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DENSITY BOUNDS FOR THE $3x+1$ PROBLEM. I. TREE-SEARCH METHOD

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Dedicated to the memory of D. H. Lehmer

ABSTRACT. The $3x+1$ function $T(x)$ takes the values $(3x+1)/2$ if x is odd and $x/2$ if x is even. Let a be any integer with $a \not\equiv 0 \pmod 3$. If $n_k(a)$ counts the number of n with $T^{(k)}(n) = a$, then for all sufficiently large k, $(1.302)^k \le n_k(a) \le (1.359)^k$. If $\pi_a(x)$ counts the number of n with $|n| \le x$ which eventually reach a under iteration by T, then for sufficiently large x, $\pi_a(x) \ge x^{.65}$. The proofs are computer-intensive.

1. INTRODUCTION

The $3x+1$ problem concerns the iteration of the function $T\colon \mathbb{Z} \to \mathbb{Z}$ defined by

$$T(x) = \begin{cases} \frac{3x+1}{2} & \text{if } x \equiv 1 \pmod 2, \\ \frac{x}{2} & \text{if } x \equiv 0 \pmod 2. \end{cases} \tag{1.1}$$

The $3x+1$ conjecture asserts that, for all $n \ge 1$, some iterate $T^{(k)}(n) = 1$. More generally, it is conjectured that T has finitely many cycles under iteration and that every $n \in \mathbb{Z}$ eventually enters a cycle (cf. Lagarias [6]). The $3x+1$ conjecture has been verified for all $n < 5.6 \times 10^{13}$ by Leavens and Vermeulen [8].

One approach to these conjectures is to study how many integers n below a given bound x have some $T^{(k)}(n) = 1$. More generally, for any $a \in \mathbb{Z}$, set

$$\pi_a(x) = \#\{n\colon |n| \le x \text{ and some } T^{(k)}(n) = a,\ k \ge 0\}. \tag{1.2}$$

It is well known that the growth of $\pi_a(x)$ depends on the residue class of $a \pmod 3$. If $a \equiv 0 \pmod 3$, then the preimages of a under iterates of T are exactly $\{2^k a\colon k \ge 1\}$; hence $\pi_a(x)$ grows logarithmically with x. The other cases are covered by the following conjecture.

Conjecture A. *For each $a \not\equiv 0 \pmod 3$, there is a positive constant c_a such that*

$$\pi_a(x) \ge c_a x \quad \textit{for all } x \ge |a|.$$

In any case, one has, for $a \not\equiv 0 \pmod 3$,

$$\pi_a(x) \ge x^{\gamma} \quad \text{for } x \ge x_0(a), \tag{1.3}$$

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for some constant $\gamma > 0$. This was first shown by Crandall [3], with $\gamma = .05$. Crandall's approach directly studies the tree of preimages of a under T. Sander [9] strengthened Crandall's approach to obtain $\gamma = .30$. Krasikov [5] introduced a different method which derives a system of difference inequalities with variables associated to congruence classes (mod 3^k). Using these inequalities for $k = 2$, he obtained $\gamma = .43$. Wirsching [10] used Krasikov's inequalities with $k = 3$ to obtain $\gamma = .48$.

In studying $\pi_a(x)$, a related problem concerns the size of the tree of preimages of a under T. Let

$$n_k(a) := \#\{n\colon T^{(k)}(n) = a\}. \tag{1.4}$$

Lagarias and Weiss [7] proved a result implying that, for $a \not\equiv 0 \pmod 3$, the average size of $n_k(a)$ as a varies is $\frac{3}{2}(\frac{4}{3})^k$. They conjectured

Conjecture B. *For each* $a \not\equiv 0 \pmod 3$,

$$n_k(a) = \left(\frac{4}{3}\right)^{k(1+o(1))} \quad \text{as } k \to \infty. \tag{1.5}$$

For a not in a cycle, they showed that

$$\frac{1}{2}(\sqrt[4]{2})^k \le n_k(a) \le 2(\sqrt{3})^k, \tag{1.6}$$

by studying all possible trees of backward iterates of depth 4.

The object of this paper and its sequel is to obtain improved bounds for $\pi_a(x)$ and $n_k(a)$, using computer-assisted proofs. This paper obtains bounds based on the tree-search approach started by Crandall, while the sequel obtains bounds for $\pi_a(x)$ derived from Krasikov's difference inequalities.

In §2 we study trees $\mathscr{T}_k^*(a)$ containing all $n \not\equiv 0 \pmod 3$ with $T^{(j)}(n) = a$ for some $j \le k$. The structure of this tree depends only on $a \pmod{3^{k+1}}$. Each leaf n of the tree is assigned a *weight* which counts the number of iterates $T^{(i)}(n) \equiv 1 \pmod 2$, for $0 \le i \le k-1$. By computer search we find, for all $k \le 30$, upper and lower bound statistics concerning the number of leaves of such trees having a fixed weight. An immediate consequence is

Theorem 1.1. *For any* $a \not\equiv 0 \pmod 3$, *and for all sufficiently large* k,

$$(1.302053)^k \le n_k(a) \le (1.358386)^k. \tag{1.7}$$

The proof of Theorem 1.1 is unavoidably computer-intensive; in effect it searches all trees of depth 30.

The upper bound and lower bound statistics for number of leaves lie within a small constant factor of $(\frac{4}{3})^k$. They appear to have a narrower distribution than that predicted by the branching process models for $3x + 1$ trees studied in [7], as we show in detail elsewhere [2].

In §3 we use Chernoff bounds to obtain lower bounds for the number of leaves in such trees having a large weight. Considering trees of depth k, we obtain a bound γ_k^* for the exponent γ in (1.3) by optimizing a "large deviations" bound for the number of heavily weighted leaves in a "worst-case" tree of depth k. Taking $k = 30$, we obtain

Theorem 1.2. *For each* $a \not\equiv 0 \pmod 3$, *there is a positive constant* c_a *such that*

$$\pi_a(x) \geq c_a x^{.65} \quad \text{for all } x \geq |a|. \tag{1.8}$$

This exponent improves on previous bounds; however, in part II we will show that Krasikov's inequalities give still better exponents.

In §3 we also obtain upper bounds for the number of leaves in any tree $\mathcal{T}_k^*(a)$ that have a large weight. Korec [4] showed for all $\beta > \beta_c := \frac{\log 3}{\log 4}$ that the set $\{n\colon \text{some } |T^{(k)}(n)| < |n|^\beta\}$ has density one. We describe an approach to lower the bound β_c using such upper bound estimates. This approach becomes effective, however, only if a certain threshold is exceeded, and it is not reached by tree depth $k = 30$.

2. $3x+1$ TREES

Throughout this section we suppose that $a \not\equiv 0 \pmod 3$. The preimages under T^{-1} of a form an infinite labelled by tree $\mathcal{T}(a)$, whose root node is labelled a and whose nodes at the kth level are labelled by $\{n\colon T^{(k)}(n) = a\}$. Note that if a is not in a cycle, then no two nodes of $\mathcal{T}(a)$ have the same label, while if a is in a cycle then labels will be repeated. The tree $\mathcal{T}(a)$ is constructed recursively using the multivalued operator

$$T^{-1}(n) = \begin{cases} \{2n\} & \text{if } n \equiv 0, 1 \pmod 3, \\ \{2n, \frac{2n-1}{3}\} & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

Each node n at level k of the tree is connected to one or two nodes at depth $k+1$ of the tree, which are labelled using the labels in $T^{-1}(n)$.

In studying asymptotic properties of $n_k(a)$, it proves convenient to throw out all preimages $n \equiv 0 \pmod 3$, and to estimate instead the quantity

$$n_k^*(a) := \#\{n\colon T^{(k)}(n) = a \text{ and } n \not\equiv 0 \pmod 3\}. \tag{2.1}$$

It is easy to show that

$$n_k^*(a) \leq n_k(a) \leq k n_k^*(a)$$

(see Lemma 3.1 of [7]); hence $n_k^*(a)$ and $n_k(a)$ have similar exponential growth rates in k as $k \to \infty$.

Thus, following [7], we study the smaller tree $\mathcal{T}^*(a)$ resulting by deleting all nodes $n \equiv 0 \pmod 3$ from $\mathcal{T}(a)$. The inverse operator $(T^*)^{-1}$ of T on the restricted domain $\{n\colon n \not\equiv 0 \pmod 3\}$ is

$$(T^*)^{-1}(n) = \begin{cases} \{2n\} & \text{if } n \equiv 1, 4, 5, \text{ or } 7 \pmod 9, \\ \{2n, \frac{2n-1}{3}\} & \text{if } n \equiv 2 \text{ or } 8 \pmod 9. \end{cases} \tag{2.2}$$

Let $\mathcal{T}_k^*(a)$ denote the depth-k subtree of $\mathcal{T}(a)$; see Figure 2.1 (next page) for $\mathcal{T}_5(4)$ and $\mathcal{T}_5^*(4)$.

We next assign *weights* to nodes and edges of the tree which keep track of $3x+1$ iterates (mod 2). An edge connecting $2n$ and n is assigned weight 0, while one connecting $\frac{2n-1}{3}$ and n is assigned weight 1. Each node of a tree (except the root) is then assigned weight equal to the sum of the weights of the edges connecting it to the root node. Thus a leaf l of $\mathcal{T}_k^*(a)$ is assigned

$$\text{weight}(l) := \#\{i\colon T^{(i)}(l) \equiv 1 \pmod 2,\ 0 \leq i \leq k-1\}. \tag{2.3}$$

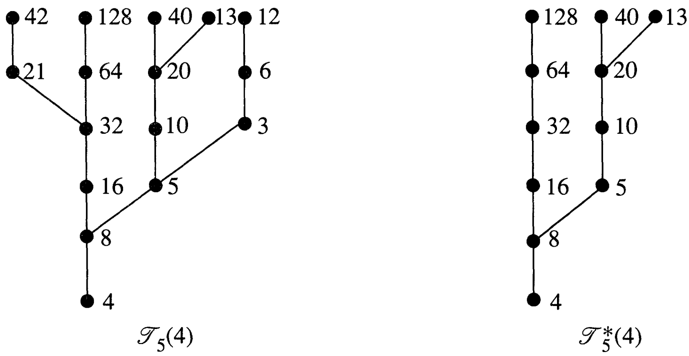

FIGURE 2.1. $3x+1$ tree $\mathcal{T}_5(4)$ and pruned tree $\mathcal{T}_5{}^*(4)$

The weight approximately measures the size of the node label, namely,

$$l \leq 3^{-\mathrm{weight}(l)} 2^k a. \tag{2.4}$$

In addition it can be shown that

$$l = (1+o(1)) 3^{-\mathrm{weight}(l)} 2^k a \quad \text{as } k \to \infty, \tag{2.5}$$

for all those l having weight $(l) \leq \frac{6}{10} k$.

The branching structure of the tree $\mathcal{T}_k{}^*(a)$, together with the weights of all its nodes and edges, is completely determined by the congruence class of a (mod 3^{k+1}); thus the number of distinct tree structures $\mathcal{T}_k{}^*(a)$ is at most $2 \cdot 3^k$.

We study various statistics concerning the leaves of the trees $\mathcal{T}_k{}^*(a)$. Let $w_j^k(a)$ count the number of leaves of $\mathcal{T}_k{}^*(a)$ having weight j. This gives the vector of weights

$$\mathbf{w}_k^*(a) := (w_0^k(a), w_1^k(a), \dots, w_k^k(a)). \tag{2.6}$$

Now let $N_k^*(a)$ count the number of leaves of $\mathcal{T}_k{}^*(a)$, and we have

$$N_k^*(a) = w_0^k(a) + w_1^k(a) + \cdots + w_k^k(a). \tag{2.7}$$

It is obvious that $n_k^*(a) \leq N_k^*(a)$, and equality holds whenever a is not in a cycle of T. Theorem 3.1 of [7] showed that the expected size $E[N_k^*(a)]$ averaged over residue classes a (mod 3^{k+1}) with $a \not\equiv 0$ (mod 3) is

$$E[N_k^*(a)] = \left(\frac{4}{3}\right)^k. \tag{2.8}$$

We study the quantities

$$N^+(k) := \max\{N_k^*(a) \colon a \ (\mathrm{mod}\ 3^{k+1}) \text{ with } a \not\equiv 0 \ (\mathrm{mod}\ 3)\},$$
$$N^-(k) := \min\{N_k^*(a) \colon a \ (\mathrm{mod}\ 3^{k+1}) \text{ with } a \not\equiv 0 \ (\mathrm{mod}\ 3)\}.$$

We also study the majorant vectors $\mathbf{w}^+(k)$ and the minorant vectors $\mathbf{w}^-(k)$ which we now define. We say that a vector $\mathbf{w} = (w_0, \dots, w_k)$ *majorizes* a vector $\mathbf{w}' = (w_0', \dots, w_k')$ if

$$\sum_{j=0}^{i} w_{k-j} \geq \sum_{j=0}^{i} w_{k-j}', \qquad 0 \leq i \leq k,$$

while $\mathbf{w}$ *minorizes* $\mathbf{w}'$ if

$$\sum_{j=0}^{i} w_{k-j} \le \sum_{j=0}^{i} w'_{k-j}, \qquad 0 \le i \le k.$$

The *majorant vector*

$$\mathbf{w}^+(k) := (w_0^+(k), w_1^+(k), \ldots, w_k^+(k))$$

is the smallest vector majorizing all the $\mathbf{w}_k^*(a)$ and is determined by the conditions

$$\text{(2.9)} \quad \sum_{j=0}^{i} w_{k-j}^+(k) = \max\left\{\sum_{j=0}^{i} w_{k-j}^k(a) \colon a \pmod{3^{k+1}} \text{ with } a \not\equiv 0 \pmod 3\right\}, \quad 0 \le i \le k.$$

Similarly, the *minorant vector*

$$\mathbf{w}^-(k) := (w_0^-(k), w_1^-(k), \ldots, w_k^-(k))$$

is determined by the conditions

(2.10)
$$\sum_{j=0}^{i} w_{k-j}^-(a) = \min\left\{\sum_{j=0}^{i} w_{k-j}^k(a) \colon a \pmod{3^{k+1}} \text{ with } a \not\equiv 0 \pmod 3\right\}, \quad 0 \le i \le k.$$

It is easy to see that these definitions imply that

$$\text{(2.11a)} \qquad N^+(k) = \sum_{j=0}^{k} w_j^+(k),$$

$$\text{(2.11b)} \qquad N^-(k) = \sum_{j=0}^{k} w_j^-(k).$$

In view of (2.8), we have

$$\text{(2.12)} \qquad N^-(k) \le \left(\frac{4}{3}\right)^k \le N^+(k), \qquad k \ge 1.$$

We computed the vectors $\mathbf{w}^+(k)$ and $\mathbf{w}^-(k)$ for $1 \le k \le 30$; the data for $w^-(k)$ and $N^-(k)$ appear in Table 2.1 (next page), and that for $\mathbf{w}^+(k)$ and $N^+(k)$ in Table 2.2 (see p. 417). Details on the computational method are given at the end of the section.

The associated growth rates are

$$\text{(2.13)} \qquad g^-(k) = N^-(k)^{1/k}; \qquad g^+(k) = N^+(k)^{1/k}.$$

They are tabulated for $1 \le k \le 30$ in Tables 2.1 and 2.2.

TABLE 2.1. Lower bounds for growth rates

k	$N^-(k)$	$g^-(k)$	minorizing vector $\mathbf{w}^-(k)$
1	1	1.000000	1 0
2	1	1.000000	1 0 0
3	1	1.000000	1 0 0 0
4	2	1.189207	1 1 0 0 0
5	2	1.148698	1 1 0 0 0 0
6	3	1.200937	1 2 0 0 0 0 0
7	4	1.219014	1 2 1 0 0 0 0 0
8	5	1.222845	1 2 2 0 0 0 0 0 0
9	6	1.220285	1 2 3 0 0 0 0 0 0 0
10	9	1.245731	1 3 3 2 0 0 0 0 0 0 0
11	11	1.243575	1 3 4 3 0 0 0 0 0 0 0 0
12	16	1.259921	1 4 5 5 1 0 0 0 0 0 0 0 0
13	20	1.259155	1 4 6 6 3 0 0 0 0 0 0 0 0 0
14	27	1.265436	1 4 8 8 5 1 0 0 0 0 0 0 0 0 0
15	36	1.269853	1 4 10 10 8 3 0 0 0 0 0 0 0 0 0 ...
16	48	1.273731	1 5 11 13 11 7 0 0 0 0 0 0 0 0 0 ...
17	64	1.277162	1 5 12 18 17 8 3 0 0 0 0 0 0 0 0 ...
18	87	1.281596	1 6 14 23 20 16 7 0 0 0 0 0 0 0 0 ...
19	114	1.283093	1 6 16 27 28 23 11 2 0 0 0 0 0 0 0 ...
20	154	1.286400	1 6 18 32 39 29 21 8 0 0 0 0 0 0 0 ...
21	206	1.288796	1 6 20 38 49 45 31 13 3 0 0 0 0 0 0 ...
22	274	1.290645	1 7 22 45 61 61 43 26 8 0 0 0 0 0 0 ...
23	363	1.292112	1 7 24 52 77 81 62 40 17 2 0 0 0 0 0 ...
24	484	1.293804	1 8 26 60 92 106 91 62 29 9 0 0 0 0 0 ...
25	649	1.295656	1 8 29 69 115 135 127 92 54 17 2 0 0 0 0 ...
26	868	1.297239	1 8 32 79 139 175 171 134 83 38 8 0 0 0 0 ...
27	1159	1.298627	1 8 35 89 164 223 232 189 131 63 22 2 0 0 ...
28	1549	1.299961	1 9 38 100 193 276 307 269 194 108 45 9 0 0 ...
29	2052	1.300807	1 9 40 113 227 339 401 366 275 171 83 25 2 0 ...
30	2747	1.302053	1 10 43 127 265 418 510 506 402 266 134 56 9 0 ...

Theorem 2.1. *For any* $k \geq 1$, *and any* $a \not\equiv 0 \pmod 3$,

$$g^-(k) \leq \liminf_{j\to\infty} N_j^*(a)^{1/j} \leq \limsup_{j\to\infty} N_j^*(a)^{1/j} \leq g^+(k). \tag{2.14}$$

In addition,

$$g^-(k) \leq \liminf_{j\to\infty} n_j^*(a)^{1/j} \leq \limsup_{j\to\infty} n_j(a)^{1/j} \leq g^+(k). \tag{2.15}$$

Proof. Since each tree of depth jk splits into trees of depth k attached to each leaf of the tree of depth $j(k-1)$, we get by an easy induction

$$N^-(k)^j \leq N_{jk}^*(a) \leq N^+(k)^j.$$

For $0 \leq l \leq k$, we obviously have

$$N^-(k)^j \leq N_{jk+l}^*(a) \leq N^+(k)^{j+1}.$$

Taking jkth roots and letting $j \to \infty$ yields (2.14).

TABLE 2.2. Upper bounds for growth rates

k	$N^+(k)$	$g^+(k)$	majorizing vector $\mathbf{w}^+(k)$
1	2	2.000000	1 1
2	3	1.732051	1 1 1
3	4	1.587401	1 1 1 1
4	6	1.565085	1 2 1 1 1
5	8	1.515717	1 2 2 1 1 1
6	10	1.467799	1 2 2 2 1 1 1
7	14	1.457916	1 3 3 2 2 1 1 1
8	18	1.435189	1 3 4 3 2 2 1 1 1
9	24	1.423498	1 3 5 5 3 2 2 1 1 1
10	32	1.414214	1 4 6 6 5 3 2 2 1 1 1
11	42	1.404650	1 4 7 9 6 5 3 2 2 1 1 1
12	55	1.396466	1 4 8 11 10 6 5 3 2 2 1 1 1
13	74	1.392474	1 5 10 14 13 10 6 5 3 2 2 1 1 1
14	100	1.389495	1 5 12 17 20 14 10 6 5 3 2 2 1 1 1
15	134	1.386140	1 5 13 21 26 23 14 10 6 5 3 2 2 1 1 1
16	178	1.382456	1 5 15 26 30 32 24 14 10 6 5 3 2 2 1 1 1
17	237	1.379403	1 6 16 31 38 41 35 24 14 10 6 5 3 2 2 1 1 1
18	311	1.375583	1 6 18 36 49 50 47 35 24 14 10 6 5 3 2 2 1 1 1
19	413	1.373035	1 7 20 42 63 65 62 49 35 24 14 10 6 5 3 2 2 1 1 1
20	548	1.370689	1 7 24 50 76 88 82 67 49 35 24 14 10 6 5 3 2 2 1 1 1
21	736	1.369361	1 8 27 58 92 118 114 96 68 50 35 24 14 10 6 5 3 2 2 1 1
22	988	1.368124	1 8 30 69 112 149 153 137 106 69 50 35 24 14 10 6 5 3 2 2 1 1 1
23	1314	1.366442	1 8 30 75 133 185 209 188 152 110 69 50 35 24 14 10 6 5 3 2 2 1 1 1
24	1744	1.364786	1 8 32 84 158 229 269 257 208 164 111 69 50 35 24 14 10 6 5 3 2 2 1 1 1
25	2309	1.363129	1 9 35 94 186 277 339 347 291 229 167 111 69 50 35 24 14 10 6 5 3 2 2 1 1 1
26	3084	1.362061	1 9 40 113 223 341 431 457 410 320 236 169 110 70 50 35 24 14 10 6 5 3 2 2 1 1 1
27	4130	1.361207	1 10 43 126 267 418 551 601 571 455 337 242 173 111 70 50 35 24 14 10 6 5 3 2 2 1 1 1
28	5500	1.360142	1 10 47 141 293 499 695 793 779 654 484 348 247 174 111 70 50 35 24 14 10 6 5 3 2 2 1 1 1
29	7336	1.359226	1 10 50 158 341 595 856 1026 1044 926 712 506 352 250 174 111 70 50 35 24 14 10 6 5 3 2 2 1 1 1
30	9788	1.358386	1 10 53 174 408 708 1053 1310 1382 1279 1025 749 517 359 251 174 111 70 50 35 24 14 10 6 5 3 2 2 1 1 1

To prove the upper bound in (2.15), use

$$n_j(a) \leq j n_j^*(a) \leq j N_j^*(a),$$

and (2.14). The lower bound in (2.15) is immediate if a is not in a cycle of T, since $n_j^*(a) = N_j^*(a)$ in this case. If a is in a cycle, then the tree $\mathcal{T}^*(a)$ contains some a' not in a cycle, say at level l. In that case

$$n_j^*(a) \geq n_{j-l}^*(a') = N_{j-l}^*(a'),$$

and the lower bound (2.15) follows from the lower bound (2.14) for $N_{j-l}^*(a')$. $\square$

Theorem 1.1 follows immediately from this result, using the $k = 30$ entries of Tables 2.1 and 2.2.

How fast do $N^+(k)$ and $N^-(k)$ grow? In order for Conjecture B to be derivable from Theorem 2.1, it is necessary that

$$\lim_{k\to\infty} g^+(k) = \lim_{k\to\infty} g^-(k) = \frac{4}{3}.$$

We restate this as the following conjecture.

Conjecture C. *Both* $N^+(k)$ *and* $N^-(k)$ *are* $(\frac{4}{3})^{k(1+o(1))}$ *as* $k \to \infty$.

This conjecture is stronger than Conjecture B, because it bounds extreme values over all trees of depth k, while Conjecture B applies to the quantities $n_k(a)$, which as $k \to \infty$ should behave like "random" trees. To compare the data with this conjecture, we give in Table 2.3 the quantities $(\frac{4}{3})^k$ and the ratios $(\frac{4}{3})^k(N^-(k))^{-1}$ and $(\frac{4}{3})^{-k}N^+(k)$. Formula (2.8) implies that these ratios must both be at least 1, for all $k \geq 1$.

TABLE 2.3. Normalized extreme values

k	$\left(\frac{4}{3}\right)^k$	$\left(\frac{4}{3}\right)^k (N^-(k))^{-1}$	$N^+(k)\left(\frac{4}{3}\right)^{-k}$
1	1.333333	1.333333	1.500000
2	1.777778	1.777778	1.687500
3	2.370370	2.370370	1.687500
4	3.160494	1.580247	1.898438
5	4.213992	2.106996	1.898438
6	5.618656	1.872885	1.779785
7	7.491541	1.872885	1.868774
8	9.988721	1.997744	1.802032
9	13.318295	2.219716	1.802032
10	17.757727	1.973081	1.802032
11	23.676969	2.152452	1.773876
12	31.569292	1.973081	1.742199
13	42.092389	2.104619	1.758038
14	56.123185	2.078636	1.781795
15	74.830914	2.078636	1.790704
16	99.774552	2.078636	1.784022
17	133.032736	2.078636	1.781516
18	177.376981	2.038816	1.753328
19	236.502641	2.074585	1.746281
20	315.336855	2.047642	1.737824
21	420.449140	2.041015	1.750509
22	560.598854	2.045981	1.762401
23	747.465138	2.059133	1.757942
24	996.620184	2.059133	1.749914
25	1328.826912	2.047499	1.737623
26	1771.769217	2.041209	1.740633
27	2362.358955	2.038273	1.748253
28	3149.811941	2.033449	1.746136
29	4199.749254	2.046614	1.746771
30	5599.665672	2.038466	1.747961

The data support Conjecture C, and even suggest the following stronger conjecture.

Conjecture C′. *There are positive constants C^+ and C^- such that*

$$C^-\left(\frac{4}{3}\right)^k \leq N^-(k) < N^+(k) \leq C^+\left(\frac{4}{3}\right)^k$$

for all sufficiently large k.

Lagarias and Weiss [7] developed branching process models intended to mimic the behavior of $3x+1$ trees. For the branching process models $\mathscr{B}[3^j]$ with $j \geq 2$ of [7] we prove elsewhere [2] that the analogue of Conjecture C is true, but the analogue of the stronger Conjecture C′ is false. That is, $3x+1$ trees empirically have a narrower variation of leaf counts than that predicted by such stochastic models. This deviation merits an explanation, and we raise this as an open question.

The computation of Tables 2.1 and 2.2 was done as follows. For a given $a \pmod{3^{k+1}}$ with $a \not\equiv 0 \pmod 3$, let $mw_k(a)$ denote the maximum weight of a leaf of the tree $\mathscr{T}_k^*(a)$. Then all trees $\mathscr{T}_k^*(a')$ with $a' \equiv a \pmod{3^{mw_k(a)+1}}$ have identical branching structure and node weights. In doing the computation we group all these trees together, specifying them by a single congruence class $a \pmod{3^{l+1}}$ where $l = mw_k(a)$, which we call a *clone*. Let R_l^k count the number of distinct clones of depth k having a maximum weight leaf of weight l. The values of R_l^k up to $k = 23$ are given in Table 2.4 (next page).

The quantities R_l^k satisfy the identity

$$\sum_{l=0}^{k} R_l^k 3^{k-l} = 2\cdot 3^k. \tag{2.16}$$

Let $R(k)$ count the total number of clones of depth k,

$$R(k) := \sum_{l=0}^{k} R_l^k. \tag{2.17}$$

Then $R(k)$ counts all possible tree structures of depth k that occur using the $3x+1$ function. Data on $R(k)$ and on $R(k)^{1/k}$ also appear in Table 2.4. By means of

$$w_i^k(a) = \begin{cases} w_i^{k-1}(2a) & \text{if } a \equiv 1, 4, 5, \text{ or } 7 \pmod 9, \\ w_i^{k-1}(2a) + w_{i-1}^{k-1}\left(\frac{2a-1}{3}\right) & \text{if } a \equiv 2, 8 \pmod 9, \end{cases}$$

for $0 \leq i \leq k$, and

$$mw_k(a) = \begin{cases} mw_{k-1}(2a) \quad \text{if } a \equiv 1, 4, 5, \text{ or } 7 \pmod 9, \\ \max\left\{mw_{k-1}(2a), mw_{k-1}\left(\frac{2a-1}{3}\right) + 1\right\} \quad \text{if } a \equiv 2 \text{ or } 8 \pmod 9, \end{cases}$$

all clones of depth k can be identified. In addition, $\mathbf{w}_k^*(\cdot)$ and $mw_k(\cdot)$ are computed in $O(kR(k))$ operations from a hash table containing $\mathbf{w}_{k-1}^*(\cdot)$ and

TABLE 2.4. R_l^k-values

k	$\sum_{l=0}^{k} R_l^k$	$\left(\sum_{l=0}^{k} R_l^k\right)^{\frac{1}{k}}$	R_l^k
1	4	4.000000	1 3
2	8	2.828427	0 5 3
3	14	2.410142	0 3 8 3
4	24	2.213364	0 2 8 11 3
5	42	2.111786	0 1 8 16 14 3
6	76	2.058112	0 0 7 22 27 17 3
7	138	2.021608	0 0 3 24 47 41 20 3
8	254	1.998040	0 0 1 17 66 86 58 23 3
9	470	1.981070	0 0 0 10 64 147 142 78 26 3
10	876	1.969021	0 0 0 3 49 189 284 218 101 29 3
11	1638	1.959794	0 0 0 0 28 183 451 497 317 127 32 3
12	3070	1.952517	0 0 0 0 9 135 555 926 809 442 156 35 3
13	5766	1.946696	0 0 0 0 1 74 520 1387 1713 1246 596 188 38 3
14	10850	1.941981	0 0 0 0 0 24 375 1628 3000 2937 1837 782 223 41 3
15	20436	1.938026	0 0 0 0 0 3 199 1471 4255 5831 4752 2614 1003 261 44 3
16	38550	1.934757	0 0 0 0 0 0 66 1019 4767 9654 10474 7344 3612 1262 302 47 3
17	72806	1.932012	0 0 0 0 0 0 9 525 4131 13012 19662 17703 10934 4869 1562 346 50 3
18	137670	1.929706	0 0 0 0 0 0 0 169 2759 13891 30899 36874 28516 15781 6426 1906 393 53 3
19	260612	1.927757	0 0 0 0 0 0 0 22 1364 11519 39599 65747 64880 44170 22185 8327 2297 443 56 3
20	493824	1.926099	0 0 0 0 0 0 0 0 415 7389 40195 98262 128421 108515 66222 30490 10619 2738 496 59 3
21	936690	1.924694	0 0 0 0 0 0 0 0 48 3484 31803 119644 218068 234608 174174 96573 41087 13352 3232 552 62 3
22	1778360	1.923498	0 0 0 0 0 0 0 0 0 968 19569 115251 310107 442990 406347 270156 137515 54417 16579 3782 611 65 3
23	3379372	1.922483	0 0 0 0 0 0 0 0 0 90 8687 86967 358136 717450 838789 673955 407052 191781 70974 20356 4391 673 68 3

$mw_k(\cdot)$ for all clones of depth $k-1$. In the actual computation, memory was exhausted by the hash table at $k = 21$, so $\mathbf{w}_l^*(\cdot)$ and $mw_l(\cdot)$ for clones of depth $l \geq 21$ were recomputed as needed.

The quantity $R(k)$ grows at a somewhat slower exponential growth rate than $2 \cdot 3^k$, which makes the computation feasible up to $k = 30$. By analogy with a branching process model in Lagarias and Weiss [7] one expects that there is a constant θ such that $R(k) = \theta^{k(1+o(1))}$ as $k \to \infty$, and empirically we estimate $1.87 < \theta < 1.92$. Here, the lower bound 1.87 comes from $R(k)^{1/(k+1)}$, which is monotonically increasing for $8 \leq k \leq 28$. Observe also that $R_l^k = 0$ for small values of l, which occurs because branching of the tree is unavoidable. By analogy with branching process models, one expects that there exists a positive constant ϕ such that $R_l^k = 0$ for $l < (\phi + o(1))k$ and $R_l^k > 0$ for $(\phi + o(1))k \leq l \leq k$, as $k \to \infty$.

3. Large deviation estimates: lower bounds and upper bounds

We use minorant vectors to get lower bounds for γ in (1.3), as follows. For any constant $\alpha \in (0, 1]$, set

$$N_j^*(a; \alpha) := \#\{l : l \text{ is a leaf in } \mathcal{T}_j^*(a) \text{ with weight}(l) \geq \alpha j\}.$$

By (2.4) all such leaves satisfy the bound

$$l \leq \exp(j(\log 2 - \alpha \log 3))a. \tag{3.1}$$

If we set $x = \exp(j(\log 2 - \alpha \log 3))a$, and let $j \to \infty$, then we obtain for any $\varepsilon > 0$ that

$$\pi_a(x) \geq x^{\gamma - \varepsilon}, \quad \text{all } x \geq x_0(\varepsilon),$$

where

$$\gamma = \frac{1}{\log 2 - \alpha \log 3} \liminf_{j \to \infty} \frac{1}{j}(\log N_j^*(a; \alpha)). \tag{3.2}$$

We next use the minorant vector $\mathbf{w}^-(k)$ to obtain an asymptotic lower bound for $N_j^*(a; \alpha)$. Form a *minorizing tree* $\mathcal{T}_k^-$ consisting of $N^-(k)$ leaves of depth one, with exactly $w_i^-(k)$ of these leaves having edges assigned the weight i, for $0 \leq i \leq k$. Now, for all $j \geq 1$, recursively construct the *concatenated minorizing tree*[1] $\mathcal{T}_k^-(j)$ by setting $\mathcal{T}_k^-(1) = \mathcal{T}_k^-$ with root node labelled 1 and then forming $\mathcal{T}_k^-(j)$ from $\mathcal{T}_k^-(j-1)$ by attaching copies of the tree $\mathcal{T}_k^-$ to each leaf of $\mathcal{T}_k^-(j-1)$. Each leaf of $\mathcal{T}_k^-(j)$ is assigned a weight consisting of the sum of edge weights from it to the root node. Let

$$\mathbf{w}^-(k)^{(*j)} := (x_0^k(j), \ldots, x_{jk}^k(j)) \tag{3.3}$$

be a vector counting the number of leaves of $\mathcal{T}_k^-(j)$ of weight i, for $0 \leq i \leq jk$. (The notation $\mathbf{w}^-(k)^{(*j)}$ is intended to indicate repeated convolution of $\mathbf{w}^-(k)$, as explained below.) Note also that the number of leaves of $\mathcal{T}_k^-(j)$ is $N^-(k)^j$. We claim that

$$\mathbf{w}^-(k)^{(*j)} \textit{ minorizes } \mathbf{w}^-(jk). \tag{3.4}$$

To prove the claim, it suffices to show that $\mathbf{w}^-(k)^{(*j)}$ minorizes each $\mathbf{w}_{jk}^*(a)$. We proceed by induction on j, it being obviously true for $j = 1$. Take any tree $\mathcal{T}_{jk}(a)$ and view it as a tree $\mathcal{T}_{(j-1)k}(a)$ with various trees $\mathcal{T}_k(b)$ attached to its leaves. By the induction hypothesis (3.4), the tree $\mathcal{T}_k^-(j-1)$ can have its leaves paired with those of $\mathcal{T}_{(j-1)k}(a)$ in such a way that each leaf of $\mathcal{T}_k^-(j-1)$ has a weight no larger than the corresponding leaf of $\mathcal{T}_{(j-1)k}(a)$, and $\mathcal{T}_{(j-1)k}(a)$ may have some unpaired leaves left over. Then replace $\mathcal{T}_{(j-1)k}(a)$ with $\mathcal{T}_k^-(j-1)$, and throw away all trees $\mathcal{T}_k(b)$ attached to the unpaired nodes; the weight vector of the resulting new tree minorizes that of the old tree $\mathcal{T}_{jk}(a)$. Next, in the resulting tree, replace each tree $\mathcal{T}_k(b)$ with the tree $\mathcal{T}_k^-$, and the weight vector of the resulting tree minorizes the one before. This final tree is $\mathcal{T}_k^-(j)$, hence we have shown that $\mathbf{w}^-(k)^{(*j)}$ minorizes $\mathbf{w}_{jk}^*(a)$, and the induction step follows.

[1]The tree $\mathcal{T}_k^-(j)$ has depth j, but we will show that its leaf counts minorize those of any $3x + 1$ tree of depth jk, see (3.4).

Now (3.4) yields the lower bound

$$N^*_{jk}(a\,;\,\alpha) \ge P^-_{j,k}(\alpha) := \sum_{i>jk\alpha} x^k_i(j). \tag{3.5}$$

The right side of (3.5) depends only on $\mathbf{w}^-(k)$ and can be estimated in a standard fashion (see Lemma 3.1 below). We can then interpolate estimates for $N^*_{jk+l}(a\,;\,\alpha)$ using

$$N^*_{jk+l}(a\,;\,\alpha) \ge N^*_{(j+1)k}\left(a\,;\,\alpha + \frac{1}{jk}\right), \qquad 0 \le l \le k.$$

We estimate the right side of (3.5) using a "large deviations" bound in probability theory. To do this, we assign a *value* to each node of the tree $\mathscr{T}_k^-$. Each leaf of weight i has value $l = 2^k 3^{-i}$. (These values actually approximate the ratio of a leaf label to the root label.) We can use this scheme to recursively assign values to all the nodes of the trees $\mathscr{T}_k^-(j)$, starting by assigning the root node the value 1. Next, let Z_k^- be a random variable which draws a leaf l of $\mathscr{T}_k^-(1)$ uniformly, and has

$$Z_k^- := \log l = k\log 2 - i\log 3. \tag{3.6}$$

The convolved random variable $(Z_k^-)^{(*j)}$ then equals $\log l$, where l is the value of a leaf of $\mathscr{T}_k^-(j)$ drawn uniformly. Now, the right side of (3.5) counts exactly those leaves of $\mathscr{T}_k^-(j)$ with $l = 2^{jk}3^{-i} \le 2^{jk}3^{-jk\alpha}$; hence

$$P^-_{j,k}(\alpha) = (N^-(k))^j \mathrm{Prob}[(Z_k^-)^{(*j)} < jk(\log 2 - \alpha\log 3)]. \tag{3.7}$$

The estimation of (3.7) is a standard "large deviations" result.

Lemma 3.1. *The random variable* $Z = Z_k^-$ *has moment generating function*

$$M_k^-(\theta) = E[e^{\theta Z}] = \sum_{i=0}^k \frac{w_i^-(k)}{N^-(k)} 2^{k\theta} 3^{-i\theta},$$

whose Legendre transform is

$$g_k^-(\beta) := \sup_{\theta\in\mathbb{R}} [\beta\theta - \log M_k^-(\theta)].$$

If $0 < \log 2 - \alpha\log 3 < \frac{1}{k}E[Z_k^-]$, *then*

$$\lim_{j\to\infty} \frac{1}{jk}(\log P^-_{j,k}(\alpha)) = \frac{1}{k}(\log N^-(k) - g_k^-(k(\log 2 - \alpha\log 3))). \tag{3.8}$$

Proof. This is just an application of Chernoff's theorem (see [7, Lemma 2.1]. □

Combining (3.2), (3.5), (3.7), and (3.8) yields the bound

$$\gamma \ge \frac{\log N^-(k) - g_k^-(k(\log 2 - \alpha\log 3))}{k(\log 2 - \alpha\log 3)}, \tag{3.9}$$

provided

$$0 < \log 2 - \alpha\log 3 < \frac{1}{k}E[Z_k^-] = \frac{1}{k}\sum_{i=0}^k \frac{iw_i^-(k)}{N^-(k)}.$$

For each value of k it remains to optimize the bound (3.9) by choosing the optimal $\alpha = \alpha_k^*$.

Data on the expected value $\frac{1}{k}E[Z_k^-]$, the optimal cutoff value α_k^*, and the resulting lower bound γ_k^* are given in Table 3.1. The quantity $\frac{1}{k}E[Z_k^-]$ is always greater than the expected growth rate of labels on a random branch of a "random" tree $\mathcal{T}_k(a)$, which is $\log 2 - \frac{1}{4}\log 3 \doteq .418494$ (cf. [7, Theorem 3.3]). The data shows that $\frac{1}{k}E[Z_k^-]$ is not a monotonically decreasing function of k. Consequently, the estimates γ_k^* are also not monotonically increasing, but tend to increase. The largest value we found was $\gamma_{30}^* = .654717$; this proves Theorem 1.2. It is natural to conjecture that $\frac{1}{k}E[Z_k^-] \to \log 2 - \frac{1}{4}\log 3$ and that $\gamma_k^* \to 1$ as $k \to \infty$.

We similarly use majorant vectors $\mathbf{w}^+(k)$ to get upper bounds on $N_j^*(a;\alpha)$.

TABLE 3.1. Lower bound exponent γ_k^* and exceptional set exponent χ_k^* for upper bound

	Lower Bounds			Upper Bounds	
k	$\frac{1}{k}E[Z_k^-]$	α_k^*	γ_k^*	$\frac{1}{k}E[Z_k^+]$	χ_k^*
1	0.693147	0.000000	0.000000	0.143841	0.693147
2	0.693147	0.000000	0.000000	0.143841	0.549306
3	0.693147	0.000000	0.000000	0.143841	0.462098
4	0.555821	0.146657	0.318622	0.189617	0.446038
5	0.583286	0.113143	0.240657	0.198772	0.413368
6	0.571079	0.123454	0.324572	0.198772	0.381467
7	0.536203	0.172320	0.380922	0.233524	0.371315
8	0.528355	0.177998	0.392520	0.243021	0.354660
9	0.530390	0.171384	0.385017	0.255737	0.344757
10	0.510045	0.208448	0.451594	0.274301	0.335695
11	0.511558	0.200535	0.443546	0.284140	0.327324
12	0.504323	0.215607	0.481701	0.291987	0.320073
13	0.498777	0.222555	0.487401	0.307148	0.314558
14	0.492607	0.233806	0.507598	0.316480	0.310239
15	0.487666	0.239897	0.521993	0.322570	0.306111
16	0.485727	0.241974	0.531764	0.327843	0.302016
17	0.482109	0.250439	0.544585	0.332942	0.298374
18	0.479177	0.254813	0.558130	0.336952	0.294522
19	0.477077	0.258955	0.564602	0.342297	0.291267
20	0.471641	0.268750	0.581699	0.347626	0.288169
21	0.469158	0.274193	0.591224	0.352461	0.285683
22	0.467338	0.277591	0.599240	0.356174	0.283427
23	0.465503	0.281793	0.606344	0.357878	0.281210
24	0.463229	0.286125	0.614848	0.360225	0.279030
25	0.461643	0.288560	0.621639	0.362450	0.276928
26	0.459970	0.292749	0.629568	0.365854	0.275026
27	0.458350	0.296715	0.636608	0.368401	0.273360
28	0.456692	0.299908	0.643504	0.369927	0.271726
29	0.455602	0.303753	0.649338	0.371744	0.270171
30	0.454481	0.305943	0.654717	0.373635	0.268692

We construct trees $\mathcal{T}_k^+$ and $\mathcal{T}_k^+(j)$ analogously to the lower bound case, using $\mathbf{w}^+(k)$ instead of $\mathbf{w}^-(k)$. The vector

$$\mathbf{w}^+(k)^{(*j)} := (y_0^k(j), \dots, y_{jk}^k(j))$$

enumerates the number of leaves in the tree $\mathcal{T}_k^+(j)$ of different weights. We then show, analogously to the lower bound case, that

$$\mathbf{w}^+(k)^{(*j)} \textit{ majorizes } \mathbf{w}^+(jk), \tag{3.10}$$

from which we conclude

$$N_{jk}^*(a;\alpha) \le P_{j,k}^+(\alpha) := \sum_{i>jk\alpha} y_i^k(j). \tag{3.11}$$

The right side of (3.11) is estimated by a Chernoff inequality argument. Let Z_k^+ be a random variable which draws a leaf l from $\mathcal{T}_k^+(1)$ uniformly and assigns the value $\log(l)$, similarly to (3.6). The convolution $(Z_k^+)^{(*j)}$ then describes the value $\log(l)$ for a random leaf of $\mathcal{T}_k^+(j)$, and we have

$$P_{j,k}^+(\alpha) = (N^+(k))^j \text{Prob}[(Z_k^+)^{(*j)} < jk(\log 2 - \alpha \log 3)].$$

The Chernoff bound formula is analogous to Lemma 3.1.

Lemma 3.2. *The random variable* $Z = Z_k^+$ *has moment generating function*

$$M_k^+(\theta) = \sum_{i=0}^{k} \frac{w_i^+(k)}{N^+(k)} 2^{k\theta} 3^{-i\theta},$$

whose Legendre transform is

$$g_k^+(\beta) := \sup_{\theta\in\mathbb{R}} [\beta\theta - \log M_k^+(\theta)].$$

If $\log 2 - \alpha \log 3 > \frac{1}{k} E[Z_k^+]$, *then*

$$\lim_{j\to\infty} \frac{1}{jk} (\log P_{j,k}^+(\alpha)) = \frac{1}{k} (\log N^+(k) - g_k^+(k(\log 2 - \alpha \log 3))). \tag{3.12}$$

Table 3.1 presents data on $\frac{1}{k}E[Z_k^+]$. It is always less than the expected growth rate $\log 2 - \frac{1}{4}\log 3 \doteq .418494$ of labels on a random branch of a "random" tree $\mathcal{T}_k(a)$. Empirically, it appears to be a monotone function of k, unlike the lower bound case. It is natural to conjecture that $\frac{1}{k}E[Z_k^+] \to \log 2 - \frac{1}{4}\log 3$ as $k \to \infty$.

Upper bound estimates for $N_j^*(a;\alpha)$ are also relevant to proving results saying that "almost all" integers decrease under iteration by T. Currently the best quantitative result of this kind is that of Korec [4].

Theorem 3.1 (Korec). *For any* $\beta > \beta_c := \frac{\log 3}{\log 4} \doteq .7925$ *the set*

$$S(\beta) := \{n \colon \textit{some } |T^{(k)}(n)| < |n|^\beta\}$$

has density one.

Korec's method actually shows that almost all $\{n \colon |n| \le x\}$ satisfy

$$|T^{(k)}(n)| \le x^\beta, \quad \text{for } k = \left[\frac{\log x}{\log 2}\right], \tag{3.13}$$

as $x \to \infty$, for any fixed $\beta > \beta_c$.

We show below that one can get improved bounds for β_c in Theorem 3.1 provided that the quantity

$$\chi_k^* := \frac{1}{k}(\log N^+(k) - g_k^+(k(\log 2 - 1/2(\log 3)))) \tag{3.14}$$

is sufficiently small. This quantity is the upper bound (3.12) with $\alpha = 1/2$, and its values are given in Table 3.1.

Consider the set of "bad elements"

$$R_\delta(x) := \left\{ n\colon |n| < x \text{ and no } T^{(j)}(x) < x^{1-\delta} \text{ for } 1 \le j < \left[\frac{\log x}{\log 2}\right]\right\}.$$

The cardinality of $R_\delta(x)$ decreases as $\delta \to 0$ and

$$\lim_{\delta\to 0} \frac{\log \#(R_\delta(x))}{\log x} = H\left(\frac{\log 2}{\log 3}\right) \doteq .94995, \tag{3.15}$$

where $H(t) = -t\log_2 t - (1-t)\log_2(1-t)$ is the binary entropy function (cf. [6, Theorem D]). Almost all $\{n\colon |n| \le x\}$ satisfy (3.13). We can get an improvement if almost all such $T^{(k)}(n)$ with $k = \left[\frac{\log x}{\log 2}\right]$ do not lie in a "bad element" set $R_\delta(x^\beta)$, for some fixed $\delta > 0$. How many such n can hit a particular "bad" element y? They must lie in the tree of preimages of y, at height $j = \frac{\log x}{\log 2}$, so we need an upper bound for the number of leaves l in such a tree, at this height, having $y \approx x^\beta$ and $l \le x$. Such leaves correspond to paths having $\alpha \ge \frac{1}{2}$ as explained in [7, §2], and we can apply[2] the upper bounds (3.11)–(3.13) to bound the number of such leaves by $\exp(\chi_k \frac{\log x}{\log 2})$. Now the number of such "bad elements" as $\beta \to \beta_c$ and $\delta \to 0$ satisfies

$$\log \#(R_\delta(x^\beta)) = \left(.94995\frac{\log 3}{\log 4} + o(1)\right)\log x;$$

hence the number of preimages $n \le x$ which these generate is at most

$$\exp\left(\left(.94995\frac{\log 3}{\log 4} + \frac{\chi_k}{\log 2}\right)\log x\right).$$

This bound will be $O(x^{1-\varepsilon'})$ for some $\varepsilon' > 0$, if and only if

$$\chi_k < \log 2 - \frac{1}{2}H\left(\frac{\log 2}{\log 3}\right)\log 3 \doteq .171331. \tag{3.16}$$

As the data of Table 3.1 show, however, for $k \le 30$ we are a long way from attaining the bound (3.16).

The assumption that $3x+1$ trees behave like the branching process models of [7] leads to the heuristic prediction that $\chi_k \to 0$ as $k \to \infty$. If so, this approach to lowering β_c should eventually work, for k large enough. The data of Table 3.1 indicate that the smallest k for which (3.16) holds will be so large that it will be impossible to compute by an exhaustive tree search.

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[2]To get a rigorous bound, one must also count a few extra leaves having $\alpha < \frac{1}{2}$, which creep in because T^{-1} has $\frac{2x-1}{3}$ instead of $\frac{2x}{3}$. However a rigorous variant of (2.5) can be used to show that these leaves make an asymptotically negligible contribution.

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