The Distribution of 3x+1 Trees

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CONTENTS

Backwards iteration of the $3x+1$ function starting from a fixed integer a produces a tree of preimages of a. Let $\mathcal{T}_k(a)$ denote this tree grown to depth k, and let $\mathcal{T}_k^*(a)$ denote the pruned tree resulting from the removal of all nodes $n \equiv 0 \bmod 3$. We previously computed the maximal and minimal number of leaves in $\mathcal{T}_k^*(a)$ for all $a \not\equiv 0 \bmod 3$ and all $k \leq 30$. Here we compare these data with predictions made using branching process models designed to imitate the growth of $3x+1$ trees, developed in [Lagarias and Weiss 1992]. We derive rigorous results for the branching process models. The range of variation exhibited by the $3x+1$ trees appears significantly narrower than that of the branching process models. We also study the variation in expected leaf-counts associated to the congruence class of $a \bmod 3^j$. This variation, when properly normalized, converges almost everywhere as $j \to \infty$ to a limit function on the invertible 3-adic integers.

1. INTRODUCTION

The well-known $3x+1$ problem concerns the behavior under iteration of the $3x+1$ function $T : \mathbb{Z} \mapsto \mathbb{Z}$ given by

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

The $3x+1$ Conjecture asserts that, for each $n \geq 1$, some iterate $T^{(k)}(n)$ equals 1; it has now been verified for all $n < 5.6 \times 10^{13}$ [Leavens and Vermeulen 1992]. For each n we call the minimal k such that $T^{(k)}(n) = 1$ the *total stopping time* of n and denote it $\sigma_\infty(n)$, letting $\sigma_\infty(n) = \infty$ if it is otherwise undefined.

The $3x+1$ function is a deterministic process that apparently exhibits pseudorandom behavior. It has been extensively studied; see the surveys [Lagarias 1985; Müller 1991]. One approach to quantify its apparent pseudorandomness is to consider

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probabilistic models for its behavior on a "random" input, and then to compare model predictions with empirical data. Any systematic discrepancies or similarities uncovered may prove helpful in eventually establishing rigorous results.

We now review several probabilistic models for the $3x+1$ iteration. Consider taking input values n drawn from the uniform distribution U_{2^k} on $[1, 2^k]$, and examine the induced probability distribution on $T^{(j)}(n)$, for $1 \le j \le [\alpha k]$, for a fixed positive α. One can rigorously prove that, when $0 < \alpha \le 1$, the successive iterates

$$\left(\log \frac{T(n)}{n}, \ldots, \log \frac{T^{[\alpha k]}(n)}{n}\right)$$

behave exactly like the trajectory of a random walk that takes i.i.d. (independent, identically distributed) steps of size $\log \frac{3}{2}$ or $\log \frac{1}{2}$ with equal probability [Lagarias 1985, § 2]. This suggests that the evolution of $3x+1$ function iterates can be modelled by a multiplicative random walk, in which from an initial point X_0 one multiplies by successive i.i.d. random variables X_i taking the values $\frac{3}{2}$ and $\frac{1}{2}$ with probability $\frac{1}{2}$ each, to obtain $Y_j := X_0 X_1 \ldots X_j$.

Such a model was first considered in [Crandall 1978], and in more detail in [Rawsthorne 1985; Wagon 1985]. The analogue in this model of the stopping time $\sigma_\infty(X_0)$ is the statistic $\sigma_\infty(X_0, \omega)$ that for a random walk ω starting from X_0 gives the smallest value of J such that $Y_J < 1$. For this model the expected value is

$$E[\sigma_\infty(X_0, \omega)] = (\tfrac{1}{2} \log \tfrac{4}{3})^{-1} \log X_0.$$

Recently Borovkov and Pfeifer [1993] gave a refined analysis showing that $\sigma_\infty(X_0, \omega)$ obeys a central limit theorem, that is, the scaled variables

$$\hat{\sigma}_\infty(X_0, \omega) := \frac{\sigma_\infty(X_0, \omega) - c_1 \log X_0}{c_2 (\log X_0)^{1/2}}, \tag{1.1}$$

in which $c_1 = (\frac{1}{2} \log \frac{4}{3})^{-1}$ and $c_2 = {c_1}^{3/2} (\frac{1}{2} \log 3)$, have distribution converging to the unit normal distribution $N(0, 1)$ as $X_0 \to \infty$. Although this model with n_0 drawn from U_{2^k} is rigorously proved to approximate the distribution of $T^{(\alpha k)}(n_0)$ only for $\alpha \le 1$, empirically it is found that the approximation seems good all the way up to $\alpha = (\frac{1}{2} \log \frac{4}{3})^{-1} \doteq 6.95212$. Furthermore the agreement with the central limit approximation (1.1) is also reasonably good. Thus this random walk model appears to accurately describe "average" trajectories of $3x+1$ iterates.

Lagarias and Weiss [1992] have introduced two types of probabilistic models intended to simulate "extreme" trajectories of $3x+1$ iterates, that is, those attaining the largest value of the quantity $\sigma_\infty(n)/\log n$ for all $n \in [1, 2^k]$. The first of these models is (the additive counterpart of) a repeated multiplicative random walk, which takes 2^k entirely independent multiplicative random walks as above, with the n-th such walk ω_n starting from $X_0 = n$. An analogous model statistic γ_k to consider is the maximum value of $\sigma_\infty(n, \omega_n)/\log n$ over $1 \le n \le 2^k$. For this model, the authors showed that with probability one the values γ_k tend to a limit γ_{RW} as $k \to \infty$; in symbols,

$$\limsup_{n\to\infty} \frac{\sigma_\infty(n, \omega_n)}{\log n} = \gamma_{\mathrm{RW}}$$

with probability one, where $\gamma_{\mathrm{RW}} \doteq 41.677647$ is the solution of a certain transcendental equation. This model has the deficiency that it assumes independence of trajectories for different starting values n_0 and n_1. This is not true of $3x+1$ trajectories: they must coalesce, since (empirically) all trajectories reach 1.

The second type of stochastic model of [Lagarias and Weiss 1992] is a branching process model that mimics backwards iteration of the $3x+1$ function, and that explicitly includes dependencies among trajectories. Backwards iteration of the $3x+1$ map is multiple-valued; given an initial value a, it produces a tree $\mathcal{T}(a)$ of preimages of a. The branching process models construct "random" trees whose structures imitate the structure of a $3x+1$ tree grown from a "random" starting point a. Lagarias and Weiss presented an infinite family $\mathcal{B}[3^j]$, for $j = 0, 1, 2, \ldots$, of increasingly refined branching process models, and proved that for these models an analogue of the asymptotically largest value of $\sigma_\infty(n)/\log n$ as $n \to \infty$ is almost surely a constant γ_{BP}, which coincides with the γ_{RW} of the preceding paragraph. Finally they observed that the existing empirical data for extremal trajectories of the $3x+1$ function, computed up to 5.6×10^{13} in [Leavens and Vermeulen 1992], is consistent with the predictions made by these two types of models.

This paper studies extremal properties of ensembles of $3x+1$ trees of depth k. A $3x+1$ tree $\mathcal{T}_k(a)$ is a rooted, labeled tree of depth k, representing the inverse iterates $T^{-j}(a)$ for $0 \le j \le k$. The inverse map $T^{-1}(n)$ is multivalued:

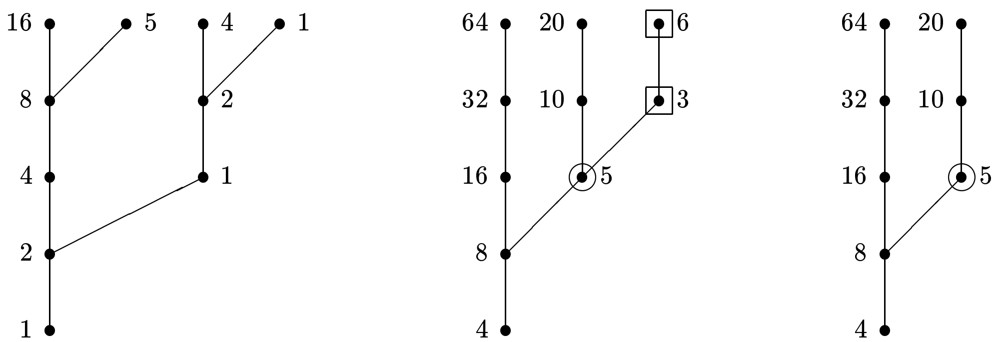
$$T^{-1}(n) = \begin{cases} \{2n\} & \text{if } n \equiv 0 \text{ or } 1 \bmod 3, \\ \{2n,\ \frac{1}{3}(2n-1)\} & \text{if } n \equiv 2 \bmod 3. \end{cases}$$

The root node a is at depth 0, and a node labeled n at level l of the tree is connected by an edge to a node labeled $T(n)$ at level $l-1$ of the tree. (We adopt a convention of "unrolling" any cycles under T, so that the same node label may appear at different levels of the tree if a cycle is present, as in Figure 1.) The formula above for $T^{-1}(n)$ reveals that the nodes labeled $n \equiv 0 \bmod 3$ give rise only to a linear chain of nodes labeled $n' \equiv 0 \bmod 3$ at higher levels. It is convenient to remove all such nodes and study a "pruned" tree $\mathcal{T}_k^*(a)$ consisting of nodes $n \not\equiv 0 \bmod 3$. Figure 1 presents some examples of $\mathcal{T}_k(a)$ and $\mathcal{T}_k^*(a)$.

We say that two pruned $3x+1$ trees $\mathcal{T}_k^*(a)$ and $\mathcal{T}_k^*(b)$ *have the same structure* if they are isomorphic as rooted trees by an isomorphism that preserves node labels modulo 2. Since the node label $n \bmod 2$ is determined by whether the lower-level node $T(n)$ that it comes from is $\frac{1}{2}n$ or $\frac{1}{2}(3n+1)$, the congruence classes $n \bmod 3$ and $T(n) \bmod 9$ suffice to determine $n \bmod 2$. From this, it easily follows that the structure of $\mathcal{T}_k^*(a)$ is completely determined by $a \bmod 3^{k+1}$. Consequently there are at most $2 \cdot 3^k$ distinct pruned tree structures $\mathcal{T}_k^*(a)$. The actual number $R(k)$ of distinct tree structures is smaller but still grows exponentially.

We study the extreme (maximum and minimum) leaf counts $N^+(k)$ and $N^-(k)$ for the ensemble of all such trees of depth k. In Section 2 we present empirical data for all $k \le 30$, which appeared in [Applegate and Lagarias 1995a]. These data suggest two conjectures concerning the asymptotic behavior of the extreme leaf counts as $k \to \infty$, which we call Conjecture C and the (stronger) Conjecture C$^\#$.

We next ask: How well do repeated trials of the branching process models of [Lagarias and Weiss 1992] reproduce these empirical $3x+1$ data? We note that only the models $\mathcal{B}[3^j]$ for $j \ge 2$ can be



(i) $\mathcal{T}_5(1)$ (ii) $\mathcal{T}_5(4)$ (iii) $\mathcal{T}_5^*(4)$

FIGURE 1. $3x+1$ trees $\mathcal{T}_k(a)$ and "pruned" $3x+1$ tree $\mathcal{T}_k^*(a)$. Nodes $n \equiv 5 \bmod 9$ are circled to indicate that they have a preimage $T^{-1}(n) \equiv 0 \bmod 3$, and nodes $n \equiv 0 \bmod 3$ are indicated with a square.

reasonable models. The models $\mathcal{B}[1]$ and $\mathcal{B}[3]$ were already shown in [Lagarias and Weiss 1992, § 6] to fail to assign the correct distribution of residue classes mod 3 to the node labels. Besides this, and more importantly, $\mathcal{B}[1]$ and $\mathcal{B}[3]$ do not possess the following "strict branching" property of pruned $3x+1$ trees: every pruned $3x+1$ tree branches after at most four steps from any node. $\mathcal{B}[1]$ and $\mathcal{B}[3]$ can produce trees having arbitrarily long chains of nodes with no branching.

As far as one can tell, all the branching process models $\mathcal{B}[3^j]$ for $j \geq 2$ provide reasonable imitations of the $3x+1$ trees. Therefore in Section 3 we study the simplest of these models, which is $\mathcal{B}[9]$. We present data for $k \leq 30$ on the expected value of extreme leaf counts for a "repeated branching process" model that takes $R(k)$ independent trials using the branching process $\mathcal{B}[9]$. (Recall that $R(k)$ is the number of distinct tree structures of depth k.) These expected values for $k \leq 30$ appear consistent with Conjecture C, but exhibit larger variability than that empirically observed for the $3x+1$ data up to $k \leq 30$.

In Sections 4 and 5 we present theoretical results about branching process models. First, in Section 4 we prove a result establishing for a large class of branching processes that there is a double-exponential dropoff of tail probabilities for values of $\log N(k)$, where $N(k)$ is the number of leaves at depth k of the process. Such results are "folklore", and we are indebted to Robin Pemantle for suggesting the method used to prove Theorem 4.1. Then, in Section 5 we prove that the analogue of Conjecture C is true for a repeated branching process model using $\mathcal{B}[9]$. We finally prove that the analogue of Conjecture $\mathrm{C}^{\#}$ is false for this repeated branching process model.

Thus we have uncovered a difference between the $3x+1$ empirical data and the branching process model: the extreme leaf count statistics for the actual $3x+1$ problem appear to have a significantly narrower range than that given by the branching process models. This seems to be the first evidence found indicating that the $3x+1$ function iterates do not behave as randomly as possible subject to "obvious" constraints.

Section 6 returns to the study of extremal leaf counts. We study the average number of leaves in pruned trees $\mathcal{T}_k^*(a)$, under the restriction $a \equiv l \bmod 3^j$, with $l \not\equiv 0 \bmod 3$. This amounts to specifying the branching structure of the first j levels of the tree $\mathcal{T}_k^*(a)$. We prove that this expected value is asymptotic to $W[l \bmod 3^j](\frac{4}{3})^k$ as $k \to \infty$, where $W[l \bmod 3^j]$ is an explicitly computable value (Theorem 6.1). The variation in $W[l \bmod 3^j]$ appears to account for nearly all of the variation in leaf sizes, and we conjecture that

$$\limsup_{k\to\infty} \left(\tfrac{4}{3}\right)^{-k} N^+(k) = \sup_{l,j} W[l \bmod 3^j],$$
$$\liminf_{k\to\infty} \left(\tfrac{4}{3}\right)^{-k} N^-(k) = \inf_{l,j} W[l \bmod 3^j].$$

We show (Theorem 6.3) that $W[l \bmod 3^j]$ interpolates to a function $W_\infty(l)$ defined almost everywhere on the invertible 3-adic integers

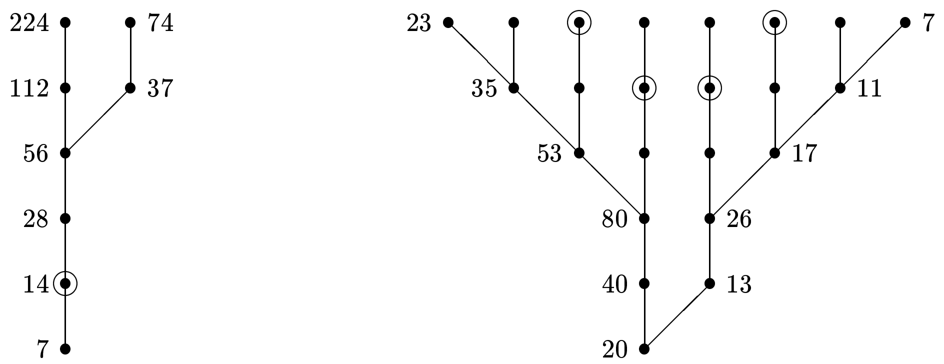
$$\mathbb{Z}_3^\times = \{l \in \mathbb{Z}_3 : l \equiv 1 \text{ or } 2 \bmod 3\}.$$

We conjecture that $W_\infty(l)$ is well-defined on all of $\mathbb{Z}_3^\times$ and is continuous and nonzero. Numerical evidence concerning $W[l \bmod 3^j]$ seems to support Conjecture $\mathrm{C}^{\#}$.

We remark that G. Wirsching [1994; 1995] has recently introduced other functions on $\mathbb{Z}_3^\times$ associated to backwards iteration of the $3x+1$ mapping. We do not know if there is any relation between these functions and the function W_∞.

2. 3x+1 TREES

In studying $3x+1$ trees we follow [Applegate and Lagarias 1995a]. Assign to each $a \not\equiv 0 \bmod 3$ the pruned tree $\mathcal{T}_k^*(a)$ of depth k whose root node is labeled a and whose other vertices at depth j for $1 \leq j \leq k$ correspond to labels in the set $\{n : n \not\equiv 0 \bmod 3 \text{ and } T^{(j)}(n) = a\}$. Each node labeled n at level j is connected to that labeled $T(n)$ at level $j-1$: see Figure 2. The branching structure of the



(i) $\mathcal{T}_5^*(7)$ attains $N^-(5) = 2$ (ii) $\mathcal{T}_5^*(20)$ attains $N^+(5) = 8$

FIGURE 2. Pruned $3x + 1$ trees. The nodes that have labels $n \equiv 5 \bmod 9$ are circled; such nodes have a preimage $n' = \frac{1}{3}(2n - 1) \equiv 0 \bmod 3$ in the corresponding unpruned tree.

pruned tree $\mathcal{T}_k^*(a)$ is completely determined by the value $a \bmod 3^{k+1}$.

Let $N_k^*(a)$ denote the number of leaves at depth k of $\mathcal{T}_k^*(a)$, and set

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

Theorem 3.1 of [Lagarias and Weiss 1992] showed that the expected size of $N_k^*(a)$ averaged over all $a \bmod 3^{k+1}$ with $a \not\equiv 0 \bmod 3$ is

$$E[N_k^*(a)] = \left(\tfrac{4}{3}\right)^k. \tag{2.1}$$

In [Applegate and Lagarias 1995a] we proposed the following conjecture:

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

To test such a conjecture it is natural to examine the normalized densities

$$D^+(k) := \left(\tfrac{4}{3}\right)^{-k} N^+(k),$$
$$D^-(k) := \left(\tfrac{4}{3}\right)^{-k} N^-(k),$$

which must necessarily satisfy $0 < D^-(k) \le 1 \le D^+(k)$ by (2.1). Table 1 gives empirical data for $k \le 30$ using the data from [Applegate and Lagarias 1995a, § 2]. These data support Conjecture C, and also appear to support the following stronger conjecture.

k	$R(k)$	$N^-(k)$	$N^+(k)$	$\left(\frac{4}{3}\right)^k$	$D^-(k)$	$D^+(k)$
1	4	1	2	1.33	0.750	1.500
2	8	1	3	1.78	0.562	1.688
3	14	1	4	2.37	0.422	1.688
4	24	2	6	3.16	0.633	1.898
5	42	2	8	4.21	0.475	1.898
6	76	3	10	5.62	0.534	1.780
7	138	4	14	7.49	0.534	1.869
8	254	5	18	9.99	0.501	1.802
9	470	6	24	13.32	0.451	1.802
10	876	9	32	17.76	0.507	1.802
11	1638	11	42	23.68	0.465	1.774
12	3070	16	55	31.57	0.507	1.742
13	5766	20	74	42.09	0.475	1.758
14	10850	27	100	56.12	0.481	1.782
15	20436	36	134	74.83	0.481	1.791
16	38550	48	178	99.77	0.481	1.784
17	72806	64	237	133.03	0.481	1.782
18	137670	87	311	177.38	0.490	1.753
19	260612	114	413	236.50	0.482	1.746
20	493824	154	548	315.34	0.488	1.738
21	936690	206	736	420.45	0.490	1.751
22	1778360	274	988	560.60	0.489	1.762
23	3379372	363	1314	747.47	0.486	1.758
24	6427190	484	1744	996.62	0.486	1.750
25	12232928	649	2309	1328.83	0.488	1.738
26	23300652	868	3084	1771.77	0.490	1.741
27	44414366	1159	4130	2362.36	0.491	1.748
28	84713872	1549	5500	3149.81	0.492	1.746
29	161686324	2052	7336	4199.75	0.489	1.747
30	308780220	2747	9788	5599.67	0.491	1.748

TABLE 1. Normalized extreme values for $3x + 1$ trees of depth k.

Conjecture C$^\#$. *There are positive constants C^+ and C^- such that*

$$C^- \leq D^-(k) < 1 < D^+(k) < C^+$$

for all sufficiently large k.

It even seems conceivable that $D^-(k)$ and $D^+(k)$ have limiting values as $k \to \infty$. In Section 6 we give further evidence that seems to support Conjecture C$^\#$ and the existence of limiting densities as $k \to \infty$.

3. BRANCHING PROCESS MODELS FOR 3x+1 TREES

We consider the question: To what extent do the branching process models $\mathcal{B}[3^j]$ for $j \geq 2$ presented in [Lagarias and Weiss 1992] accurately imitate the behavior of $3x+1$ trees? These models are multitype Galton–Watson processes [Athreiya and Ney 1972; Harris 1963]. Recall that such a process describes the evolution of a population of individuals of several types over generations, where each individual lives one generation. Each individual independently gives rise to progeny in the next generation of several types according to a specified probability distribution. The branching process tree describes the descendents of a single individual at generation 0, and level l of the tree includes all individuals in generation l. Edges connect individuals to their progeny in the next generation. Such a process is completely described by the probability distribution of individuals of each type.

The multitype Galton–Watson branching process $\mathcal{B}[9]$ has individuals of six types, one for each congruence classes mod 9 that is nonzero mod 3. They evolve as pictured in Figure 3. Individuals labeled 1, 4, 5 and 7 evolve deterministically, having one child of specified type, while individuals of type 2 or 8 always have two children, one of specified type, while the other's type can be one of three, with equal probability. Figure 3 also has edge labels reflecting whether $T^{-1}(n)$ is $2n$ or $\frac{1}{3}(2n-1)$, that is, whether $T^{-1}(n)$ is even or odd. The edge labels are completely determined by the types of the individuals at the two ends of the edge, hence are determined by the Galton–Watson process.

The model $\mathcal{B}[9]$ permits an unambiguous assignment of node labels to all nodes of a branching process tree, provided that a root node label is given. If n is a node label at level l and n' is a node it is connected to at level $l+1$, we assign $n' = 2n$ or $\frac{2}{3}n$ according to whether the edge connecting n to n' is labeled even or odd. The Galton–Watson process with the node labels added and interpreted as locations of the individuals on the line $\mathbb{R}$ becomes a *branching random walk*; this is the term used for these models in [Lagarias and Weiss 1992]. The node labels are needed in that reference in order that the branching process can be viewed as imitating the growth of $3x+1$ iterates, but they play no role in this paper.

Now let X_k be a random variable equal to the number of leaves at depth k of a sample tree drawn from the branching process $\mathcal{B}[9]$, starting from a

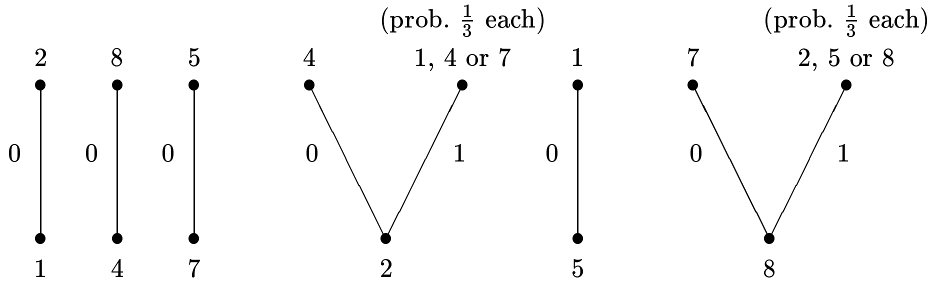


FIGURE 3. Transitions of the branching process $\mathcal{B}[9]$. The parent (bottom) always yields a child by the map $n \mapsto 2n$ (edge label 0), and it yields a child by the multivalued map $n \mapsto \frac{1}{3}(2n-1)$ (edge label 1) if $n = 2$ or 8 mod 9.

single individual of type drawn uniformly from the set $\{1, 2, 4, 5, 7, 8\}$. We are going to consider extreme value statistics for the quantity $(\frac{4}{3})^{-k} X_k$ for a specified number of repeated independent draws of such trees at depth k.

How many independent draws should one allow in such a "repeated branching process" model? A naïve model is to take $2 \cdot 3^k$ draws, which corresponds to allowing all residue classes a mod 3^{k+1} with $a \not\equiv 0$ mod 3. An alternative is to take instead the smaller number $R(k)$ of possible distinct $3x+1$ tree structures $\mathcal{T}^*(a)$ of depth k. The quantities $R(k)$ still grow exponentially in k, and based on the data for $k \leq 30$, Applegate and Lagarias [1993] estimated (empirically) that

$$1.87 < \liminf_{k \to \infty} R(k)^{1/k} < 1.92.$$

How do the data in Table 1 compare with the predictions from the branching process model $\mathcal{B}[9]$? To obtain as exact a numerical comparison with Table 1 as possible, we computed, for $k \leq 30$, the quantities

$$E[\tilde{N}^-(k)] := E[\min\{X_k : \text{ take } R(k) \text{ i.i.d. draws}\}],$$
$$E[\tilde{N}^+(k)] := E[\max\{X_k : \text{ take } R(k) \text{ i.i.d. draws}\}],$$

using the values of $R(k)$ from Table 1, drawing the root node uniformly from $\{1, 2, 4, 5, 7, 8\}$. The results appear in Table 2.

In this table, both $\tilde{D}^+(k) = (\frac{4}{3})^{-k} E[\tilde{N}^+(k)]$ and $\tilde{D}^-(k) = (\frac{4}{3})^{-k} E[\tilde{N}^-(k)]$ exhibit some initial fluctuations, and then $\tilde{D}^-(k)$ appears to steadily decrease with k, while $\tilde{D}^+(k)$ appears to steadily increase with k. This contrasts with the analogous quantities in Table 1, which appear to be roughly constant. If we computed these expected values $E[\tilde{N}^-(k)]$ and $E[\tilde{N}^+(k)]$ using $2 \cdot 3^k$ draws instead of $R(k)$ draws, the disagreement with Table 1 would be even greater.

In Section 5 we prove theoretical results concerning the analogues of Conjectures C and C$^\#$ for the branching process model $\mathcal{B}[9]$. We prove that the analogue of Conjecture C holds for these statistics, using a result on tail probabilities for leaf count distributions for a general class of branching processes, proved in Section 4. We prove that the analogue of Conjecture C$^\#$ doesn't hold, and that $\tilde{D}^-(k) \to 0$ and $\tilde{D}^+(k) \to \infty$ as $k \to \infty$.

k	$E[\tilde{N}^-(k)]$	$E[\tilde{N}^+(k)]$	$(\frac{4}{3})^k$	$\tilde{D}^-(k)$	$\tilde{D}^+(k)$
1	1.00	2.00	1.33	0.750	1.500
2	1.00	2.77	1.78	0.562	1.557
3	1.00	3.96	2.37	0.422	1.669
4	2.00	5.46	3.16	0.633	1.728
5	2.00	7.55	4.21	0.475	1.792
6	3.00	9.99	5.62	0.534	1.778
7	3.07	14.31	7.49	0.409	1.911
8	4.00	19.20	9.99	0.401	1.923
9	5.00	26.45	13.32	0.375	1.986
10	7.00	35.97	17.76	0.394	2.026
11	8.32	48.63	23.68	0.352	2.054
12	10.81	65.53	31.57	0.342	2.076
13	12.92	89.17	42.09	0.307	2.118
14	17.12	119.58	56.12	0.305	2.131
15	22.49	162.12	74.83	0.300	2.166
16	30.16	218.52	99.77	0.302	2.190
17	38.42	294.11	133.03	0.289	2.211
18	49.91	395.94	177.38	0.281	2.232
19	64.49	533.21	236.50	0.273	2.255
20	85.41	715.96	315.34	0.271	2.270
21	112.45	963.62	420.45	0.268	2.292
22	148.38	1294.74	560.60	0.265	2.310
23	193.77	1739.01	747.47	0.259	2.327
24	254.38	2335.64	996.62	0.255	2.344
25	334.18	3135.96	1328.83	0.252	2.360
26	441.25	4207.62	1771.77	0.249	2.375
27	581.63	5647.11	2362.36	0.246	2.390
28	766.94	7575.10	3149.81	0.243	2.405
29	1009.74	10159.40	4199.75	0.240	2.419
30	1331.40	13623.43	5599.67	0.238	2.433

TABLE 2. Expected values of the branching process. The quantites $E[\tilde{N}^\pm(k)]$ are defined in the opposite column, and calculated as explained in the sidebar on the next page. The last two columns are defined by $\tilde{D}^\pm(k) = (\frac{4}{3})^{-k} E[\tilde{N}^\pm(k)]$.

4. TAIL PROBABILITIES FOR LEAF COUNT DISTRIBUTIONS

We consider multitype Galton–Watson processes $\mathcal{G}$ having n types of individuals. In such a process an individual of type i lives for exactly one time period t and gives rise to a set of progeny of various types at time $t+1$. We assume that $\mathcal{G}$ has a finite *mean matrix* $\boldsymbol{M} = [\boldsymbol{M}_{i,j}]_{1\le i,j\le n}$, where $\boldsymbol{M}_{i,j}$ gives the expected number of progeny of type j produced by an individual of type i. We assume that $\mathcal{G}$ is *positively regular*, which means that some power $\boldsymbol{M}^k$ has all entries strictly positive. Under the positive regularity assumption the mean matrix $\boldsymbol{M}$ has a maximal real eigenvalue ρ of multiplicity one, which we call the *growth rate* of $\mathcal{G}$. Let $N_i(k)$ denote the total number of individuals at time k of a process starting from a single individual of type i at time 0. We say that $\mathcal{G}$ has *finite second moments* if $E[N_i(1)^2] < \infty$ for $1 \le i \le n$.

We prove below a result showing that the upper and lower tails of the logarithm of the leaf count distributions $N_i(k)$ of multitype Galton–Watson processes have double-exponential decay in k as $k \to \infty$, provided that the processes satisfy some mild extra conditions, which we now introduce. A multitype Galton–Watson process is *boundedly branching* if there is an upper bound L on the number of progeny that an individual (of any type) can have in one time period. It is *strictly branching* if an individual always has at least two progeny in each time period.

Theorem 4.1. *Let $\mathcal{G}$ be a multitype Galton–Watson process with n types that is positively regular, has finite mean matrix $\boldsymbol{M}$ with maximal real eigenvalue ρ, and is supercritical* ($\rho > 1$).

(i) *If $\mathcal{G}$ is boundedly branching, there exist for any $r > \rho$ positive constants α and δ, depending on r, such that*
$$\operatorname{Prob}\{N_i(k) > r^k\} \le \exp(-\alpha(1+\delta)^k)$$
for $1 \le i \le n$ and all $k \ge 1$.

(ii) *If $\mathcal{G}$ is strictly branching and has finite second moments, there exist for any $r < \rho$ positive constants α and δ, depending on r, such that*
$$\operatorname{Prob}\{N_i(k) < r^k\} \le \exp(-\alpha(1+\delta)^k)$$
for $1 \le i \le n$ and all $k \ge 1$.

REMARKS ON TABLE 2

Although a branching process of the type we are considering has a double-exponential number of possible trees at depth k, the $E[\tilde{N}^{\pm}(k)]$ entries in Table 2 were computed in single-exponential time as follows: Let X_k^i, for $i \bmod 9$, be a random variable counting the number of leaves at depth k of a sample tree drawn from the branching process $\mathcal{B}[9]$, starting from a single individual of type i. Let $P[X_k^i = x] := \operatorname{Prob}\{X_k^i = x\}$. Then the distributions of X_k^i and X_k were computed from the recursion

$$\begin{aligned}
&P[X_0^i = 1] = 1,\\
&P[X_k^i = x] = P[X_{k-1}^{2i} = x] \quad \text{if } i = 1,4,5,7,\\
&P[X_k^2 = x] = \sum_{y=0}^{\infty} P[X_{k-1}^{2i} = x-y]\left(\frac{P[X_{k-1}^1 = y] + P[X_{k-1}^4 = y] + P[X_{k-1}^7 = y]}{3}\right),\\
&P[X_k^8 = x] = \sum_{y=0}^{\infty} P[X_{k-1}^{2i} = x-y]\left(\frac{P[X_{k-1}^2 = y] + P[X_{k-1}^5 = y] + P[X_{k-1}^8 = y]}{3}\right),\\
&P[X_k = x] = \tfrac{1}{6}\sum_{i \bmod 9} P[X_k^i = x].
\end{aligned}$$

The cumulative distribution function $f_k(t)$ of the number of leaves was then computed. Finally the cumulative distributions of the minimum and maximum of $R(k)$ draws were computed using $1-(1-f_k(t))^{R(k)}$ and $f_k(t)^{R(k)}$, respectively. The entire computation took about 15 minutes on a 150 MHz MIPS R4400 processor.

Before giving the proof, we note that the conclusion of either part of the theorem certainly require some extra restriction on the Galton–Watson process $\mathcal{G}$ beyond being positively regular and supercritical. Concerning (i), suppose a single-type Galton–Watson process $\mathcal{G}$ has the probability p_m of m offspring satisfying $p_m = cm^{-4}$ for large m (so $\mathcal{G}$ has a finite second moment). Then

$$\operatorname{Prob}\{N_1(k) > r^k\} \geq \operatorname{Prob}\{N_1(1) > r^k\} \geq p_{r^k} \geq cr^{-4k},$$

for sufficiently large r, which violates the conclusion in (i). Concerning (ii), if $\mathcal{G}$ is not strictly branching, and $p_1 > 0$, then

$$\operatorname{Prob}\{N_1(k) < r^k\} \geq (p_1)^k,$$

which violates the conclusion in (ii).

Proof. (i) Suppose that $r > \rho$ is given. By hypothesis there is a finite bound L for the maximum number of progeny that a single individual can have in one time period. The argument we give does not depend on the type of the individual at time 0, so we omit explicit reference to it.

Let $N^{(i)}(k)$ denote the number of individuals of type i at time k, and define the *type vector* $\boldsymbol{v}(k)$ at period k by

$$\boldsymbol{v}(k) := (N^{(1)}(k), N^{(2)}(k), \ldots, N^{(n)}(k)).$$

Also let $N^{(i,j)}(k, k+1)$ denote the number of individuals of type j at period $k+1$ that are progeny of an individual of type i at period k.

Suppose that $N(k) > r^k$. We claim that there is a constant k_0 depending on r and a constant $\delta > 0$ such that, for all $k \geq k_0$, there is some intermediate time l with $0 \leq l \leq k-1$ and a pair (i, j) of types with $\boldsymbol{M}_{i,j} \neq 0$, such that

$$N^{(i)}(l) \geq (1+\delta)^k \tag{4.1}$$

and

$$N^{(i,j)}(l, l+1) \geq (1+\delta)\boldsymbol{M}_{i,j} N^{(i)}(l). \tag{4.2}$$

We argue by contradiction, and suppose there were no such time l. Set $\boldsymbol{e} = (1, 1, \ldots, 1)$ and observe that all the type vectors satisfy coordinatewise the inequality

$$\boldsymbol{v}(l+1) \leq (1+\delta)\boldsymbol{v}(l)\boldsymbol{M} + (1+\delta)^k L\boldsymbol{e},$$

because the first term on the right bounds the contribution to $\boldsymbol{v}(l+1)$ of individuals of type j at time $l+1$ that are progeny of those types i at time l for which (4.2) doesn't hold, while the second term on the right bounds the contribution from types i for which (4.1) doesn't hold. Iterating this inequality for $0 \leq l \leq k-1$ starting with $\boldsymbol{v}(0) \leq \boldsymbol{e}$, we have

$$\boldsymbol{v}(k) \leq L(1+\delta)^k \boldsymbol{e} \times (\boldsymbol{I} + (1+\delta)\boldsymbol{M} + (1+\delta)^2\boldsymbol{M}^2 + \cdots + (1+\delta)^k \boldsymbol{M}^k)$$

(where $\boldsymbol{I}$ is the identity). By Perron–Frobenius theory the matrix $\boldsymbol{M}$ has spectral radius ρ, and by the positive regularity hypothesis its set of eigenvalues on the circle $|z| = \rho$ consists of a single simple eigenvalue at $z = \rho$. Therefore there is a constant c_0 with

$$\boldsymbol{e}\boldsymbol{M}^k \leq c_0 \rho^k \boldsymbol{e}.$$

Thus the preceding inequality for $\boldsymbol{v}(k)$ yields

$$\boldsymbol{v}(k) \leq c_0(k+1)L(1+\delta)^{2k}\rho^k \boldsymbol{e},$$

hence

$$N(k) = \boldsymbol{v}(k)\boldsymbol{e}^T \leq c_0 n(k+1)L(1+\delta)^{2k}\rho^k.$$

If we therefore choose δ so that $1 < 1+\delta < \sqrt{r/\rho}$, this bound contradicts $N(k) > r^k$ provided that $k \geq k_0$, proving the claim.

To bound $\operatorname{Prob}\{N(k) > r^k\}$ it thus suffices to bound the probability of the event (4.1) and (4.2) occurring over all triples (i, j, l). Now the random variable $N^{(i,j)}(l, l+1)$ is a sum of $N^{(i)}(l)$ independent draws from an integer-valued probability distribution $\{p_m\}$, where p_m is the probability that an individual of type i on $\mathcal{G}$ has exactly m progeny of type j. By definition the distribution $\{p_m\}$ has expected value $E[p] = \boldsymbol{M}_{i,j}$, and we also know that $p_m = 0$ for all $m \geq L$. Now we can apply Chernoff's theorem (as quoted in [Lagarias and Weiss 1992, p. 234]) with $N^{(i)}(l)$ draws to obtain the bound

$$\begin{aligned}\operatorname{Prob}\{N^{(i,j)}(l,\, l+1) \geq (1+\delta)E[p]N^{(i)}(l)\}\\ \leq \exp(-\alpha N^{(i)}(l)), \quad (4.3)\end{aligned}$$

where $\alpha = -g((1+\delta)E[p])$ with

$$g(a) := \sup_{\theta\in\mathbb{R}}\Bigl\{\theta a - \log\sum_{m=0}^{L} p_m e^{m\theta}\Bigr\}.$$

We check that $\alpha > 0$. Certainly $g(a) \geq 0$, by taking $\theta = 0$ above, and the strict convexity of

$$\log\sum_{m=0}^{L} p_m e^{m\theta}$$

allows one to check that for $a > E[p]$ the minimizer on the right side is not at $\theta = 0$, hence $\alpha > 0$.

Now combining (4.1), (4.2) and (4.3) we get

$$\operatorname{Prob}\{N(k) > r^k\} \leq n^2 k \exp(-\alpha(1+\delta)^k),$$

valid for $k \geq k_0$. Decreasing α and δ towards 0 as necessary, we obtain the conclusion of part (i).

(ii) Suppose that $r < \rho$ is given. The assumption that the process is strictly branching guarantees that $N_i(t) \geq 2^t$ for all $t \geq 1$ and $1 \leq i \leq n$. Now view a tree of depth k as consisting of a rooted tree of depth t that has $N(t)$ subtrees, each of depth $l := k - t$, growing from each of its leaves. All of these subtrees grow independently, and each of them can have at most r^k leaves, because the whole tree has r^k leaves by hypothesis. Using the fact that $N_i(t) \geq 2^t$ for all $t \geq 1$, we obtain the bound

$$\begin{aligned}&\operatorname{Prob}\{N_i(k) < r^k\}\\ &\quad\leq (\operatorname{Prob}\{\text{depth-}l\text{ subtree has} < r^k \text{ leaves}\})^{N_i(t)}\\ &\quad\leq \bigl(\max_{1\leq j\leq n}\{\operatorname{Prob}\{N_j(l) < r^k\}\}\bigr)^{2^t}. \quad (4.4)\end{aligned}$$

We choose $t = \alpha k$ for a small α and wish to bound the probability that a tree of depth $l = (1-\alpha)k$ has no more than r^k leaves. Since $\boldsymbol{M}$ is positively regular and second moments exist, the Kesten–Stigum theorem [Kesten and Stigum 1966, Theorem 1] applies to give positive constants u_i such that

$$E[N_i(l)] = (u_i + o(1))\rho^l \quad \text{as } l \to \infty. \qquad (4.5)$$

Furthermore, by the finite second moment assumption, there is a finite upper bound on the second moment of $N_i(l)/\rho^l$ valid for all $l \geq 1$ [Harris 1963, Theorem 9.2]. Hence by Chebyshev's inequality there is a constant $\gamma < 1$ such that

$$\operatorname{Prob}\{N_i(l) < E[N_i(l)]\} \leq \gamma$$

for all $l \geq 1$ and $1 \leq i \leq n$. To apply this in (4.4), it suffices to arrange that $E[N_i(l)] > r^k$. Now (4.5) implies that there is a positive constant c^* such that for $1 \leq i \leq n$,

$$E[N_i(l)] \geq c^*\rho^l$$

for all $l \geq 1$. Write $r = \rho^{\bar{c}}$ with $0 < \bar{c} < 1$ and choose

$$l = \bar{c}k - \log_2(c^*),$$

the point being that with this choice we have

$$E[N_j(l)] \geq c^*\rho^l \geq r^k$$

for $1 \leq j \leq n$, the last inequality depending on the fact that $\rho \geq 2$. Thus, for $1 \leq j \leq n$, we get

$$\operatorname{Prob}\{N_j(l) < r^k\}] \leq \operatorname{Prob}\{N_j(l) < E[N_j(l)]\} \leq \gamma$$

for all $l \geq 1$. Setting $\gamma = \exp(-\alpha^*)$, we get from (4.4) that

$$\begin{aligned}\operatorname{Prob}\{N(k) < r^k\} &\leq \exp(-\alpha^* 2^{k-l})\\ &= \exp(-\alpha^* c^* c^{(1-i)k})\\ &\leq \exp(-\alpha(1+\delta)^k)\end{aligned}$$

with $\alpha > 0$ and $\delta > 0$. □

5. APPLICATION TO $3x+1$ BRANCHING PROCESS MODELS

We consider now a "repeated branching process" model in which the model $\mathcal{B}[9]$ is grown to depth k, making $S(k)$ independent trials. The statistics that we are interested in are the minimum and maximum of the number of leaves over these $S(k)$ trials. We are interested in the case that $S(k)$ grows exponentially in k, so we consider $S(k) = \lfloor \tau^k \rfloor$, where $\tau > 1$ is a fixed constant. The relevant random variables are

$$\tilde{N}_\tau^-(k) = \min\{X_k : \text{take } \lfloor \tau^k \rfloor \text{ i.i.d. draws from } \mathcal{B}[9]\},$$
$$\tilde{N}_\tau^+(k) = \max\{X_k : \text{take } \lfloor \tau^k \rfloor \text{ i.i.d. draws from } \mathcal{B}[9]\}.$$

The scaled random variables $(\frac{4}{3})^k(\tilde{N}_\tau^-(k))^{-1}$ and $(\frac{4}{3})^{-k}\tilde{N}_\tau^+(k)$ are analogous to $(D^-(k))^{-1}$ and $D^+(k)$ in Table 1.

We first prove that an analogue of Conjecture C holds for this "repeated branching process" model using $\mathcal{B}[9]$.

Theorem 5.1. *For any fixed $\tau > 1$, with probability one, the branching process $\mathcal{B}[9]$ has*

$$\lim_{k\to\infty} (\tilde{N}_\tau^-(k))^{1/k} = \lim_{k\to\infty} (\tilde{N}_\tau^+(k))^{1/k} = \tfrac{4}{3}.$$

Proof. The process has mean matrix

$$\boldsymbol{M} := \begin{array}{c|cccccc|} \text{Type} & 1 & 4 & 7 & 2 & 5 & 8 \\ \hline 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 1 \\ 7 & 0 & 0 & 0 & 0 & 1 & 0 \\ 2 & \frac{1}{3} & \frac{4}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 5 & 1 & 0 & 0 & 0 & 0 & 0 \\ 8 & 0 & 0 & 1 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \hline \end{array} \qquad (5.1)$$

with left-eigenvector $\boldsymbol{v} = (1,1,1,1,1,1)$, and $\boldsymbol{M}^4$ has positive entries so $\mathcal{B}[9]$ is positively regular: compare [Lagarias and Weiss 1992, Theorem 3.2]. It is certainly *boundedly branching*, so part (i) of Theorem 4.1 applies to give, for $r > \frac{4}{3}$,

$$\text{Prob}\{\tilde{N}_\tau^+(k) \ge r^k\} \le \tau^k \exp(-\alpha(1+\delta)^k).$$

Since $\sum_{k=1}^{\infty} \tau^k \exp(-\alpha(1+\delta)^k)$ converges, we conclude that, with probability one,

$$\limsup_{k\to\infty} (\tilde{N}_\tau^+(k))^{1/k} \le \rho = \tfrac{4}{3} \qquad (5.2)$$

The key point of the proof concerns the strict branching property. Although $\mathcal{B}[9]$ is not strictly branching, repeated application of it for four time periods is. This is easy to check using the branching data in Figure 3. The repeated branching process $\mathcal{G} = \mathcal{B}[9]^{(*4)}$ has mean matrix $\boldsymbol{M}^4$, which has growth rate ρ^4, and it has finite second moments since it is boundedly branching. Now part (ii) of Theorem 4.1 applies to $\mathcal{G}$, to show that

$$\text{Prob}\{\tilde{N}_\tau^-(4k) < r^k\} \le \tau^k \exp(-\alpha(1+\delta)^k)$$

for any $r < (\frac{4}{3})^4$. As in the argument above, we conclude that, with probability one,

$$\liminf_{k\to\infty} (\tilde{N}_\tau^-(4k))^{1/k} \ge \left(\tfrac{4}{3}\right)^4.$$

Since $N(k) \le N(k+i) \le 2^i N(k)$ for $0 \le i \le 3$, we conclude that, with probability one,

$$\liminf_{k\to\infty} (\tilde{N}_\tau^-(k))^{1/k} \ge \rho = \tfrac{4}{3}.$$

Combining this with (5.2) and using the fact that $\tilde{N}_\tau^-(k) \le \tilde{N}_\tau^+(k)$ in any sampling of trees, we conclude that $\lim_{k\to\infty} (\tilde{N}_\tau^+(k))^{1/k}$ and $\lim_{k\to\infty} (\tilde{N}_\tau^-(k))^{1/k}$ both exist and equal $\frac{4}{3}$ with probability one. $\square$

Remark. This proof applies to all the branching process models $\mathcal{B}[3^j]$ with $j \ge 2$, because all the processes $\mathcal{B}[3^j]^{(*4)}$ have the strict branching property for $j \ge 2$. It does not apply to the branching processes $\mathcal{B}[1]$ and $\mathcal{B}[3]$, because they have no iterate possessing the strict branching property. In fact the lower bound (5.2) is false for $\mathcal{B}[1]$ and $\mathcal{B}[3]$ whenever $\tau > \frac{4}{3}$.

We now show that the analogue of Conjecture C$^{\#}$ is false for the "repeated branching process" model using $\mathcal{B}[9]$.

Theorem 5.2. *For any fixed $\tau > 1$, the branching process $\mathcal{B}[9]$ has*

$$\lim_{k\to\infty} \left(\tfrac{4}{3}\right)^{-k} \tilde{N}_\tau^-(k) = 0,$$
$$\lim_{k\to\infty} \left(\tfrac{4}{3}\right)^{-k} \tilde{N}_\tau^+(k) = +\infty.$$

Proof. Let W_k^m, for m mod 9, enumerate the number of leaves of type m of a random tree of depth k drawn from $\mathcal{B}[9]$, with root node drawn uniformly from $\{1, 2, 4, 5, 7, 8\}$. Set

$$\boldsymbol{W}_k := (W_k^1, W_k^2, W_k^4, W_k^5, W_k^7, W_k^8),$$

so that $X_k = W_k^1 + W_k^2 + W_k^4 + W_k^5 + W_k^7 + W_k^8$. Let $\boldsymbol{w}_k$ denote the probability distribution of the random vector $(\frac{4}{3})^{-k}\boldsymbol{W}_k$. Now $E[X_1 \log X_1] < \infty$, hence the Kesten–Stigum theorem applies to show that the distributions $\boldsymbol{w}_k$ converge weakly to a limiting distribution $\boldsymbol{w}_\infty$, which is of the form

$$\boldsymbol{w}_\infty = w \cdot \boldsymbol{v},$$

where $\boldsymbol{v}$ is a constant vector and w is a one-dimensional positive random variable that is absolutely continuous, except for a possible jump at the origin. (The jump at the origin represents the probability of extinction.) Furthermore $\boldsymbol{v}$ is the (unique) left eigenvector corresponding to the maximal real eigenvalue ρ of the mean matrix $\boldsymbol{M}$ of the Galton–Watson process; in our case $\boldsymbol{M}$ is given in (5.1), and $\boldsymbol{v} = \boldsymbol{e} = (1, 1, \dots, 1)$.

The conditional distribution

$$w_i := \{w \mid \text{initial type } i\}$$

has expectation

$$E[w \mid \text{initial type } i] = u_i,$$

where $\boldsymbol{u}$ is a right eigenvector of $\boldsymbol{M}$, and the jump q_i at the origin depends on the type i. The q_i are just probabilities of extinction, so in the case of $\mathcal{B}[9]$ there are no jumps (all $q_i = 0$), and *each conditional distribution w_i is strictly positive* on $\mathbb{R}^+$, by [Athreiya and Ney 1972, § V.6, Theorem 2(iv)]. (A detailed proof of the positivity of w for the single-type Galton–Watson process appears in [Athreiya and Ney 1972, § II.5, Theorem 2]. See also [Kesten and Stigum 1966, Lemma 7].)

Now the random variables

$$\left(\tfrac{4}{3}\right)^{-k}\tilde{N}_\tau^-(k) \qquad \text{and} \qquad \left(\tfrac{4}{3}\right)^{-k}\tilde{N}_\tau^+(k)$$

sample values in the tails of the distributions $\boldsymbol{w}_k$, that is, values that lie outside any fixed region $(\varepsilon, 1-\varepsilon)$ in the cumulative distribution for large enough k. Since the $\boldsymbol{w}_k$ converge weakly to $\boldsymbol{w}_\infty$, it follows from the strict positivity of w on $\mathbb{R}^+$ that, as $k \to \infty$, we have

$$\left(\tfrac{4}{3}\right)^{-k}\tilde{N}_\tau^-(k) \to 0,$$
$$\left(\tfrac{4}{3}\right)^{-k}\tilde{N}_\tau^+(k) \to \infty.$$

Theorem 5.2 follows. □

6. AVERAGE LEAF COUNTS AND CONJECTURE C$^\#$

We return to the study of $3x+1$ trees, and study fluctuations in the leaf counts of such trees caused by the branching pattern at the base of the tree, in its first j levels. That is, we estimate the expected size of pruned $3x+1$ trees $\mathcal{T}_k^*(a)$ whose root node lies in a fixed congruence clase l mod 3^j. This expected value is

$$E_k^*[l \bmod 3^j] := 3^{j-(k+1)} \sum_{\substack{a \bmod 3^{k+1} \\ a \equiv l \bmod 3^j}} N_k^*(a)$$

for $j \geq 1$.

Theorem 6.1. *For each $j \geq 1$ and $l \not\equiv 0 \bmod 3$ there is a positive constant $W[l \bmod 3^j]$ such that*

$$E_k^*[l \bmod 3^j] = (W[l \bmod 3^j] + o(1))\left(\tfrac{4}{3}\right)^k \tag{6.1}$$

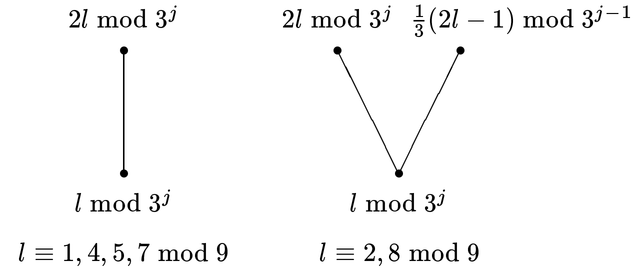
as $k \to \infty$.

Proof. We will use the formula (corresponding to $j = 0$)

$$\frac{1}{2 \cdot 3^k} \sum_{\substack{a \bmod 3^{k+1} \\ a \not\equiv 0 \bmod 3}} N_k^*(a) = \left(\tfrac{4}{3}\right)^k, \tag{6.2}$$

which is proved in [Lagarias and Weiss 1992, Theorem 3.1].

We first establish recursions for the quantities $E_k^*[l \bmod 3^j]$. The recursions are based on the bottom branching of the $3x+1$ tree, which depends on $l \bmod 9$, and is as follows:



This gives the recursion

$$N_k^*(a) = N_{k-1}^*(2a) + \psi(a \bmod 9) N_{k-1}^*\big(\tfrac{1}{3}(2a-1)\big),$$

in which

$$\psi(l \bmod 9) := \begin{cases} 0 & \text{if } l \equiv 1,4,5,7 \bmod 9 \\ 1 & \text{if } l \equiv 2,8 \bmod 9 \end{cases}$$

is an indicator function for the presence of a branch of the tree with edge label 1. Summing this recursion over all $a \bmod 3^{k+1}$ we get, for $k \geq j \geq 2$,

$$E_k^*[l \bmod 3^j] = E_{k-1}^*[2l \bmod 3^j] + \psi(l \bmod 9) E_{k-1}^*[\tfrac{1}{3}(2l-1) \bmod 3^{j-1}]. \quad (6.3)$$

If $j \geq 2$ but $1 \leq k < j$ then

$$E_k^*[l \bmod 3^j] = E_k^*[l \bmod 3^k].$$

The case $j=1$ must be treated separately. The recursions become

$$E_k^*[1 \bmod 3] = E_{k-1}^*[2 \bmod 3],$$
$$E_k^*[2 \bmod 3] = E_{k-1}^*[1 \bmod 3] + \tfrac{2}{3}\big(\tfrac{4}{3}\big)^{k-1},$$

where (6.2) was used to obtain the last equation. We have $E_1^*[1 \bmod 3] = 1 = \frac{3}{4}\big(\frac{4}{3}\big)$ and $E_1^*[2 \bmod 3] = \frac{5}{3} = \frac{5}{4}\big(\frac{4}{3}\big)$, from which we deduce

$$E_k^*[l \bmod 3] = w_l(k)\big(\tfrac{4}{3}\big)^k$$

for $l = 1,2$, in which $w_1(k)$ and $w_2(k)$ obey the recurrences

$$w_1(k) = \tfrac{3}{4} w_2(k-1),$$
$$w_2(k) = \tfrac{3}{4} w_1(k-1) + \tfrac{1}{2}.$$

This yields $w_2(k) = \frac{9}{16} w_2(k-2) + \frac{1}{2}$, from which one easily deduces

$$w_1(k) = \tfrac{6}{7} + O\big(\big(\tfrac{3}{4}\big)^k\big),$$
$$w_2(k) = \tfrac{8}{7} + O\big(\big(\tfrac{3}{4}\big)^k\big). \quad (6.4)$$

Now (6.1) follows for $j=1$ with

$$W[1 \bmod 3] = \tfrac{6}{7} \quad \text{and} \quad W[2 \bmod 3] = \tfrac{8}{7}. \quad (6.5)$$

For $j \geq 2$, let $W[l \bmod 3^j]$ be defined recursively in j as the unique solution to the system of linear equations

$$W[l \bmod 3^j] = \tfrac{3}{4}\big(W[2l \bmod 3^j] + \psi(l \bmod 9) W[\tfrac{1}{3}(2l-1) \bmod 3^{j-1}]\big). \quad (6.6)$$

The quantities $W[\frac{1}{3}(2l-1) \bmod 3^{j-1}]$ are known, and this linear system has matrix $\boldsymbol{I} - \frac{3}{4}\boldsymbol{P}$, where $\boldsymbol{P}$ is a certain permutation matrix, which is clearly invertible since $(\boldsymbol{I} - \frac{3}{4}\boldsymbol{P})^{-1} = \boldsymbol{I} + \frac{3}{4}\boldsymbol{P} + \big(\frac{3}{4}\boldsymbol{P}\big)^2 + \cdots$.

Next, define the quantities $\Delta_k[l \bmod 3^j]$ by

$$E_k^*[l \bmod 3^j] = \big(W[l \bmod 3^j] + \Delta_k[l \bmod 3^j]\big)\big(\tfrac{4}{3}\big)^k,$$

and set

$$\bar{\Delta}_k[3^j] := \max_{l \not\equiv 0 \bmod 3} \big|\Delta_k[l \bmod 3^j]\big|.$$

We claim that there are positive constants c_j such that

$$\bar{\Delta}_k[3^j] \leq c_j \big(\tfrac{7}{8}\big)^k. \quad (6.7)$$

If so, then (6.1) follows.

For $j=1$ this holds for all $k \geq 1$ by (6.4), choosing a suitable value for c_1.

We prove (6.7) for $j \geq 2$ by induction on j, where for each j we verify it for all k by induction on $k \geq 1$. The constants c_j are defined recursively by

$$c_j = \max\big(6c_{j-1}, \max_{1 \leq k \leq j} \bar{\Delta}_k[3^j]\big(\tfrac{8}{7}\big)^k\big).$$

Assume (6.7) is true for $j-1$ and all k. For j and $1 \leq k < j$, (6.7) holds by the definition of c_j. For $j \geq k$, the recursions (6.3) give

$$\Delta_k[l \bmod 3^j] = \tfrac{3}{4}\big(\Delta_{k-1}[2l \bmod 3^j] + \psi(l \bmod 9)\Delta_{k-1}[\tfrac{1}{3}(2l-1) \bmod 3^{j-1}]\big).$$

In particular the recursions yield the inequality

$$\bar{\Delta}_k[3^j] \le \tfrac{3}{4}\bar{\Delta}_{k-1}[3^j] + \tfrac{3}{4}\bar{\Delta}_{k-1}[3^{j-1}].$$

This gives, by the induction hypothesis,

$$\bar{\Delta}_k[3^j] \le \tfrac{3}{4}c_j\left(\tfrac{7}{8}\right)^{k-1} + \tfrac{3}{4}c_{j-1}\left(\tfrac{7}{8}\right)^{k-1} \le c_j\left(\tfrac{7}{8}\right)^{k},$$

since $c_j \ge 6c_{j-1}$, completing the induction step. (One can prove that $\bar{\Delta}_k[3^j]$ is $O\big((\frac{3}{4})^{(1+\varepsilon)k}\big)$ for any $\varepsilon > 0$, by a similar argument.) □

The densities $W[l \bmod 3^j]$ are determined recursively by solving the linear system (6.6). For $j = 2$, we obtain

$$\left.\begin{aligned} W[1 \bmod 9] &= \tfrac{3456}{3367}, & W[2 \bmod 9] &= \tfrac{4608}{3367},\\ W[4 \bmod 9] &= \tfrac{3258}{3367}, & W[8 \bmod 9] &= \tfrac{4344}{3367},\\ W[7 \bmod 9] &= \tfrac{1944}{3367}, & W[5 \bmod 9] &= \tfrac{2592}{3367}. \end{aligned}\right\} \quad (6.8)$$

We now show, for later use, that the quantities $W[l \bmod 3^j]$ satisfy, for all $j \ge 1$, the mean value formula

$$\frac{1}{2\cdot 3^{j-1}} \sum_{\substack{l \bmod 3^j\\ l\not\equiv 0 \bmod 3}} W[l \bmod 3^j] = 1. \quad (6.9)$$

This holds for $j = 1$ by (6.5). For $j \ge 2$, summing up (6.6) over all $l \bmod 3^j$ we get

$$\tfrac{1}{4} \sum_{\substack{l \bmod 3^j\\ l\not\equiv 0 \bmod 3}} W[l \bmod 3^j] = \tfrac{3}{4} \sum_{\substack{l' \bmod 3^{j-1}\\ l'\not\equiv 0 \bmod 3}} W[l' \bmod 3^{j-1}].$$

Now (6.9) follows by induction on j, because its left-hand side equals, by the equation just given,

$$\frac{1}{2\cdot 3^{j-2}} \sum_{\substack{l' \bmod 3^{j-1}\\ l'\not\equiv 0 \bmod 3}} W[l' \bmod 3^{j-1}] = 1.$$

Using the quantities $W[l \bmod 3^j]$ we can obtain asymptotic bounds on the number of leaves in extremal trees.

Corollary 6.2. *Let $D^{\pm}(k) = \left(\frac{4}{3}\right)^{-k} N^{\pm}(k)$. For each $j \ge 1$, we have*

$$\limsup_{k\to\infty} D^+(k) \ge W_j^+ := \max_{l\not\equiv 0 \bmod 3} W[l \bmod 3^j],$$
$$\liminf_{k\to\infty} D^-(k) \le W_j^- := \min_{l\not\equiv 0 \bmod 3} W[l \bmod 3^j].$$

Proof. Extreme values on leaf counts satisfy obvious inequalities in relation to mean values. □

The limit $j \to \infty$ in Corollary 6.2 yields

$$\limsup_{k\to\infty} D^+(k) \ge W_\infty^+ := \limsup_{j\to\infty} W_j^+,$$
$$\liminf_{k\to\infty} D^-(k) \le W_\infty^- := \liminf_{j\to\infty} W_j^-.$$

In order for Conjecture $C^{\#}$ to hold, W_∞^+ and W_∞^- must satisfy

$$0 < W_\infty^- < 1 < W_\infty^+ < \infty. \quad (6.10)$$

This is unproved, but would follow from the Limit Function Conjecture stated below.

Table 3 presents data on the extreme values W_j^- and W_j^+, as well as on the quantities

$$\eta_j^+ := \max_{l\equiv l' \bmod 3^{j-1}} \left| W[l \bmod 3^j] - W[l' \bmod 3^j] \right|$$

which bound how fast W_j^- and W_j^+ are changing as $j \to \infty$. It also gives the quantities $l \bmod 3^j$ attaining W_j^+ and W_j^-, with l expressed in base 3, as well as $l \bmod 3^{j-1}$ attaining η_j^+.

On comparing the values in Table 3 with the extreme densities $D^+(k)$ and $D^-(k)$ in Table 1, we see that by $k = 9$ the values W^+ and W^- seem to be accounting for nearly all of the observed variation in $D^+(k)$ and $D^-(k)$. (Note that $W_8^- < D^-(8)$; this is not contradictory because W_8^- is an asymptotic limit as $k \to \infty$. However we must have $D^-(8) \le \min_l E_8^*[l \bmod 3^8](\frac{3}{4})^8$.)

The data in Table 3 suggest that the quantities $W[l \bmod 3^j]$ may explain all the extremal variation in leaf count sizes in an asymptotic sense. We therefore propose the following conjecture.

j	$\min l \pmod{3^j}$	W_j^-	$\max l \pmod{3^j}$	W_j^+	$\max l \pmod{3^{j-1}}$	η_j^+
1	1_3	0.857	2_3	1.143	–	0.286
2	21_3	0.577	02_3	1.369	2_3	0.599
3	221_3	0.528	202_3	1.493	22_3	0.407
4	2221_3	0.517	0202_3	1.561	222_3	0.302
5	02221_3	0.504	12122_3	1.611	2222_3	0.209
6	202221_3	0.503	212122_3	1.649	22222_3	0.166
7	1002221_3	0.498	1212122_3	1.672	222222_3	0.116
8	21002221_3	0.497	21212122_3	1.690	2222222_3	0.085
9	221002221_3	0.494	202020202_3	1.704	22222222_3	0.062
10	1221002221_3	0.493	0202020202_3	1.714	222222222_3	0.045
11	21221002221_3	0.491	20202020202_3	1.721	2222222222_3	0.033

TABLE 3. Extreme densities $W[l \bmod 3^j]$.

Extremal Limit Conjecture. *$D^+(k)$ and $D^-(k)$ satisfy $\limsup_{k\to\infty} D^+(k) = W_\infty^+$ and $\liminf_{k\to\infty} D^-(k) = W_\infty^-$.*

We observe that the recursion for $W[l \bmod 3^j]$ has a regular structure. These quantities interpolate to a function defined almost everywhere on the invertible 3-adic integers

$$\mathbb{Z}_3^\times = \{\alpha \in \mathbb{Z}_3 : \alpha \equiv 1 \text{ or } 2 \bmod 3\},$$

as we now show. We view $\mathbb{Z}_3^\times$ as a measure space with the 3-adic measure μ with $\mu(\mathbb{Z}_3) = 1$, so that $\mu(\mathbb{Z}_3^\times) = \frac{2}{3}$.

Theorem 6.3. *For μ-almost all $\alpha = \sum_{j=0}^\infty a_j 3^j \in \mathbb{Z}_3^\times$, the limit*

$$W_\infty(\alpha) := \lim_{j\to\infty} W[\alpha \bmod 3^j] \tag{6.11}$$

exists.

Proof. Let $\mu^\times = \frac{3}{2}\mu$, so that $\mu^\times(\mathbb{Z}_3^\times) = 1$ is a probability measure. Define for $j \geq 1$ the functions $W_j : \mathbb{Z}_3^\times \to \mathbb{R}$ by

$$W_j(\alpha) := W[\alpha \bmod 3^j],$$

and view $\{W_j : j \geq 1\}$ as random variables on $\mathbb{Z}_3^\times$ with respect to $\mu^\times$. We claim that $\{W_j : j \geq 1\}$ is a martingale with respect to the σ-fields $\{\mathcal{F}_j : j \geq 1\}$ with $\mathcal{F}_j = \{\text{residue classes mod } 3^j\}$. The martingale property is that, for each residue class $\alpha \bmod 3^j$,

$$E[W_{j+1}(\beta) \mid \beta \equiv \alpha \bmod 3^j] = W_j(\alpha),$$

which is equivalent to

$$\frac{1}{3}\sum_{k=0}^{2} W[\alpha + k\cdot 3^j \bmod 3^{j+1}] = W[\alpha \bmod 3^j]. \tag{6.12}$$

To establish (6.12), we define

$$X[l \bmod 3^j] := W[l \bmod 3^j] - W[l \bmod 3^{j-1}].$$

The recursion (6.6) for $l \bmod 3^j$, subtracted from that for $l \bmod 3^{j+1}$, gives

$$\begin{aligned} X[l \bmod 3^{j+1}] = \tfrac{3}{4}\big(&X[2l \bmod 3^{j+1}] \\ &+ \psi(l \bmod 9) X[\tfrac{1}{3}(2l-1) \bmod 3^j]\big). \end{aligned} \tag{6.13}$$

We now prove by induction on $j \geq 1$ that

$$A[l \bmod 3^{j+1}] := \sum_{k=0}^{2} X[l + k\cdot 3^j \bmod 3^{j+1}] = 0 \tag{6.14}$$

for all $l \bmod 3^{j+1}$. The base case $j = 1$ is verified by direct computation, using (6.8). For the induction step, (6.13) summed over l, $l + 3^j$, and $l + 2\cdot 3^j$ gives

$$\begin{aligned} A[l \bmod 3^{j+1}] = \tfrac{3}{4}\big(&A[2l \bmod 3^{j+1}] \\ &+ \psi(l \bmod 9) A[\tfrac{1}{3}(2l-1) \bmod 3^j]\big). \end{aligned}$$

The last term $A[\frac{1}{3}(2l-1) \bmod 3^j]$ vanishes by the induction hypothesis, so the equation becomes the invertible linear system

$$(\boldsymbol{I} - \tfrac{3}{4}\boldsymbol{P})\big(A[l \bmod 3^{j+1}]\big) = \boldsymbol{0}.$$

This gives (6.14). Substituting the definition of $X[l \bmod 3^{j+1}]$ in (6.14) gives (6.12); hence $\{W_j : j \geq 1\}$ is a martingale.

The mean value formula (6.9) gives

$$E\big[|W_j|\big] = E[W_j] = \int_{\mathbb{Z}_3^\times} W_j(\alpha) d\mu^\times(\alpha) = 1$$

for $j \geq 1$. Now the Martingale Convergence Theorem [Billingsley 1979, Theorem 35.4] applies to $\{W_j : j \geq 1\}$, so the theorem follows. □

We may define the limit function $W_\infty(\alpha)$ for all $\alpha \in \mathbb{Z}_3^\times$ by

$$W_\infty(\alpha) = \limsup_{j\to\infty} W[\alpha \bmod 3^j].$$

Here $W_\infty(\alpha) \geq 0$ and the value $+\infty$ is allowed. The Martingale Convergence Theorem also gives

$$\begin{aligned} E[W_\infty] &= \int_{\mathbb{Z}_3^\times} W_\infty(\alpha)\, d\mu^\times(\alpha) \\ &= E\big[|W_\infty|\big] = E\big[|W_1|\big] = 1. \end{aligned} \tag{6.15}$$

The data in Table 3 suggest that η_j^+ tends to 0 rapidly enough that $\sum_{j=0}^\infty \eta_j^+ < \infty$, in which case $W[\alpha \bmod 3^j]$ would converge uniformly to $W_\infty(\alpha)$ for all $\alpha \in \mathbb{Z}_3^\times$. Therefore we propose:

Limit Function Conjecture. *The function $W_\infty : \mathbb{Z}_3^\times \to \mathbb{R}$ is continuous and nonzero, and*

$$W_\infty(\alpha) = \lim_{j\to\infty} W[\alpha \bmod 3^j]$$

for all $\alpha \in \mathbb{Z}_3^\times$.

If this conjecture is true, then taking the limit as $j \to \infty$ in (6.6) shows that $W_\infty(\alpha)$ satisfies the functional equation

$$W_\infty(\alpha) = \tfrac{3}{4}\big(W_\infty(2\alpha)+\psi(\alpha \bmod 9)W_\infty(\tfrac{1}{3}(2\alpha-1))\big). \tag{6.16}$$

Since $\mathbb{Z}_3^\times$ is compact, this conjecture also implies that

$$W_\infty^+ = \sup_{\alpha\in\mathbb{Z}_3^\times} W_\infty(\alpha) < \infty$$

and

$$W_\infty^- = \inf_{\alpha\in\mathbb{Z}_3^\times} W_\infty(\alpha) > 0.$$

Since (6.15) and (6.16) imply that $W_\infty(\alpha)$ cannot be the constant function 1, we must have $W_\infty^- < 1 < W_\infty^+$, and (6.10) follows. Thus the Limit Function Conjecture and the Extremal Limit Conjecture together imply Conjecture $C^\#$.

Finally, we note some resemblance of the recursion (6.6) to the Krasikov inequalities studied in [Applegate and Lagarias 1995b].

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