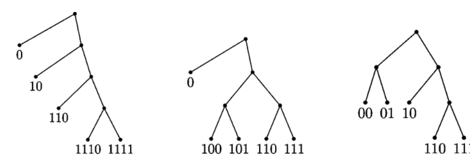
Counting Huffman sequences (Definition 2), we count $(a_0, a_1, \ldots)$ where a_i is the number of words of length i, or the number of occurrences of the fraction $\frac{1}{t^i}$, $i \geq 0$. Here, with $t = 2$, these sequences are

$$(0, 1, 1, 1, 2), (0, 1, 0, 4), (0, 0, 3, 2).$$

From this, one can write down the compact Huffman codes

$$
\begin{aligned}
C_1 &= \{0, 10, 110, 1110, 1111\} \\
C_2 &= \{0, 100, 101, 110, 111\} \\
C_3 &= \{00, 01, 10, 110, 111\}.
\end{aligned}
$$

The canonical trees (see Definition 3) are the following:



The bounded degree sequences counted in Definition 4 are $(1, 1, 1, 1)$, $(1, 1, 2)$, and $(1, 2, 1)$. The proper words in Definition 5 can be found as follows: From the bijection and the bounded degree sequences above, we find that the c_i are given by $(0, 0, 0, 0)$, $(0, 0, 1)$, and $(0, 1, 0)$. Therefore, the proper words u are $(1, 1, 1)$, $(1, 1, 0)$, and $(1, 0, 1)$, with $m = 3, l = 3$ for the first word, and $m = 3$, $l = 2$, both for the second and third words.

III. Review on Results on the Growth of $f_t(r)$

A. First Elementary Bounds

As far as we are aware of, Bende [4] and Norwood [31] (both in 1967), were the first to examine the sequence $f_2(r)$, and they observed the connection to coding theory and trees. (Minc's paper [29] was, of course, earlier but had less interest in the sequence itself.) Bende asked about the asymptotic growth. Erdős in his review of Bende's paper (Mathematical Reviews) also wrote it is "desirable" to know the asymptotic.

The early 1970's saw a considerable number of contributions to the problem, such as Boyd [6], Even and Lempel [13], and Gilbert [17].

A trivial upper bound for the number of rooted canonical trees on $|V|$ vertices is $2^{\binom{|V|}{2}}$. A much more precise bound is the number of all trees. The number of binary trees on $|V|$ vertices is determined by the Catalan numbers $\frac{1}{n+1}\binom{2n}{n} = O(4^n n^{-3/2})$ and the number of nonisomorphic trees is asymptotically $\sim C_2\, C_1^n n^{-5/2}$, where $C_1 = 2.955\ldots$ and $C_2 = 0.5349\ldots$, see [33].

A trivial lower bound comes from observing that Definition 4 shows that $f_2(r) \geq F_r$, where F_r is the number of ways of partitioning $r - 1$ into ones and twos. It is known that this is the rth Fibonacci number so that $f_2(r) \geq 0.4472 \times 1.61803^r$ (for sufficiently large r). Using simple estimates on the complex roots of equations such as $x^4 - x^3 - x^2 - 1 = 0$ or $x^3 - x^2 - 2x + 1 = 0$, Clowes *et al.* [12] proved that there are positive constants C_1, C_2 such that $C_1 1.755^r \leq f_2(r) \leq C_2 1.802^r$ holds.

Similarly, a lower bound on $f_t(r)$ can be obtained by partitioning $r - 1$ into 1's, 2's... and t's. By means of the generating series of $\frac{1}{1-z-z^2-\cdots-z^t}$ and determining a real root of the equation $1 - z - z^2 - \cdots - z^t = 0$ near 0.5, the corresponding generalized Fibonacci number $F_{t,r}$ can be shown to be about $c_t \rho_t^r$, where $\rho_t \approx 2 - \frac{1}{2^t - \frac{t}{2}}$, and c_t is a positive constant. In our main theorem, we refine an analysis of this type considerably.

B. Improved Elementary Bound on $f_t(r)$

When evaluating $f_t(r)$, according to the Definition 2 of Huffman sequences, it suffices to investigate in which way a solution counted by $f_t(r - t + 1)$ can be split. Let $S_t(r)$ denote the set of all sequences counted by $f_t(r)$. Generally, $(a_0, a_1, \ldots, a_i, \ldots, a_l)$ can be split into $(a_0, a_1, \ldots, a_i - 1, a_i + t, \ldots, a_l)$, whenever $a_i > 0$. Starting from a complete set of solutions, i.e., $S_t(r - t + 1)$, one only needs to branch each sequence at the last two positions, in order to compile a complete set of solutions, $S_t(r)$. The reason for this is that all elements of $S_t(r)$ obtained from branching at any of the earlier positions will be obtained from another member of $S_t(r - t + 1)$ by branching at the last two positions. Before we generally prove this, let us look at an example. Let us determine $S_2(6)$, starting from the three elements of $S_2(5) = \{01112, 0104, 0032\}$

$$\begin{aligned} &0111|2 \to 0111|12, \quad 011|12 \to 011|04, \\ &010|4 \to 010|32, \qquad 003|2 \to 003|12, \\ &00|32 \to 00|24. \end{aligned}$$

There is no need to consider

$$\begin{aligned} 0|1112 \to 0|0312 \text{ or } 01|112 \to 01|032 \\ \text{or } 0|104 \to 0|024 \end{aligned}$$

as these are obtained otherwise.

To see this generally, let us consider the step from $f_t(r - t + 1)$ to $f_t(r)$: If $(a_0, a_1, a_2, a_3, \ldots, a_l) \in S_t(r - t + 1)$, i.e., $\sum_{i=0}^{l} a_i = r - t + 1$, with $a_l > 0$, we need to check if $(a_0, a_1, \ldots, a_i - 1, a_{i+1} + t, a_{i+2}, \ldots, a_l) \in S_t(r)$ will be reached by branching an appropriate element of $S_t(r - t + 1)$ in any of the last two positions only.

Note that $(a_0, a_1, \ldots, a_i - 1, a_{i+1} + t, a_{i+2}, \ldots, a_{l-1} + 1, a_l - t) \in S_t(r - t + 1)$. Hence, one reaches $(a_0, a_1, \ldots, a_i - 1, a_{i+1} + t, a_{i+2}, \ldots, a_{l-1}, a_l) \in S_t(r)$ by branching in the last two positions only. We may also observe that this gives a trivial upper bound of $f_t(r) \le 2^{\frac{r-1}{t-1}}$.

Using the aforementioned observation of branching at two positions only, Narimani and Khosravifard [30] describe a recursive algorithm to create all codes counted by $f_t(r)$.

The first terms of the sequence $f_2(r)$ are

$$t = 2 : 1, 1, 1, 2, 3, 5, 9, 16, 28, 50, 89, 159, \ldots.$$

The values of $f_3(r)$ are zero, whenever r is even. The nontrivial part of the sequence for odd r, i.e., $g_3(n)$, starts with

$$t = 3 : 1, 1, 1, 2, 4, 7, 13, 25, 48, 92, 176, \ldots$$

(see also [35]). For general t, the sequence is only nonzero for $r = 1 + (t - 1)n$. For convenience, one examines $g_t(n) = f_t(1 + n(t - 1))$ instead, see Definition 4. For reference purposes,

TABLE I
VALUES OF $g_t(n)$ FOR $2 \le t \le 10$ AND $1 \le n \le 20$

t	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
2	1	1	1	2	3	5	9	16	28	50	89	159	285	510	914	1639	2938	5269	9451	16952
3	1	1	1	2	4	7	13	25	48	92	176	338	649	1246	2392	4594	8823	16945	32545	62509
4	1	1	1	2	4	8	15	29	57	112	220	432	848	1666	3273	6430	12632	24816	48754	95783
5	1	1	1	2	4	8	16	31	61	121	240	476	944	1872	3712	7362	14601	28958	57432	113904
6	1	1	1	2	4	8	16	32	63	125	249	496	988	1968	3920	7808	15552	30978	61705	122910
7	1	1	1	2	4	8	16	32	64	127	253	505	1008	2012	4016	8016	16000	31936	63744	127234
8	1	1	1	2	4	8	16	32	64	128	255	509	1017	2032	4060	8112	16208	32384	64704	129280
9	1	1	1	2	4	8	16	32	64	128	256	511	1021	2041	4080	8156	16304	32592	65152	130240
10	1	1	1	2	4	8	16	32	64	128	256	512	1023	2045	4089	8176	16348	32688	65360	130688

we list the first values of the sequences $g_t(n)$ in Table I. In these tables, one can easily notice the aforementioned observation, $g_t(n) = f_t(r) \le 2^{\frac{r-1}{t-1}} = 2^n$.

The sequences $g_2(n)$, $g_3(n)$, and $g_4(n)$ have been included into the OEIS (sequences A002572, A176485, and A176503). (The latter two sequences only after the appearance of the Paschke *et al.* paper [35].)

C. Asymptotic Growth, Previous Results

Boyd (1975) [6], Komlos, W. Moser and Nemetz (1984) [26], Flajolet and Prodinger (1987) [15], all independently, gave an asymptotic

$$f_2(r) \sim R\rho^r$$

where $R \approx 0.14185$ and $\rho \approx 1.7941471$. Boyd and Flajolet and Prodinger additionally gave an error term $f_2(r) = R\rho^r + O(\tilde{\rho}^r)$, where Boyd proves $\tilde{\rho} = 1.55$, and Flajolet and Prodinger proved that this even holds for $\tilde{\rho} = \frac{10}{7}$. Boyd and Komlos *et al.* also briefly study the case of more general t. Boyd mentions that some error term can be achieved, but does not give an explicit error term. Komlos *et al.* state an asymptotic only.

As noted previously: as $f_t(r)$ is positive only for $r = 1 + n(t - 1)$, one examines $g_t(n) = f_t(1 + n(t - 1))$ instead.

In particular, Komlos *et al.* observed that $g_t(n) \sim K_t \rho_t^n$ with $\rho_t \to 2$, as t increases. Flajolet and Prodinger [15] also refer to other areas, where the sequence $f_2(r)$ naturally occurs.

Building upon [15], but not making use of [6] nor [26], Tangora (1991) [38] generalized the results to prime values of t.

Another string of references follows from Gilbert's experimental observation that $f_2(r) \approx 0.148(1.791)^r$, see [17]. The observation was based on the values for $r \le 30$, and is relatively close to the true asymptotic $f_2(r) \sim 0.1418\ldots(1.7941\ldots)^r$. However, the aforementioned approximations have been referred to in the more recent coding literature, see, for example, [1], [24], [25], [30], [34], and [36].

More recently Burkert (2010) [9] and Paschke, Burkert, Fehribach (2011) [35] studied $f_2(r)$ and $f_t(r)$, respectively, unfortunately with inferior results and unfortunately making no use of the earlier work.[1]

D. Numerical Discussion of the Results in Section IV

In the results that we describe in detail in Section IV, we state a rather precise asymptotic formula, with two main terms, and

[1]The oversights some decades ago can be easily explained due to the fact that the results were discovered independently by people with interests in number theory, coding theory, or graph theory. Boyd's paper [6] has a number theoretic title, the Komlos *et al.* paper [26] a coding title and appeared in a less accessible journal. Using standard tools such as MathSciNet, Zentralblatt, Google Scholar, Online Encyclopedia of Integer Sequences (OEIS), we found a considerable corpus of literature referring to the result that $f_t(r) \sim K_t \cdot \rho_t^r$.

an error term, which is *exponentially* smaller. As an example, one finds an approximation

$$f_2(n) \approx R\rho^n + R_2\rho_2^n$$

with

$$\begin{aligned}\rho &= 1.794147187541686\\ \rho_2 &= 1.279549134726681\\ R &= 0.1418532020854094\\ R_2 &= 0.06124104103121269.\end{aligned}$$

Let us evaluate $f_2(50) \approx 699427308155.394\cdots = 6.99\ldots 10^{11}$. While the error analysis of Theorem 7 (below) gives an error of $|f_2(50)-(R\rho^{50}+R_2\rho_2^{50})| \leq 36.6\cdot 1.123^{50} \leq 12092$, the absolute error is much smaller and, in this case, the aforementioned approximation predicts the *correct* value of $f_2(50) = 699427308155$. For comparison, Boyd has an error term of $\leq 578(1.55)^{50}$ which is in this case larger than the main term. The best available previous error term by Flajolet and Prodinger $O(\tilde{\varrho}^r)$ would give (assuming for simplicity the O constant is bounded by 1) an error of about $(\frac{10}{7})^{50} \approx 5.56\cdot 10^7$.

As this is a "small" example, let us analyze how many correct bits the approximation $f_2(n) \sim K_2\rho^n + O(\tilde{\varrho}^r)$ generates, asymptotically when n tends to infinity. As the error term is $O(\tilde{\varrho}^r) = O(MT^C)$, where "$MT$" denotes the "main term," and $C = \frac{\log\tilde{\varrho}}{\log\varrho} \approx \frac{\log(10/7)}{\log 1.79414718} \approx 0.61019$. In other words, the proportion of correct bits that the main term generates is 38.98%.

Now, let us analyze, for comparison, the quality of the new approximation

$$f_2(n) \approx R\rho^n + R_2\rho_2^n + O(r_3^n)$$

with an error term of $\leq 36.6\times 1.123^n$. The error term is in terms of the main term: $O(MT^C)$ with $C = \frac{\log r_3}{\log\varrho} \approx \frac{\log 1.123}{\log 1.79414718} \approx 0.198456$. In other words, now the two main terms generate at least 80.154% correct bits. Experimentally, the absolute error is even smaller, but the fact that in the example $f_2(50)$ the approximation was actually precise may have been somewhat accidental.

A corollary of our main theorem (Theorem 7) is the following: As t increases, the proportion of correct bits generated by the main term tends to 1. This can be seen from Theorem 7 where ρ tends to 2, and r_3 tends to 1. In fact, $C_t = \frac{\log r_3}{\log\varrho} \approx \frac{\frac{\log 2}{t}}{\log(2-\frac{1}{2^{t+1}})} \approx \frac{1}{t}$.

For each fixed t, an analysis of this type can be performed, based on some finite amount of computation. We have worked out the details for $t \leq 15$. For larger t, our uniform asymptotic analysis, which includes the size of the constants in terms of t, is perhaps, from a theoretical point of view, even more valuable.

E. Note on Algorithms and Complexity

The question of the complexity of the evaluation of $f_2(r)$ is raised by Even and Lempel [13]. They give an algorithm to determine $f_2(r)$ in $O(r^3)$ additions. This appears to be the only algorithm with a statement about its complexity. Even and Lempel also state another algorithm giving a complete list of the $f_2(r)$ elements.

Huffman *et al.* [21] describe another algorithm to give a complete list.

A tree-based algorithm for generating the binary compact codes is described by Khosravifard *et al.* [24]. Narimani and Khosravifard [30] describe a recursive algorithm to create all t-ary codes of length r by those of length $r-t+1$.

IV. New Computational and Analytic Results

We generalize the generating function approach of Flajolet and Prodinger [15] to the case of arbitrary t. In particular, our Theorem 6 corresponds to their Theorem 2. Although the proof is similar, we prefer to include it in order to be self-contained and to include some more details of the proof.

The asymptotic result (our Theorem 7), however, needs more than a simple generalization: On the one hand, dealing with all $t \geq 30$ simultaneously needs a careful asymptotic analysis in t with exact error terms. On the other hand, the technical details have been omitted in [15]. Finally, the second-order term is completely new. Moreover, for $t \geq 3$, no explicit error term was known (in any of the references). So, for $t \geq 3$, not even any proportion of digits was known.

In the following, a tree will always be a t-ary rooted canonical tree. The set of t-ary canonical trees is denoted by $\mathcal{T}$. The number of internal vertices (non-leaves) of a tree T is denoted by $n(T)$. We are interested in the generating function

$$F(q) = \sum_{n\geq 0} g_t(n)q^n = \sum_{T\in\mathcal{T}} q^{n(T)}.$$

Here, the sum goes over trees of arbitrary size, and q is a variable. The aforementioned expression is an element of the ring of formal power series. (Later, we evaluate the power series for $q < |q_0|$, where q_0 is the dominant pole, and prove its convergence.)

This generating function can be computed explicitly.

Theorem 6: Setting $[k] := 1+t+t^2+\cdots+t^{k-1}$, we have

$$F(q) = \frac{\sum_{j=0}^{\infty}(-1)^j q^{[j]}\prod_{i=1}^{j}\frac{q^{[i]}}{1-q^{[i]}}}{\sum_{j=0}^{\infty}(-1)^j\prod_{i=1}^{j}\frac{q^{[i]}}{1-q^{[i]}}}.$$

The proof of this theorem will be given in Section V. In Section VI, we give the proof of the following theorem which gives a very precise asymptotic expression for $g_t(n)$, based on the aforementioned generating function. In view of the numerous asymptotic approximations, we point out that this is the first result containing two main terms and an explicit error term.

We used this exact formula for comparing the asymptotic approximations with the exact values of $g_t(n)$. Our straightforward implementation of this formula in Sage (Version 5.3) [37] easily allows us to compute very large values: For $t = 2$, we computed the exact values of $f_2(r)$, using the formal power series in the range $r \leq 2^{15}$. The program completed in only 135.94 s. For comparison, our asymptotic formula in the same range took 19.93 s. The exact evaluation using formal power series is also memory intensive. We stopped the computation at the argument 2^{15} due to memory constraints of 8 GB.

TABLE II

VALUES FOR SMALL VALUES OF t. STARRED ($*$) ENTRIES CORRESPOND TO VALUES SATISFYING THE ASYMPTOTIC ESTIMATES OF THEOREM 7. THE VALUES COULD BE GIVEN WITH MUCH HIGHER PRECISION. THERE IS SOME UNCERTAINTY ABOUT THE LAST DIGIT

t	ρ	ρ_2	r_3	R	R_2	R_3
2	1.794147187541686	1.279549134726681	1.123	0.1418532020854094	0.06124104103121269∗	36.6
3	1.920712538405631∗	1.211479378117327	1.098	0.1338681353605138∗	0.05040725710011751∗	39.0
4	1.964624757813775∗	1.165158374565692	1.083	0.1305243270109503∗	0.04239969309700251∗	58.4
5	1.983293986764127∗	1.134459698442781	1.074	0.1284678647212778∗	0.03633182386516354∗	70.7
6	1.991897175722647∗	1.113019849812048	1.068	0.1271299952558400∗	0.03168855397536632∗	50.0
7	1.996015107731262∗	1.097324075593615	1.063	0.1262776860399922∗	0.02807600275247040∗	59.6
8	1.998025544625657∗	1.085389242111509	1.059	0.1257503987658994∗	0.02520568904841775∗	48.1
9	1.999017663916874∗	1.076032488551186	1.056	0.1254328058843682∗	0.02287594728315024∗	24.0
10	1.999510161506312∗	1.068511410911158	1.053	0.1252458295005635∗	0.02094759256441895∗	19.7
11	1.999755441055006∗	1.062339511503337∗	1.050	0.1251378340222618∗	0.01932397366876184∗	20.1
12	1.999877817773010∗	1.057186165846774∗	1.047	0.1250764428075050∗	0.01793689446751572∗	26.6
13	1.999938935019296∗	1.052819586914068∗	1.044	0.1250420050254539∗	0.01673722535920120∗	80.6
14	1.999969474502513∗	1.049072853620226∗	1.042	0.1250229006766309∗	0.01568876914448585∗	43.3
15	1.999984739115025∗	1.045822904924682∗	1.040	0.1250124013324635∗	0.01476426249364319∗	39.0

Theorem 7 (Main Theorem): For $t \geq 2$, the following holds:

$$g_t(n) = R\rho^{n+1} + R_2\rho_2^{n+1} + R_3 r_3^n \varepsilon_1(t,n). \tag{IV.1}$$

Here, $\rho > \rho_2 > r_3$ and R, R_2, R_3 are positive real constants to be specified in the following, and depending on t. Here and below, $\varepsilon_j(\ldots)$, $j = 1, \ldots$, denote real functions with $|\varepsilon_j(\ldots)| \leq 1$ for all valid values of the indicated parameters.

For $t \geq 16$, we have

$$\begin{aligned} \rho &= 2 - \frac{1}{2^{t+1}} - \frac{t+3}{2^{2t+3}} \\ &\quad - \frac{3t^2+19t+24}{2^{3t+6}} + \frac{0.28t^3}{2^{4t}}\varepsilon_2(t) && \text{(IV.2)} \\ \rho_2 &= 1 + \frac{L}{t} - \frac{L-L^2}{2t^2} + \frac{4L^3+3L^2+6L}{24t^3} \\ &\quad + \frac{2L^4+54L^3-27L^2-6L}{48t^4} + \frac{0.26}{t^5}\varepsilon_3(t) && \text{(IV.3)} \\ r_3 &= 1 + \frac{L}{t} - \frac{L-L^2}{2t^2} && \text{(IV.4)} \\ R &= \frac{1}{8} + \frac{t-2}{2^{t+5}} + \frac{2t^2+3t-5}{2^{2t+7}} \\ &\quad + \frac{9t^3+45t^2+20t-68}{2^{3t+10}} + \frac{t^4}{50\cdot 2^{4t}}\varepsilon_4(t) && \text{(IV.5)} \\ R_2 &= \frac{1}{4t} - \frac{4L+1}{8t^2} + \frac{0.77}{t^3}\varepsilon_5(t) && \text{(IV.6)} \\ R_3 &= 5t^4 && \text{(IV.7)} \end{aligned}$$

where $L = \log 2$.

For $3 \leq t \leq 15$, (IV.1) holds with (IV.2), (IV.5), and (IV.6) and the values for ρ_2, r_3, and R_3 given in Table II.

For $t = 2$, (IV.1) holds with (IV.6) and the values for ρ, ρ_2, r_3, R, and R_3 given in Table II.

For simplicity, the functions ε_j can be thought of as $O(1)$ terms. Some of our proofs indeed depend on explicit values of the error bounds. For this reason, we had to compute absolute O-constants in any case, and decided to include these in the statement of the theorem.

The asymptotic result focuses on the first and the second exponential terms ρ^{n+1} and ρ_2^{n+1} and no effort has been made to improve the error term r_3^n: note that for large t, it is not much smaller than the second-order term ρ_2^{n+1}. For Table II, the values r_3 have been improved by a computer calculation in comparison with (IV.4), also leading to a stronger value of the constant R_3 in comparison with (IV.7). In principle, this type of improvement is possible for any fixed $t \geq 16$ as well.

The asymptotic expansions of ρ, ρ_2, R, and R_2 can always be refined by further iterating the fixed-point equations in the proof of Proposition 10. So, for fixed k, we could refine the estimates for ρ and R to a precision of $t^k 2^{-tk}$ and the estimates for ρ_2 and R_2 to a precision of t^{-k}.

V. GENERATING FUNCTION

This section is devoted to the proof of Theorem 6.

Proof of Theorem 6: In the proof of the theorem, we will actually consider more refined statistics in order to derive a functional equation for a more general generating function.

The height of a vertex in a rooted tree is defined to be its distance from the root. So, the root has height 0. The height $\mathsf{height}(T)$ of a tree T is defined to be the maximal height of its vertices.

For a rooted tree T, we set $m(T)$ to be the number of leaves of maximum height of T.

We will derive a functional equation for the generating function

$$G(q,u) = \sum_{T\in\mathcal{T}} q^{n(T)} u^{m(T)}$$

i.e., u counts the number of leaves of maximal height and q counts the number of internal vertices. By definition, we have $F(q) = G(q,1)$.

To derive the functional equation for $G(q,u)$, we partition $\mathcal{T}$ with respect to the height and consider

$$G_k(q,u) = \sum_{\substack{T\in\mathcal{T}\\ \mathsf{height}(T)=k}} q^{n(T)} u^{m(T)}.$$

Obviously, we have

$$G(q,u) = \sum_{k\geq 0} G_k(q,u).$$

A tree T of height k corresponds to exactly $m(T)$ trees T'_j, $j \in \{1,\ldots,m(T)\}$, of height $k+1$: T'_j arises from T by replacing j of the $m(T)$ leaves of maximum height by vertices with t attached leaves. On the other hand, all trees T' of height $k+1$ are uniquely described by this process.

Thus, we have

$$\begin{aligned} G_{k+1}(q,u) &= \sum_{\substack{T\in\mathcal{T}\\ \mathsf{height}(T)=k}} \sum_{j=1}^{m(T)} q^{n(T)+j}u^{jt} \\ &= \sum_{\substack{T\in\mathcal{T}\\ \mathsf{height}(T)=k}} q^{n(T)}\cdot qu^t\cdot \frac{1-(qu^t)^{m(T)}}{1-qu^t} \\ &= \frac{qu^t}{1-qu^t}\left(G_k(q,1)-G_k(q,qu^t)\right). \qquad \text{(V.1)}\end{aligned}$$

We have $G_0(q,u)=u$, so summing over all $k\geq 0$ yields

$$G(q,u)-u=\frac{qu^t}{1-qu^t}(G(q,1)-G(q,qu^t)). \qquad \text{(V.2)}$$

The generating function $G(q,u)$ is certainly convergent for $|u|\leq 1$ and $|q|<1/2$, as can be seen from (V.1).

We now keep q with $|q|<1/2$ fixed and consider everything as a function of u with $|u|\leq 1$. We use the abbreviations $h(u)=qu^t/(1-qu^t)$ and $g(u)=G(q,u)$. We rewrite the functional equation (V.2) as

$$g(u)=u+h(u)g(1)-h(u)g(qu^t). \qquad \text{(V.3)}$$

By iterating (V.3) r times, we obtain

$$\begin{aligned} g(u) &= a_r(u)+b_r(u)g(1)+c_r(u)g(q^{[r+1]}u^{t^{r+1}}) \\ a_r(u) &= \sum_{j=0}^{r}(-1)^j q^{[j]}u^{t^j}\prod_{i=0}^{j-1}h(q^{[i]}u^{t^i}) \\ b_r(u) &= \sum_{j=0}^{r}(-1)^j\prod_{i=0}^{j}h(q^{[i]}u^{t^i}) \\ c_r(u) &= (-1)^{r+1}\prod_{i=0}^{r}h(q^{[i]}u^{t^i})\end{aligned}$$

for $r\geq 0$. As $|h(u)|\leq \frac{|q|}{1-|q|}<1$ holds for all $|u|\leq 1$, the limits

$$\begin{aligned} a(u) &= \sum_{j=0}^{\infty}(-1)^j q^{[j]}u^{t^j}\prod_{i=0}^{j-1}h(q^{[i]}u^{t^i}) \\ b(u) &= \sum_{j=0}^{\infty}(-1)^j\prod_{i=0}^{j}h(q^{[i]}u^{t^i})\end{aligned}$$

exist and we have

$$\lim_{r\to\infty} c_r(u)g(q^{r+1}u^{t^{r+1}})=0.$$

Thus, we obtained

$$g(u)=a(u)+b(u)g(1).$$

Setting $u=1$ yields

$$F(q)=G(q,1)=g(1)=\frac{a(1)}{1-b(1)}.$$

■

VI. Asymptotics, Proof of Theorem 7

After some preparatory lemmas, at the end of this section, we prove Theorem 7.

We will use the following notations in order to work with the generating function F:

$$\begin{aligned} f_j(q) &= \frac{q^{[j]}}{1-q^{[j]}} \\ N_K(q) &= \sum_{0\leq k<K}(-1)^k q^{[k]}\prod_{j=1}^{k}f_j(q) \\ D_K(q) &= \sum_{0\leq k<K}(-1)^k\prod_{j=1}^{k}f_j(q) \\ N(q) &= \sum_{0\leq k}(-1)^k q^{[k]}\prod_{j=1}^{k}f_j(q) \\ D(q) &= \sum_{0\leq k}(-1)^k\prod_{j=1}^{k}f_j(q).\end{aligned}$$

The quantities have been defined such that $F(q)=N(q)/D(q)$. The names N and D refer to their roles as numerator and denominator, respectively.

We intend to work with the finite sums D_K and N_K for fixed values of K, so we need upper bounds for the approximation errors.

Lemma 8: Let $K\geq 0$ and $|q|^{[K+1]}<1/2$. Then

$$\begin{aligned} &|N(q)-N_K(q)| \\ &\quad\leq \left(\frac{1-|q|^{[K+1]}}{1-2|q|^{[K+1]}}\prod_{j=1}^{K}\frac{1}{1-|q|^{[j]}}\right)|q|^{[K]+\sum_{j=1}^{K}[j]} \qquad \text{(VI.1a)} \\ &|D(q)-D_K(q)| \\ &\quad\leq \left(\frac{1-|q|^{[K+1]}}{1-2|q|^{[K+1]}}\prod_{j=1}^{K}\frac{1}{1-|q|^{[j]}}\right)|q|^{\sum_{j=1}^{K}[j]}. \qquad \text{(VI.1b)}\end{aligned}$$

These bounds are decreasing in t and increasing in $|q|$.

Proof: As $|f_j(q)|\leq f_j(|q|)$ and $f_j(|q|)$ is decreasing in j, we have

$$\begin{aligned} &|D(q)-D_K(q)| \\ &\quad\leq \sum_{k=K}^{\infty}\prod_{j=1}^{K}f_j(|q|)\prod_{j=K+1}^{k}f_j(|q|) \\ &\quad\leq \prod_{j=1}^{K}f_j(|q|)\sum_{k=K}^{\infty}f_{K+1}(|q|)^{k-K} \\ &\quad= \frac{1}{1-f_{K+1}(|q|)}\prod_{j=1}^{K}f_j(|q|)\end{aligned}$$

which, upon inserting the definition of f_j, yields (VI.1b). The approximation bound (VI.1a) for the numerator follows along the same lines; we get an additional factor $q^{[K]}$. ■

We will also need estimates for the derivative $D'(q)$ (we recall the abbreviation $L=\log 2$ introduced in Theorem 7).

Lemma 9: Let $t\geq 30$ and $q\in\mathbb{C}$ with $1/2\leq |q|\leq 1/r_3$, where $r_3=1+\frac{L}{t}-\frac{L-L^2}{2t^2}$ (cf., (IV.4)). Then

$$|D'(q)-D_4'(q)|\leq \frac{1}{2^{t^2}}.$$

Proof: Let $q = 1/z$ with $r_3 \le |z| \le 2$. Then, $f_j(q) = f_j(1/z) = \frac{1}{z^{[j]}-1}$ and $|f_j(q)| = 1/|z^{[j]}-1| \le 1/(r_3^{[j]}-1)$. We use standard estimates on logarithms and exponential function which arise by truncating Taylor series of these functions and by bounding the truncation error. This results in

$$\begin{aligned} r_3 - 1 &\ge \frac{1}{2t} \\ r_3^{[2]} - 1 &= \exp\Big((1+t)\log\Big(1+\frac{L}{t}-\frac{L-L^2}{2t^2}\Big)\Big) \\ &\quad - 1 \ge 1 \\ r_3^{[3]} - 1 &\ge 2^t && \text{(VI.2a)} \\ r_3^{[4]} - 1 &\ge 2^{t^2+t/2}. && \text{(VI.2b)} \end{aligned}$$

We have

$$\begin{aligned} &|D'(1/z) - D_4'(1/z)| \\ &\le |z| \sum_{k=4}^{\infty} \prod_{j=1}^{k} f_j(1/|z|) \Big(\sum_{j=1}^{k} \frac{[j]}{1-(1/|z|)^{[j]}}\Big) \\ &\le 2 \sum_{k=4}^{\infty} \frac{t\big(4t + 4\sum_{j=2}^{k}[j]\big)}{2^{-1+t(k-1)/2+(k-3)t^2}} \\ &\le \sum_{k=4}^{\infty} \frac{kt^{k+1}}{2^{(k-3)t^2+t(k-1)/2-4}} \\ &\le \frac{1}{2} \sum_{k=4}^{\infty} \frac{1}{2^{t^2(k-3)}} \le \frac{1}{2^{t^2}}. \end{aligned}$$

■

The exponential growth of the coefficients $g_t(n)$ of $F(q)$ is directly related to the dominating pole $1/\rho$ of $F(q)$. So, we now investigate the location of the poles of $F(q)$. Essentially, this is equivalent to finding the zeros of the denominator of $F(q)$.

Proposition 10: Let $t \ge 2$. Then, there are exactly two poles $1/\rho$ and $1/\rho_2$ of $F(q)$ with $|q| \le 1/r_3$, where r_3 has been defined in (IV.4) (or Table II for $t \in \{2, 3\}$).

Both $1/\rho$ and $1/\rho_2$ are simple poles of $F(q)$. The dominant pole $1/\rho$ of $F(q)$ is asymptotically given by (IV.2) (or Table II for $t = 2$).

The residue of $F(q)$ at $1/\rho$ is $-R$ where R is asymptotically given by (IV.5) (or Table II for $t = 2$).

The pole $1/\rho_2$ is given by (IV.3) (or Table II for $2 \le t \le 15$), the residue of $F(q)$ at $1/\rho_2$ is $-R_2$, where R_2 is given in (IV.6).

Finally, we have

$$|F(q)| \le 5t^4 \qquad \text{(VI.3)}$$

for all q with $|q| = 1/r_3$.

We first outline the proof of Proposition 10; the details follow below. We rewrite the equation $D(q) = 0$ into a fixed-point equation $q = Q(q)$ (cf., (VI.4)). It turns out that the dominant pole $1/\rho$ is an attractive fixed point of Q. Therefore, inserting preliminary bounds for $1/\rho$ improves these bounds. After several iterations ("bootstrapping", cf., [19, Sec. 4.1.2]), we get very precise bounds for $1/\rho$. The second pole $1/\rho_2$, however, is a repellent fixed point of Q. Inverting the fixed-point equation yields $q = Q^{-1}(q)$ and $1/\rho_2$ is indeed an attractive fixed point of Q^{-1}. However, inverting Q involves extracting a $(t+1)$-st root, so several branches occur. In order to pick the correct branch, additional inequalities are required. After establishing these, precise bounds for $1/\rho_2$ are obtained. We repeatedly use power series estimates in order to get the required inequalities. In order to sharpen these estimates, we first assume that $t \ge 30$.

Proof: In the proof of this proposition, some more functions $\varepsilon_j(\ldots)$ occur. We first allow complex values for the $\varepsilon_j(\ldots)$; it will later turn out that those occurring in Theorem 7 have only real values.

In the following, we consider the case $t \ge 30$. The remaining cases $2 < t < 30$ are much easier and will be discussed at the end of this proof. Assume that $1/z$ is a pole of $F(q)$ with $|z| \ge 1 + a/t$ for some $2 \ge a \ge L$. As $N(q)$ is holomorphic for $|q| < 1$, cf., Lemma 8, $1/z$ must be a root of $D(q)$. Using $K = 3$, we get

$$\begin{aligned} 0 = 1 - \frac{1}{z-1} + \frac{1}{z-1}\frac{1}{z^{t+1}-1} \\ + (D(1/z) - D_3(1/z)) \end{aligned}$$

which is equivalent to

$$2 - z = \frac{1}{z^{t+1}-1} + (z-1)(D(1/z) - D_3(1/z)). \qquad \text{(VI.4)}$$

Taking absolute values, (VI.1b) yields

$$\begin{aligned} 2 - |z| &\le |2 - z| \\ &\le \frac{1}{|z|^{[2]}-1}\Bigg(1 + \frac{1}{|z|^{[3]}-1}\cdot\frac{1}{1-\frac{1}{|z|^{[4]}-1}}\Bigg). \qquad \text{(VI.5)} \end{aligned}$$

We have

$$\begin{aligned} |z|^{[2]} &\ge \left(1+\frac{a}{t}\right)^{t+1} \\ &= \exp\left((t+1)\log\left(1+\frac{a}{t}\right)\right) \\ &\ge \exp\left((t+1)\left(\frac{a}{t}-\frac{a^2}{2t^2}\right)\right) \\ &= \exp\left(a + \frac{a - a^2/2}{t} - \frac{a^2}{2t^2}\right) \\ &\ge \exp\left(a + \frac{b}{t}\right) \\ &\ge e^a\left(1+\frac{b}{t}\right) \qquad \text{(VI.6)} \end{aligned}$$

for $b = a - 31a^2/60 > 0$. By (VI.2a) and (VI.2b), we have

$$\frac{1}{|z|^{[3]}-1}\cdot\frac{1}{1-\frac{1}{|z|^{[4]}-1}} \le \frac{1.00001}{2^t}. \qquad \text{(VI.7)}$$

Consider now the case $a = L$. Then, (VI.5)–(VI.7) yield

$$2 - |z| \le \frac{1}{1+\frac{2b}{t}}\left(1+\frac{1.00001}{2^t}\right) \le 1 - \frac{4}{5t}. \qquad \text{(VI.8)}$$

We conclude that $|z| \ge 1 + \frac{4}{5t}$. So, using now $a = 4/5$, (VI.5)–(VI.7) yield

$$2 - |z| \le \frac{1}{e^{4/5}-1}\left(1+\frac{1.00001}{2^t}\right) \le 0.82$$

and therefore $|z| \geq 1.18$. Inserting this and (VI.7) in (VI.5) now yields

$$\begin{aligned} 2-|z| &\leq |2-z| \\ &\leq \frac{1}{1.18^{t+1}-1}\left(1+\frac{1.00001}{2^t}\right) \\ &\leq \frac{0.86}{1.18^t}. \end{aligned}$$

We conclude that $z = 2+O(1.18^{-t})$. We now rewrite (VI.4) as

$$z = 2 - \frac{1}{z^{t+1}-1} + O(2^{-t^2}). \tag{VI.9}$$

Inserting $z = 2 + O(1.18^{-t})$ in the right-hand side of (VI.9) yields

$$\begin{aligned} z &= 2 - \frac{1}{(2+O(1.18^{-t}))^{t+1}-1} \\ &= 2 - \frac{1}{2^{t+1}}\left(1+O(t\,1.18^{-t})\right). \end{aligned}$$

We now repeat the process: We insert this estimate on the right-hand side of (VI.9) and get a better estimate. After a few iterations (and taking care of all implicit constants), we finally get (IV.2). Inserting the lower and the upper bounds of (IV.2) into $D_3(q)$ (and taking into account $D(q)-D_3(q)$), we see that $D(q)$ changes sign within the interval, so there is certainly a root $1/z$ of $D(q)$ fulfilling (IV.2).

Inserting this asymptotic expression into $D'(q)$ and using Lemma 9, we get

$$|D'(1/z)+4| \leq 1.04t2^{-t} \tag{VI.10}$$

for $t \geq 30$. This shows that there is at most one zero of $D(1/z)$ within the bounds of the asymptotic expression (IV.2): if there were two, say $1/z_1$ and $1/z_2$, then

$$\begin{aligned} &4\left|\frac{1}{z_2}-\frac{1}{z_1}\right| \\ &= \left|D(1/z_2)-D(1/z_1)+4\left(\frac{1}{z_2}-\frac{1}{z_1}\right)\right| \\ &= \left|\int_{[1/z_1,1/z_2]}(D'(q)+4)\,dq\right| \\ &\leq 1.04t2^{-t}\left|\frac{1}{z_2}-\frac{1}{z_1}\right| \end{aligned}$$

which implies $1/z_1 = 1/z_2$. Here, we integrate over the straight line from $1/z_1$ to $1/z_2$. The estimate (VI.10) also shows that there can only be a simple root. Thus, we have shown that the only root $1/z$ of D with $|z| \geq 1+L/t$ is a simple zero with z as in (IV.2). The residue (IV.5) follows upon inserting (IV.2) into $N(1/z)/D'(1/z)$. Note that this also shows that the dominant zero of the denominator does not cancel out against a zero of the numerator.

Now assume that $|D(1/z)| \leq 1/t^3$ holds for some z with $r_3 \leq |z| \leq 1+L/t$. Inserting these bounds into (VI.5), we get

$$\begin{aligned} |z-2| \leq 1 - \frac{L}{t} &+ \frac{4L^3-3L^2+12L}{12t^2} \\ &+ \frac{1.5}{t^3}\varepsilon_6(t,z) =: r'. \end{aligned} \tag{VI.11}$$

The intersection point with positive imaginary part of the circle of radius $1+L/t$ centered at the origin with the circle of radius r' centered at 2 is denoted by ξ. We obtain

$$\xi = 1 + \frac{4L + i\sqrt{\frac{16}{3}L^3-4L^2+16L}}{4t} + \frac{2.23}{t^2}\varepsilon_7(t).$$

In particular, we have

$$|z-1| \leq |\xi - 1| \leq \frac{1.14}{t} \tag{VI.12}$$

and

$$|\arg(z)| \leq |\arg\xi| \leq |\log\xi| \leq \frac{1.18}{t}. \tag{VI.13}$$

As $|D(1/z)| \leq 1/t^3$, we have (after multiplication with $z-1$)

$$0 = z - 2 + \frac{1}{z^{t+1}-1} + \frac{2.01}{t^3}\varepsilon_8(t,z).$$

Solving for z^{t+1} yields

$$z^{t+1} = 1 + \frac{1}{2-z-\frac{2.01}{t^3}\varepsilon_8(t,z)}.$$

As $z = 1 + \frac{1.14}{t}\varepsilon_9(t,z)$ by (VI.12), we obtain

$$z^{t+1} = 2 + \frac{1.19}{t}\varepsilon_{10}(t,z).$$

We conclude that

$$z = \exp\left(\frac{2\ell\pi i}{t+1} + \frac{1}{t+1}\log\left(2+\frac{1.19}{t}\varepsilon_{10}(t,z)\right)\right) \tag{VI.14}$$

for some integer ℓ with $-\frac{t+1}{2} < \ell \leq \frac{t+1}{2}$. In particular, we have

$$\arg z = \frac{2\ell\pi}{t+1} + \frac{1}{t+1}\Im\log\left(1+\frac{1.19}{2t}\varepsilon_{10}(t,z)\right)$$

which, in view of (VI.13), implies $\ell = 0$. Thus, (VI.14) simplifies to

$$\begin{aligned} z &= \exp\left(\frac{1}{t+1}\log\left(2+\frac{1.19}{t}\varepsilon_{10}(t,z)\right)\right) \\ &= 1 + \frac{L}{t} + \frac{1.63}{t^2}\varepsilon_{11}(t,z). \end{aligned}$$

We may now repeat the argument a few times to finally obtain

$$z = 1 + \frac{L}{t} - \frac{L-L^2}{2t^2} + \frac{4L^3+3L^2+6L}{24t^3} + \frac{3.45}{t^4}\varepsilon_{12}(t,z).$$

Thus, we have $|z| > r_3$. We have therefore shown that

$$|D(q)| \geq \frac{1}{t^3} \qquad \text{for} \qquad |q| = 1/r_3.$$

So, we now assume that $D(1/z) = 0$ for some z with $r_3 \leq |z| < 1+L/t$. Repeating the aforementioned steps with $1/t^3$ replaced by 0 gives the slightly better bound $z = \rho_2$ with ρ_2 as in (IV.3).

Inserting the real upper and lower bounds implied by (IV.3) into $D_3(q)$ and taking the error $D(q) - D_3(q)$ into account shows that the sign of $D(q)$ changes sign in this interval, so there is a real root $1/z = 1/\rho_2$ of $D(q)$ fulfilling (IV.3).

For the z in (IV.3), we get

$$D'(1/z) = \frac{2}{L}t^2 + 1.07t\varepsilon_{13}(t,z)$$

which implies that there is exactly one simple zero $1/z$ of $D(q)$ with z fulfilling (IV.3). By the same argument as earlier, this is the only zero $1/z$ with $r_3 \leq |z| < 1 + L/t$. Computing $N(1/z)/D'(1/z)$ finally yields the residue given in (IV.6).

We already know that $|D(q)| \geq 1/t^3$ for all q with $|q| = 1/r_3$. We also get $|N(q)| \leq 5t$. This yields (VI.3).

We now turn to the case $2 \leq t < 30$. Here, the asymptotic estimates can be replaced by concrete numbers. In fact, we only have to find zeros of the denominator, where the infinite series is truncated and the error is estimated as in Lemma 8. We use the interval arithmetic built in Sage [37], which uses correct rounding and therefore keeps track of rounding errors.

We start with the unit square in $\mathbb{C}$. We carry out a bisection process discarding those intervals where no zero can occur. More precisely, given a square $I \subseteq \mathbb{C}$, we compute the image $D(I)$ of the complex interval I under the denominator D (computing $D_K(I)$ for a suitable K using the interval arithmetic and adding the error obtained in Lemma 8). If zero is not contained in the resulting interval containing $D(I)$, there is no zero of D in I, so I can be discarded. If I lies outside the circle with radius $1/r_3$, we also discard I, because we are not interested in large zeros of the denominator. Otherwise, we bisect I.

This procedure leads to two small intervals (of diameter $<10^{-10}$) containing all roots of the denominator. Within these small intervals, we obtained good bounds for the derivative D'; so, we can conclude (by the same arguments as in the case $t \geq 30$) that there can only be one root in each of these intervals and that these roots have to be simple. Both of these intervals intersect the real axis. By computing the signs of D at the ends of the intersection of the complex intervals with the real axis and observing a sign change, we conclude that the roots are simple roots. The standard real bisection method is then used to improve the real bounds. ■

Using Proposition 10, the proof of Theorem 7 only requires a standard application of results from complex analysis.

Proof of Theorem 7: This is a consequence of singularity analysis [14], cf., also [16].

In this simple case, this also follows from Cauchy's integral formula and the residue theorem: By Cauchy's integral formula, we have

$$g_t(n) = \frac{1}{2\pi i}\oint_{|q|=1/10} \frac{F(q)}{q^{n+1}}\,dq.$$

Shifting the line of integration to $|q| = 1/r_3$ and taking the residues at $1/\rho$ and $1/\rho_2$ into account, the residue theorem (and Proposition 10) yield

$$g_t(n) = R\rho^{n+1} + R_2\rho_2^{n+1} + \frac{1}{2\pi i}\oint_{|q|=1/r_3} \frac{F(q)}{q^{n+1}}\,dq.$$

Estimating the latter integral using Proposition 10 finally gives

$$\frac{1}{2\pi i}\oint_{|q|=1/r_3} \frac{F(q)}{q^{n+1}}\,dq = \varepsilon_1(t,n)5t^4r_3^n.$$

■

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