3x + 1 inverse orbit generating functions almost always have natural boundaries

by

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1. Introduction. The 3x + 1 function is given by

(1.1)
$$T(n) = T_1(n) := \begin{cases} \frac{3n+1}{2} & \text{if } n \text{ is odd,} \\ \frac{n}{2} & \text{if } n \text{ is even.} \end{cases}$$

The 3x + 1 problem (or Collatz problem) concerns the behavior of this map under iteration, restricted to the domain of positive integers \mathbb{N}^+ . This domain is invariant under iteration, and it contains the periodic orbit $\{1,2\}$ of T, which is the only periodic orbit known on \mathbb{N}^+ at present. The 3x + 1 Conjecture (or Collatz Conjecture) asserts that every positive integer under iteration enters this periodic orbit. The 3x + 1 Conjecture appears to be intractable at present: see for example [14, 20], and for recent viewpoints [16] and [9].

The 3x - 1 function is given by

(1.2)
$$T_{-1}(n) := \begin{cases} \frac{3n-1}{2} & \text{if } n \text{ is odd,} \\ \frac{n}{2} & \text{if } n \text{ is even.} \end{cases}$$

It satisfies $T_{-1}(n) = -T_1(-n)$. There is an analogous 3x - 1 problem concerning its behavior under iteration on the positive integers \mathbb{N}^+ , which has recently been studied by Berg and Opfer [6]. This function has three known periodic orbits on \mathbb{N}^+ , which are

$$\{1\}, \{5,7,10\}, \{17,25,37,55,82,41,61,91,136,68,34\}.$$

The 3x-1 Conjecture asserts that every integer $m \ge 1$ under iteration by T_{-1} eventually enters one of these three periodic orbits. This conjecture also appears intractable at present.

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More generally, one may consider iteration of the 3x + k function, where $k \equiv \pm 1 \pmod{6}$, given by

(1.3)
$$T_k(n) := \begin{cases} \frac{3n+k}{2} & \text{if } n \text{ is odd,} \\ \frac{n}{2} & \text{if } n \text{ is even.} \end{cases}$$

The 3x + k functions were studied in [15], in connection with rational cycles for the 3x+1 function. Those periodic orbits of the $3x \pm k$ function restricted to the domain of all integers n having (n, k) = 1 are known to correspond to those rational cycles for the 3x + 1 problem whose members each have denominator k, when written in lowest terms.

We let $T^{\circ j}(m)$ denote the jth iterate of a map $T: \mathbb{Z} \to \mathbb{Z}$, and denote the forward orbit of m by

$$\mathcal{O}_k^+(m) := \{ n : n = T_k^{\circ j}(m) \text{ for some } j \ge 0 \}.$$

In terms of forward orbits the 3x+1 Conjecture asserts that $1 \in \mathcal{O}_1^+(m)$ for each integer $m \geq 1$. Additionally we define the *backward orbit* (or *inverse orbit*) of m by

$$\mathcal{O}_k^-(m) := \{n: T_k^{\circ j}(n) = m \text{ for some } j \ge 0\}.$$

The set $\mathcal{O}_k^-(m)$ comprises the forward orbit of m under the (multivalued) inverse map

(1.4)
$$T^{\circ -1}(n) = T_1^{\circ -1}(n) := \begin{cases} \{2n\} & \text{if } n \equiv 0, 1 \pmod{3}, \\ \{2n, \frac{2n-1}{3}\} & \text{if } n \equiv 2 \pmod{3}. \end{cases}$$

The 3x + 1 Conjecture formulated in terms of backward orbits asserts that $\mathcal{O}_1^-(1) = \mathbb{N}^+$.

The main objects of study of this paper are the backward orbit generating functions

(1.5)
$$f_{k,m}(z) := \sum_{n \in \mathcal{O}_k^-(m) \cap \mathbb{N}^+} z^n$$

with $k \equiv \pm 1 \pmod{6}$ and $m \in \mathbb{Z}$. The functions $f_{k,m}(z)$ are analytic functions of z in the open unit disk $\{z \in \mathbb{C} : |z| < 1\}$, and we consider the problem of when these generating functions are analytically continuable to larger domains in the complex plane.

Our main result, Theorem 1.1 below, formulates conditions characterizing for the 3x + k problem when the generating function of a finite union of backward orbits is a rational function of z. There is a known dichotomy for analytic continuation of a class of functions including the type above: they either are rational functions or else have the unit circle as a natural boundary to analytic continuation (the Pólya–Carlson theorem). Using this dichotomy we deduce that for each $k \in \mathbb{Z}$ with (k, 6) = 1 and for almost

all $m \ge 1$, the functions $f_{k,m}(z)$ have the unit circle $\{|z| = 1\}$ as a natural boundary to analytic continuation.

The functions $f_{k,m}(z)$ encode data on the orbit intersected with the positive integers. However with the proper choice of two such functions one can recover the orbit on the negative integers as well. To see this, we first note that the 3x + k function and the 3x - k function are conjugate under the involution $J: \mathbb{Z} \to \mathbb{Z}$ with J(x) = -x, i.e.

$$T_k \circ J = J \circ T_{-k}$$

an operation which exchanges positive and negative integers. Consequently, the behavior of the function T_k restricted to the negative integers exactly matches that of T_{-k} restricted to the positive integers, with the latter encoded by the generating function above. Thus the two generating functions $f_{k,m}(z)$ and $f_{-k,-m}(z)$ between them give full information (1) for the inverse orbit $\mathcal{O}_k^-(m)$ on \mathbb{Z} .

For the special case $k=\pm 1$ corresponding to the 3x+1 function and the 3x-1 function respectively, the positive integers \mathbb{N}^+ and negative integers $\mathbb{N}^-=-\mathbb{N}^+$ are each bi-invariant sets for T_k , i.e. they are closed under forward and backward iteration. The conjugacy function J above shows that the 3x-1 function on \mathbb{N}^+ has iterates matching those of the 3x+1 function on the negative integers. In this special case we need only consider $m \geq 1$, using $f_{1,m}(z)$ and $f_{-1,m}(z)$. For all $m \leq -1$ we have $f_{1,m}(z) = f_{-1,m}(z) \equiv 0$.

1.1. Main results. The results of this paper concern properties of generating functions for the set union of a finite number of backward orbits of the 3x + k map.

We first observe that the backward orbits of a general function $T: X \to X$ have a trichotomy of possible behaviors: Two distinct such orbits $\mathcal{O}_T^-(m_1)$ and $\mathcal{O}_T^-(m_2)$ either are disjoint or have one of them properly contained in the other. These three outcomes correspond to one of:

- (i) $m_1 \in \mathcal{O}_T^-(m_2);$
- (ii) $m_2 \in \mathcal{O}_T^-(m_1);$
- (iii) neither (i) nor (ii) holds.

It follows from this trichotomy that for any map T on a countable set X, the set union S of any finite collection of backward orbits can always be partitioned into a finite set of disjoint backward orbits of single elements, whose set union equals that of the whole collection.

Our main result characterizes when a finite union of backward orbits has generating function that is a rational function.

⁽¹⁾ For the functions T_k that we consider, no orbit contains m = 0 except for the single point orbit $\{0\}$.

THEOREM 1.1. Consider the 3x + k map T_k for an integer $k \equiv \pm 1 \pmod{6}$. The following two conditions on a set union $S = \bigcup_{i=1}^{\ell} \mathcal{O}_k^-(m_i)$ of a finite set of backward orbits $\{\mathcal{O}_k^-(m_i): 1 \leq i \leq \ell\}$ of T_k are equivalent:

(1) The generating function of S restricted to \mathbb{N}^+ , which is

$$g(z) := \sum_{n \in \mathcal{S} \cap \mathbb{N}^+} z^n,$$

is a rational function of z.

(2) There is a set X of residue classes modulo |k| and a positive integer k_0 such that the rational function

$$h(z) = \sum_{\substack{n>0\\ n \, (\text{mod } |k|) \in X}} z^n = \sum_{\substack{a \in X\\1 \le a \le |k|}} \frac{z^a}{1 - z^{|k|}}$$

has power series coefficients agreeing with g(z) for all $n \geq k_0$, so that g(z) - h(z) is a polynomial of degree at most $k_0 - 1$. That is, the set of all $n \geq k_0$ belonging to S contains exactly those $n \geq k_0$ that belong to the union of the arithmetic progressions modulo |k| in X.

If the equivalent conditions (1), (2) hold, then the set X of residue classes in (2) is necessarily closed under the action of the maps $r \mapsto 2r$ and $r \mapsto 3r$ acting on residue classes modulo |k|.

We prove Theorem 1.1 in Section 3. The proof uses the Skolem–Mahler–Lech theorem, whose statement we recall in Section 2, together with the trichotomy above. The logical status of this result is interesting: At present we do not know of a single case of a value k and a set union \mathcal{S} where either of conditions (1) or (2) hold unconditionally. However if the 3x+1 Conjecture is true then for k=1 there exist infinitely many examples of finite unions of backward orbits \mathcal{S} where conditions (1)–(2) hold. See Section 6 for discussion of the general case $k \equiv \pm 1 \pmod{6}$.

We deduce from Theorem 1.1 several consequences about backward orbit generating functions having natural boundaries, given in Theorems 1.2–1.4 below.

First we consider natural boundaries for the 3x + 1 function.

THEOREM 1.2. Consider the 3x+1 map T_1 on the positive integers \mathbb{N}^+ . For the inverse orbit generating functions $f_{1,m}(z) = \sum_{n \in \mathcal{O}_1^-(m)} z^n$ with starting value $m \geq 1$ the following hold:

- (1) For each $m \geq 1$ except possibly m = 1, 2, 4 and 8 the generating function $f_{1,m}(z)$ has the unit circle $\{|z| = 1\}$ as a natural boundary to analytic continuation.
- (2) If the 3x + 1 Conjecture is true, then for m = 1, 2, 4 and 8 the generating function $f_{1,m}(z)$ analytically continues to a rational function

of z. If the 3x+1 Conjecture is false, then each of these four functions has the unit circle $\{|z|=1\}$ as a natural boundary to analytic continuation.

Secondly, we consider natural boundaries for the 3x-1 function.

THEOREM 1.3. Consider the 3x-1 map T_{-1} on the positive integers \mathbb{N}^+ . For every starting value $m \geq 1$, the backward orbit generating function

$$f_{-1,m}(z) = \sum_{n \in \mathcal{O}_{-1}^{-}(m)} z^n$$

has the unit circle $\{|z|=1\}$ as a natural boundary to analytic continuation.

This result proves a conjecture of Berg and Opfer [6, Conjecture 2.4], which concerns analytic continuability of the three functions $\eta_1(z) = f_{-1,1}(z)$, $\eta_2(z) = f_{-1,5}(z)$ and $\eta_3(z) = f_{-1,17}(z)$. Theorems 1.2 and 1.3 are proved in Section 4 and make use of the Pólya–Carlson theorem given in Section 2.

Finally, in Section 5 we establish an analogous result for the general case $k \equiv \pm 1 \pmod{6}$, which is less specific about exceptional cases.

THEOREM 1.4. Consider the 3x + k map T_k with $k \equiv \pm 1 \pmod{6}$ on the positive integers \mathbb{N}^+ . Then for all but finitely many starting values $m \geq 1$ the backward orbit generating function $f_{k,m}(z)$ has the unit circle $\{|z| = 1\}$ as a natural boundary to analytic continuation.

Establishing Theorem 1.4 involves two additional difficulties. First, the orbits of T_k for general k are more complicated than those for $k=\pm 1$; they can have several collections of residue classes modulo |k| that are forward-and-backward invariant sets for the general 3x+k function; cf. Lemma 5.1. (There is only one such class for $k=\pm 1$.) Second, some orbits may simultaneously contain infinitely many positive integers and infinitely many negative integers. This latter fact necessitated our definition of orbit generating functions in (1.5) to require intersecting the orbit with the set of positive integers.

1.2. Complexity of backward orbits in the 3x + 1 problem. The 3x + 1 Conjecture asserts that the backward orbit $\mathcal{O}_1^-(1)$ has a simple form. However this simplicity of form seems to be an illusion that hides the difficulty of the problem. The results above show that most backward orbits $\mathcal{O}_1^-(m)$ for variable m have considerable complexity, that is, they cannot have the regular structure required for the backward orbit generating function to be a rational function.

Indeed, the backward orbits of the 3x + k maps for different k appear to have an extremely complicated structure. The complexity of backward orbits was noted already for the 3x - 1 problem by Berg and Opfer [6, Fig. 1].

They presented numerical data of membership in the three disjoint backward orbits $\mathcal{O}_{-1}^-(1)$, $\mathcal{O}_{-1}^-(5)$, $\mathcal{O}_{-1}^-(17)$ in blocks of consecutive integers. Each of these three orbits appears experimentally to contain a positive density of integers, and the members of the different backward orbits appear to interlace in a complicated way on these blocks of integers. It would be interesting to formulate and study statistics that measure the amount of intertwining complexity between two disjoint backward orbits of a fixed function T_k .

1.3. Effective computability issues. The computational problem of deciding whether, given input data (k, m), the function $f_{k,m}(z)$ has $\{|z| = 1\}$ as a natural boundary is not known to be effectively computable. There does exist a computational algorithm $(^2)$ which, given k as input, if it halts, will list a finite exceptional set $E_k \subset \mathbb{Z}$ and a proof that for all integers m not in E_k , the generating function $f_{k,m}(z)$ has the unit circle as a natural boundary to analytic continuation. This algorithm is described at the end of Section 5. Standard conjectures analogous to the 3x+1 Conjecture would imply that this algorithm will always halt. At present it remains an open problem to prove (or disprove) that this algorithm always halts.

There are two obstacles to proving effective computability for individual inputs (k, m):

- (1) There is no effective algorithm known which, when given m_1 and m_2 , will determine whether the backward orbits of m_1 and m_2 under T_k are disjoint.
- (2) It is not known whether each bi-invariant component of the 3x + k map contains a finite cycle, although conjecturally this is always the case [15, Sect. 3.1].

Each of these obstacles appears to be an intractable problem at present.

1.4. Contents of paper. In Section 2 we recall several well-known results on the structure of power series with integer coefficients. These concern conditions for being rational functions or for having a natural boundary to analytic continuation. In Section 3 we prove Theorem 1.1, in Section 4 we prove Theorems 1.2 and 1.3, and in Section 5 we prove Theorem 1.4.

In Section 6 we complement Theorem 1.2 by showing that standard conjectures on the iteration of the 3x + k maps imply that there will exist infinitely many cases where a finite sum of backward orbit generating functions is a rational function.

In the concluding section we describe other known results for different analytic generating functions associated to 3x + k mappings which are (or may sometimes be) rational functions.

⁽²⁾ By an algorithm we mean a procedure which can be programmed on a Turing machine. Such a procedure, however, is not certified to halt on all inputs.

2. Preliminary facts. The proofs of the paper use several well-known results in analytic function theory.

2.1. Fabry gap theorem. The following basic result on natural boundaries of analytic functions given by lacunary expansion can be applied to very special cases of backward orbits above.

THEOREM 2.1 (Fabry gap theorem). Let $f(z) = \sum_{j=0}^{\infty} a_j z^{n_j}$ be a power series with positive finite radius of convergence R, and having gaps between its exponents n_j in the sense that

$$\lim_{j \to \infty} \frac{n_j}{j} = \infty.$$

Then the disk $B_R(0) = \{|z| < R\}$ is a maximal domain of holomorphy for f(z), i.e. the circle |z| = R is a natural boundary to analytic continuation.

The original 1896 result of Fabry [13] proved this theorem under the weaker assumption that the exponents are lacunary in the sense that there is a constant C > 1 such that $n_{k+1}/n_k > C$ for all sufficiently large k. The stronger result stated above was established by Faber [12] in 1906 (see Remmert [19, p. 256]). There are now much stronger gap theorem results known, showing that if the average gap size tends to infinity then there is a natural boundary (again see [19, p. 256]).

Theorem 2.1 has an immediate application to the 3x + k problem, based on the observation that for any $k \equiv \pm 1 \pmod{6}$ the backward orbit of any $m \equiv 0 \pmod{3}$ is $\mathcal{O}_k^-(m) = \{2^k m : k \geq 0\}$. It follows that for any positive $m \equiv 0 \pmod{3}$ the generating function of its inverse orbit

$$f_{k,m}(z) = \sum_{n \in \mathcal{O}_{b}^{-}(m)} z^{n} = \sum_{n=0}^{\infty} z^{m2^{n}}$$

satisfies the hypotheses of the Fabry gap theorem, so has $\{|z|=1\}$ as a natural boundary.

For the 3x+1 function T_1 , it has been conjectured that for $m \not\equiv 0 \pmod{3}$ the expected number of inverse iterates below x is asymptotically bounded below by c(m)x for a positive constant c(m) (see [1, Conjecture A]). If such a conjecture were true, then the existing gap-type theorems do not apply to infer the existence of a natural boundary to analytic continuation. The main results of this paper are proved without appeal to the Fabry gap theorem.

2.2. Pólya–Carlson theorem. The following dichotomy theorem was conjectured by Pólya [17] in 1916, and proved by Carlson [7] in 1921.

THEOREM 2.2 (Pólya–Carlson theorem). Let $f(z) = \sum_{n=0}^{\infty} a_n z^n$ have integer coefficients and have radius of convergence R = 1. Then exactly one of the following holds:

- (i) The power series f(z) has the circle $\{|z|=1\}$ as a natural boundary to analytic continuation.
- (ii) The power series f(z) can be analytically continued to a rational function of the form $p(z)/(1-z^m)^n$ for a polynomial $p(z) \in \mathbb{Z}[z]$ with m, n positive integers.

This result has since been strengthened and extended in various ways: see Remmert [19, p. 265] and Bell, Coons and Rowland [2].

2.3. Skolem–Mahler–Lech theorem. The Skolem–Mahler–Lech theorem has many different incarnations, for which see van der Poorten [18] and Everest et al. [10, Chap. 2]. It can be formulated in terms of zeros of recurrence sequences or zeros of Taylor series coefficients of rational functions; for more recent algebraic-geometric versions, see [3]. We will use the following version.

THEOREM 2.3 (Skolem-Mahler-Lech theorem). Let $R(z) \in \mathbb{C}(z)$ be a rational function. Suppose that R(z) is holomorphic at z=0 and let its Taylor series expansion around z=0 be

$$R(z) = \sum_{n=0}^{\infty} c_n z^n.$$

Then the set of indices of vanishing Taylor coefficients $Z(R; z = 0) := \{n : c_n = 0\}$ can be partitioned into a finite (possibly empty) set of complete half-infinite arithmetic progressions $P(a; d)^+ := \{n : n \equiv a \pmod{d} \text{ with } n > 0\}$, for some modulus d, up to the inclusion or exclusion of a finite set.

Proof. This is a consequence of two results given in [10]. The first is a result showing that the Taylor coefficients of a rational function R(z) satisfy a linear recurrence with constant coefficients, with a converse stating that any Taylor expansion having this property is the Taylor expansion of a rational function [10, Theorem 1.5]. The second result is the recurrence sequence form of the Skolem–Mahler–Lech theorem [10, Theorem 2.1]. For a detailed proof of the latter result, see [18]. \blacksquare

Rather remarkably, the known proofs of the Skolem–Mahler–Lech theorem use p-adic methods for some suitably chosen prime p, despite this theorem statement being an assertion over the complex numbers.

At present there is no general algorithm known to effectively determine the set of zero coefficients of a rational function. There does exist an effectively computable algorithm to determine a set of arithmetic progressions satisfying the conclusion of the theorem, and in particular, there is an effectively computable algorithm to determine whether the exceptional set Z(R; z=0) is finite or infinite. Evertse, Schlickewei and Schmidt [11] establish an effective upper bound on the number of exceptional zeros in the

case where Z(R; z = 0) is finite; they do not, however, obtain a bound on the size of such zeros.

3. Backward orbits of 3x + k maps and the SML property. It is convenient to restate the conclusion of the Skolem–Mahler–Lech theorem as asserting a general property of sequences.

DEFINITION 3.1. We say that a sequence $\{c_n : n \geq 0\}$ of complex numbers has the *SML property* if the set $\{n \geq 0 : c_n = 0\}$ can be partitioned into a finite set of half-infinite arithmetic progressions

(3.1)
$$P^{+}(a;d) := \{n : n \equiv a \pmod{d} \text{ with } n > 0\}$$

plus or minus a finite set (possibly the empty set).

Proof of Theorem 1.1. We set $\mathcal{O} := \mathcal{S} \cap \mathbb{N}^+ = (\bigcup_{i=1}^{\ell} \mathcal{O}_k^-(m_i)) \cap \mathbb{N}^+$. By the remark just before Theorem 1.1, we may assume without loss of generality that the $\mathcal{O}_k^-(m_i)$ are pairwise disjoint sets.

Suppose first that property (2) holds. Then letting the members of X be the least nonnegative residues in the congruence classes modulo |k| we may write

$$g(z) := \sum_{n \in \mathcal{O}} z^n = \sum_{j=0}^{k_0 - 1} a_i z^j + \sum_{j \in X} \frac{z^{k_0 + j}}{1 - z^{|k|}},$$

which certifies that g(z) is a rational function, so property (1) holds.

Suppose next that property (1) holds. Then by hypothesis

$$g(z) = \sum_{j=1}^{\ell} f_{k,m_j}(z) = \sum_{n=1}^{\infty} c_n z^n$$

is a rational function, so the Skolem–Mahler–Lech theorem applies to show that

$$S := \{m : c_m = 0\} := \mathbb{N}^+ \setminus \mathcal{O}$$

has the SML property, i.e. its members are eventually periodic modulo some finite modulus $d \ge 1$:

(3.2)
$$n \in S \implies n + d \in S \text{ for all } n \ge n_0(d).$$

That is, S coincides with the set union of a finite set of complete arithmetic progressions

(3.3)
$$P(a_i; d) := \{ n \ge 1 : n \equiv a_i \pmod{d} \},$$

up to the inclusion or exclusion of a finite set of exceptional values.

We call a modulus d admissible for a set $S' \subseteq \mathbb{N}^+$ if it has the eventual periodicity property (3.2). Note that d is admissible for S' if and only if d is admissible for its complement $(S')^c := \mathbb{N}^+ \setminus S'$. Most sets $S' \subset \mathbb{N}^+$ have no

admissible modulus, but we now know that the S above does have one, and here $S^c = \mathbb{N}^+ \setminus S = \mathcal{O}$.

Consider now the minimal admissible modulus d for S. For this value we have a partition of all residue classes modulo d as $X \cup Y$, defined by

$$X := \{i \pmod{d} : P(i; d) \cap S \text{ is finite}\},$$

$$Y := \{i \pmod{d} : P(i; d) \cap S^c \text{ is finite}\}.$$

In particular, a coset $j \pmod{d}$ contains infinitely many elements of \mathcal{O} if and only if this coset belongs to X; and then all but finitely many $j \pmod{d}$ belong to \mathcal{O} .

Claim 1. The minimal admissible modulus d for S is odd.

Proof. Suppose to the contrary that d = 2d' were even. By minimality there must exist a residue class $i \pmod{d}$ such that $i \pmod{d} \in X$ while $i + d' \pmod{d} \in Y$.

We assert that $2i \pmod{d} \in X$. Pick a modulus m_j such that there are infinitely many inverse iterates of m in the class $i \pmod{d}$. Now if $n \in \mathcal{O}_k^-(m_j)$ then $2n \in \mathcal{O}_k^-(m_j)$. This gives infinitely many elements of \mathcal{O} in $2i \pmod{d}$, whence this residue class is in X. We conclude that all sufficiently large members of P(2i;d) belong to X.

However

$$T_k(2i + dn) = T_k(2(i + d'n)) = i + d'n,$$

hence half of the elements of P(2i;d), those with n odd, arise as preimages under T_k of the residue class P(i+d';d). Since all sufficiently large elements of \mathcal{O} are the preimage under T_k of some other element of \mathcal{O} , we conclude that infinitely many elements of \mathcal{O} fall into the class $i+d' \pmod{d}$, whence this class also belongs to X. But this contradicts the hypothesis that this class belonged to Y, and Claim 1 follows. \blacksquare

Claim 2. The minimal admissible modulus d for S is not divisible by 3.

Proof. Suppose to the contrary that d = 3d' were divisible by 3. Then there must exist a residue class $i \pmod{d} \in X$, with at least one of $i + d' \pmod{d}$ and $i + 2d' \pmod{d}$ in Y. By Claim 1, d is odd, so by replacing i by i + d if necessary we may assume that i is odd. The residue class $i \pmod{d}$ in X contains all sufficiently large elements of the form n = i + 2dn', and since these are in \mathcal{O} and are odd numbers, with at most ℓ exceptions we have

$$T_k(n) = \frac{3i+k}{2} + 3dn' \in \mathcal{O}.$$

This construction exhibits infinitely many numbers $\frac{3i+k}{2} \pmod{d}$ in \mathcal{O} , so

it follows that $\frac{3i+k}{2} \pmod{d}$ belongs to X. In a similar fashion one has

$$T_k(i+2d'+2dn') = \frac{3i+k}{2} + d'(3n'+1) \subset P\left(\frac{3i+k}{2};d\right)$$

and also

$$T_k(i+d'+(d+2dn')) = \frac{3i+k}{2} + d'(3n'+2) \subset P\left(\frac{3i+k}{2};d\right).$$

Thus each residue class $i+d' \pmod d$ and $i+2d' \pmod d$ contains infinitely many elements of \mathcal{O} , so both these residue classes must belong to X. This contradicts the fact that one of these classes is in Y, and Claim 2 follows.

Claim 3. The modulus d = |k| is an admissible modulus for S.

Proof. We have (|k|, 6) = 1. Since we now know the minimum admissible modulus d for S has (d, 6) = 1, by splitting into smaller residue classes as necessary we may obtain an admissible modulus d' such that |k| divides d', and (d', 6) = 1. We now redefine $d \ge 1$ to be the minimal admissible modulus having the property that |k| divides d. The claim asserts that d = |k|.

Since (d, 6) = 1, both 2 and 3 are invertible modulo d. By applying forward iteration, since $n \in \mathcal{O}_k^-(m_j)$ implies $T_k(n) \in \mathcal{O}_k^-(m_j)$ with at most one exception, and since each residue class modulo d contains infinitely many even integers and infinitely many odd integers, we conclude that

$$i \pmod{d} \in X \implies \frac{i}{2} \pmod{d} \in X.$$

Since each congruence class modulo d contains infinitely many odd numbers, we also have

$$i \pmod{d} \in X \implies \frac{3i+k}{2} \pmod{d} \in X.$$

By applying a single step of backward iteration of T_k , and observing that each residue class modulo d contains infinitely many integers in each residue class modulo 6, we obtain

$$i \pmod{d} \in X \implies 2i \pmod{d} \in X,$$

 $i \pmod{d} \in X \implies \frac{2i-k}{3} \pmod{d} \in X.$

These results show that the set of residue classes (mod d) in X is closed under the action of the transfomations $S_1(r) = 2r$ and $S_2(r) = \frac{3r+k}{2}$, as well as under their inverses $(S_1)^{-1}(r) = \frac{r}{2}$ and $(S_2)^{-1}(r) = \frac{2r-k}{3}$. Now set $S_3(r) := S_1 \circ S_2(r) = 3r + k$, with inverse map $(S_3)^{-1}(r) = \frac{r-k}{3}$. One calculates the commutator map

$$S_1S_3(S_1)^{-1}(S_3)^{-1}(r) = r + k$$
 and $S_3S_1(S_3)^{-1}(S_1)^{-1}(r) = r - k$.

We deduce that for all sufficiently large members of X,

$$n \in X \implies n + |k| \in X.$$

This fact shows that we may choose the modulus d = |k|, proving Claim 3.

Claim 3 implies that d is admissible for $\mathbb{N}^+ \setminus S = \mathcal{O}$, so property (2) holds.

We have shown properties (1) and (2) are equivalent. If property (1) holds then Claim 3 shows that the set of residue classes in $X \pmod{|k|}$ is invariant under the action of the maps $x \mapsto 2x$ and $x \mapsto 3x + k \equiv 3x \pmod{|k|}$. Since (|k|, 6) = 1, these maps are invertible, whence it follows that the complementary set Y of residues modulo |k| is invariant under these maps as well.

This completes the proof of Theorem 1.1.

4. Natural boundaries for backward orbits of the $3x \pm 1$ functions. We use Theorem 1.1 to show the existence of natural boundaries for the generating functions of most backward orbits for the $3x \pm 1$ functions, as stated in Theorems 1.2 and 1.3.

Proof of Theorem 1.2. By the Pólya–Carlson theorem, for $\mathcal{O}_1^-(m)$ the associated generating function $f_{1,m}(z)$ will have $\{|z|=1\}$ as a natural boundary if and only if $f_{1,m}(z)$ is not a rational function. By Theorem 1.1, the orbit generating function $f_{1,m}(z)$ will be a rational function if and only if the backward orbit $\mathcal{O}_1^-(m)$ is eventually periodic modulo 1, i.e. it contains all sufficiently large integers n. Thus to show a particular backward orbit $\mathcal{O}_1^-(m)$ for $m \geq 1$ has a generating function $f_{1,m}(z)$ that is not a rational function, it suffices to show there is another backward orbit $\mathcal{O}_1^-(m')$ disjoint from it for some $m' \geq 1$. We treat two cases, which between them establish assertions (1) and (2).

CASE 1: The 3x+1 Conjecture is false. In this case there exists a backward orbit $\mathcal{O}_1^-(m')$ of positive integers disjoint from $\mathcal{O}_1^-(1)$, and both these orbits are infinite. Then for each $m \geq 1$ the function $f_{1,m}(z)$ is not a rational function of z, since the backward orbit $\mathcal{O}_1^-(m)$ must be disjoint from at least one of the orbits $\mathcal{O}_1^-(1)$ or $\mathcal{O}_1^-(m')$, preventing eventual periodicity modulo 1.

Case 2: The 3x + 1 Conjecture is true. In this case, for m = 1, 2, 4, 8 we have

$$f_{1,m}(z) = \left(\sum_{n=1}^{\infty} z^n\right) - p_m(z) = \frac{z}{1-z} - p_m(z),$$

in which $p_m(z) = 0, z, z + z^2$ and $z + z^2 + z^4$ respectively, so these $f_{1,m}(z)$ are rational functions. All remaining $m \in \mathbb{N}^+ \setminus \{1, 2, 4, 8\}$ necessarily belong

to one of the two backward orbits $m \in \mathcal{O}_1^-(5)$ or $m \in \mathcal{O}_1^-(16)$, which are infinite and disjoint. It follows that the elements of $\mathcal{O}_1^-(m)$ for such m are not eventually periodic modulo 1, whence the contrapositive of Theorem 1.1 implies $f_{1,m}(z)$ is not a rational function.

Proof of Theorem 1.3. For the 3x-1 function, it is known that $\mathcal{O}_{-1}^-(1)$, $\mathcal{O}_{-1}^-(5)$ and $\mathcal{O}_{-1}^-(17)$ are infinite disjoint sets. It follows that for any $m \geq 1$, the elements in the backward orbit $\mathcal{O}_{-1}^-(m)$ cannot be eventually periodic modulo 1. The contrapositive of Theorem 1.1 for k=-1 implies that $f_{-1,m}(z)$ is not a rational function. By the Pólya–Carlson theorem it then must have the unit circle $\{|z|=1\}$ as a natural boundary to analytic continuation. \blacksquare

5. Natural boundaries for backward orbits of the 3x + k functions. We first discuss additional complexity in the iteration of general 3x + k maps compared with the $3x \pm 1$ maps, and then prove Theorem 1.4.

The behavior of general 3x + k maps under iteration exhibits three features not occurring for the $3x \pm 1$ maps. The first of these features is that the larger domain \mathbb{Z} splits into various bi-invariant sets for T_k . To describe it, we denote a complete (two-sided) arithmetic progression in \mathbb{Z} by

(5.1)
$$P^{\pm}(a;d) := \{n \in \mathbb{Z} : n \equiv a \pmod{|d|}\};$$
 compare with (3.3).

LEMMA 5.1. For $k \equiv \pm 1 \pmod{6}$, the congruence classes modulo |k| partition into minimal invariant sets under the action of the finite group G(2,3) generated by multiplication by 2 and by 3 acting on the multiplicative semigroup $(\mathbb{Z}/k\mathbb{Z}, \times)$. For $1 \leq a \leq |k|$, all of the sets

$$X_{a,k} := \bigcup_{i,j>1} P^{\pm}(2^i 3^j a; |k|)$$

in \mathbb{Z} are forward-invariant and backward-invariant sets under the map T_k , that project modulo |k| onto a set invariant under G(2,3) in $(\mathbb{Z}/k\mathbb{Z},\times)$.

Proof. Because of (|k|, 6) = 1, the two transformations acting on the finite group $\mathbb{Z}/k\mathbb{Z}$ given by $S_1(r) = 2r$ and $S_2(r) = (3r + k)/2$ are invertible, and so generate a group. The proof of Claim 3 above shows that this group is also generated by $S_1(r) = 2r$ and $S_3(r) = 3r$. The projections on $\mathbb{Z}/k\mathbb{Z}$ of the sets $X_{a,k}$ are minimal sets closed under the action of these latter two generators. The forward and backward invariance of these sets immediately follows from this fact. ■

The second additional feature of general 3x + k maps is that for positive divisors d of k, each of the sets

$$S_{d,k} := \bigcup_{a:(a,|k|)=d} P^{\pm}(a;|k|)$$

is bi-invariant for T_k , and is a disjoint union of classes $X_{a,k}$. Furthermore, the map M_d of multiplication by d has

$$M_d(S_{1,k/d}) = S_{d,k}.$$

It defines a conjugacy map between $T_{k/d}$ and T_k restricted to these invariant sets, i.e.

$$M_{k/d}T_{k/d}(n) = T_k M_{k/d}(n)$$
 for all $n \in S_{1,k/d}$.

This conjugacy also applies at the level of the smaller bi-invariant sets $X_{a,k}$, for if (a,k)=d then

$$M_d(X_{a/d,k/d}) = X_{a,k}.$$

The third additional feature is that 3x + k maps may contain backward orbits that have infinite intersection with both \mathbb{N}^+ and with the negative integers \mathbb{N}^- . As an example of a backward orbit unbounded for positive and negative integers, take any k > 0 with $k \equiv 5 \pmod{6}$ and the backward orbit $\mathcal{O}_k^-(1)$. We have $\frac{2-k}{3} \in \mathcal{O}_k^-(1)$, hence

$$\{(2-k)2^j, 2^j : j \ge 1\} \cup \{2^j : j \ge 1\} \subset \mathcal{O}_k^-(1).$$

There are only finitely many such exceptional orbits, and each of them contains an odd integer in the "critical interval" [-k, -1].

Proof of Theorem 1.4. We treat separately the action of T_k on each biinvariant subset $X_{a,k}$ of $\mathbb Z$ given by Lemma 5.1. There are finitely many such subsets, so it suffices to prove for each $X_{a,k}$ that for all but finitely many $m \in X_{a,k}$ with $m \geq 1$, the generating function $f_{k,m}(z)$ has $\{|z|=1\}$ as a natural boundary. By the Pólya-Carlson theorem this is equivalent to the assertion that $f_{k,m}(z)$ is a rational function for only finitely many $m \in X_{a,k}$ with $m \geq 1$. (Here the condition $m \geq 1$ must be imposed in the hypothesis of Theorem 1.4 because there always exist infinitely many negative m with $\mathcal{O}_k^-(m) \subset \mathbb{N}^-$, whence $f_{k,m}(z) = 0$ is a rational function.)

Now suppose that $m \in X_{a,k} \cap \mathbb{N}^+$ is such that $f_{k,m}(z)$ is a rational function. Then by criterion (2) of Theorem 1.2, the backward orbit $\mathcal{O}_k^-(m)$ (which is infinite) must contain all sufficiently large positive integers in $X_{a,k}$. However a backward orbit $\mathcal{O}_k^-(m)$ cannot have this property whenever there exists another $m' \in X_{a,k} \cap \mathbb{N}^+$ such that $\mathcal{O}_k^-(m')$ is disjoint from $\mathcal{O}_k^-(m)$. Since all backward orbits on positive integers are infinite, the finitely many elements $(X_{a,k} \cap \mathbb{N}^+) \setminus \mathcal{O}_k^-(m)$ must by trichotomy have backward orbits intersecting $\mathcal{O}_k^-(m)$, and therefore containing it. By replacing m with such an element, we may enlarge the backward orbit, and thus in a finite number

of steps arrive at a single positive element m' whose backward orbit $\mathcal{O}_k^-(m)$ contains all of $X_{a,k} \cap \mathbb{N}^+$. We now study this backward orbit; note that it may contain some negative integers. There are two cases to consider.

CASE 1: The backward orbit $\mathcal{O}^-(m')$ is a tree. This tree must necessarily branch at a lowest point where both subtrees at the branch contain infinitely many positive integers, otherwise its density on the positive integers in $X_{a,k}$ would be zero, contradicting that it covers all positive integers in $X_{a,k}$. That is, there can be at most a finite number of branchings where only one of the two branch subtrees contains positive integers. Go to the lowest such branching where both subtrees have positive integers, hence infinitely many such integers. Let m_1 and m_2 be the lowest nodes in these two subtrees. Now $\mathcal{O}_k^-(m_1)$ and $\mathcal{O}_k^-(m_2)$ cover all but finitely many elements of $X_{a,k} \cap \mathbb{N}^+$ and each certifies that all nodes in the other have backward orbit generating functions having $\{|z|=1\}$ as a natural boundary.

Case 2: The backward orbit $\mathcal{O}^-(m')$ contains a periodic orbit. In this case m' itself must be in the periodic orbit, and $\mathcal{O}^-(m')$ consists of this periodic orbit plus a finite number of trees that enter it under forward iteration. Let m_1, \ldots, m_k denote the lowest node in each such tree that does not belong to the periodic orbit. If there are more than two such trees containing a positive element, then together they certify that all positive elements m'' in all these trees have generating functions $f_{k,m''}(z)$ having $\{|z|=1\}$ as a natural boundary. In this case only the elements of the periodic orbit itself have $f_{k,m''}(z)$ being a rational function. If, however, there is exactly one tree entering the periodic orbit, then we must go backward to the first branching node in this tree such that both subtrees contain positive elements, and repeat the argument of Case 1. This latter situation will occur for the 3x+1 function if the 3x+1 Conjecture is true, with m'=1 in that case. \blacksquare

- 6. Existence of finite backward orbits covering almost all positive integers. Standard conjectures for the 3x + k problem on the integers when (k, 6) = 1 (see [15]) assert that the following hold:
 - (i) (Finite Cycles Conjecture) There are only finitely many periodic orbits of T_k on the integers \mathbb{Z} .
 - (ii) (Divergent Trajectories Conjecture) There are no divergent trajectories of T_k , i.e. for no integer m is its forward orbit $\mathcal{O}_k^+(m)$ of infinite cardinality.

The first conjecture follows from the Finite Primitive Cycles Conjecture made in [15], taken over all the divisors of k. The second conjecture is a generalization of the Divergent Trajectories Conjecture given for the 3x + 1

problem in [14, Sect. 2.7]; the heuristic argument justifying it applies just as well to the 3x + k problem with gcd(k, 6) = 1.

We will show that these two conjectures together imply the existence of infinitely many collections of orbits satisfying hypotheses (1)–(2) of Theorem 1.1. We make some preliminary definitions.

DEFINITION 6.1. Two analytic functions f(z) and g(z) will be called rationally equivalent if their difference f(z) - g(z) is a rational function. Otherwise they are rationally inequivalent.

DEFINITION 6.2. Two collections of analytic functions $(f_1(z), \ldots, f_n(z))$ and $(g_1(z), \ldots, g_m(z))$ are called rationally equivalent if there is a one-to-one correspondence of rationally equivalent pairs $(f_i(z), g_{\sigma(i)}(z))$ where, if the sequences are of unequal length, one is padded with zeros to be the same length, and σ is a permutation of indices of that length. Otherwise the collections are rationally inequivalent.

THEOREM 6.3. Suppose that the Finite Cycles Conjecture and the Divergent Trajectories Conjecture both hold for T_k with $k \equiv \pm 1 \pmod{6}$. Then for each set X of residue classes modulo |k| that is closed under the action of the maps $r \mapsto 2r$ and $r \mapsto 3r$ acting on residue classes modulo |k|, there are infinitely many different finite collections of inverse orbit generating functions of disjoint backward orbits of the form $\{\mathcal{O}_k^-(m_i): 1 \leq i \leq \ell\}$ (with all $m_i > 0$) that are pairwise rationally inequivalent, such that:

- (1) all orbits $\mathcal{O}_k^-(m_i)$ take values only in residue classes in X;
- (2) all sufficiently large positive integers in congruence classes in X belong to their set union $S := \bigcup_{i=1}^{\ell} \mathcal{O}_k^-(m_i)$.

In each of these cases the associated generating function $g_{\mathcal{S}}(z) := \sum_{n \in \mathcal{S} \cap \mathbb{N}^+} z^n$ is a rational function.

Proof. The truth of the Divergent Trajectories Conjecture implies that each integer enters a periodic orbit under forward iteration. The truth of the Finite Cycles Conjecture predicts that there are finitely many cycles. Choose cycle generators $\{m_i : 1 \leq i \leq \ell\}$, taking m_i to be the element of smallest absolute value in each cycle, making it positive if there is a tie.

We need only consider those backward orbits $\mathcal{O}_k^-(m_i)$ that contain infinitely many positive integers, which is the same as those that contain at least one positive integer. The collection of these finite sets of backward orbits whose members m_i belong to a fixed minimal set $X_{a,k}$ in Lemma 5.1 will cover $X_{a,k} \cap \mathbb{N}^+$. They are disjoint backward orbits, and

$$\sum_{m_i \in X_{a,k}} f_{k,m_i}(z) = \sum_{n \in X_{a,k} \cap \mathbb{N}^+} x^n,$$

the right side of which is a rational function. Thus we obtain a finite sum of generating functions of elements in each $X_{a,k}$ that is a rational function.

To get infinitely many distinct such identities we trace back along their trees of inverse iterates. We note that at each node of the tree one has the set partition identity

$$\mathcal{O}^{-}(m) = \{m\} \cup \bigcup_{\{m' : T_k(m') = m\}} \mathcal{O}_k^{-}(m').$$

This identity allows us to replace the generating function of the left side element by the sum of generating functions of the right side. We may then drop the generating function of the one-element set (which is a polynomial), and we get another identity giving a sum of backward orbit generating functions equal to a rational function. Whenever a branching of the backward iterate trees occurs, we split the partition of $X_{a,k}$ into one larger set. Some of these inverse iterate trees must infinitely branch, otherwise there will not be enough elements in the inverse image to cover all elements of $X_{a,k} \cap \mathbb{N}^+$. Thus it is possible to obtain an infinite set of finite collections of backward orbit sets on $X = X_{a,k}$ for which property (2) holds, which are linearly ordered under set inclusion ("nested").

Now let \mathcal{P}_k denote the kth partition into backward orbit sets obtained this way in a nested set of partitions into inverse orbits. We may arrange that the base partition \mathcal{P}_1 contains at least two distinct backward orbits, whence its set of inverse orbit generating functions is rationally inequivalent to the single rational function

$$R(x) := \sum_{n \in X_{a,k} \cap \mathbb{N}^+} x^n,$$

in the sense of Definition 6.2. This inequivalence holds using Theorem 1.1. We see that condition (2) of that theorem does not hold for such subsets because $X_{a,k}$ is a minimal bi-invariant set closed under the action of multiplication by 2 and 3 (mod |k|) (via Lemma 5.1), and the node splitting guarantees there exist infinitely many integers that lie in each of the inverse orbits in the partition \mathcal{P}_1 . In going from \mathcal{P}_k to \mathcal{P}_{k+1} a single node is split, and one inverse orbit is replaced by two inverse orbits, and a polynomial is discarded from the right side of the identity, which is the generating function of $X_{a.k} \cap \mathbb{N}^+$ with a finite number of terms removed.

For $X_{a,k}$ it remains to show all the partitions \mathcal{P}_k give pairwise rationally inequivalent generating functions in the sense of Definition 6.2. To show this, we assert that each time a node is split we get a new collection of inverse orbits whose associated collection of generating functions \mathcal{P}_{k+1} is pairwise rationally inequivalent to each \mathcal{P}_j , $1 \leq j \leq k$, previously constructed. By the nesting property of the partitions, this rational inequivalence condition is

really equivalent to checking that any nontrivial subset of each partition \mathcal{P}_k separately does not have a generating function that is a rational function. To verify the latter property we check that condition (2) of Theorem 1.1 does not hold for the generating function attached to any strict nontrivial subset of the partition. By induction on $k \geq 1$ we really only need to check this property for those subsets of \mathcal{P}_{k+1} that contain exactly one of the two new inverse orbits formed by the splitting at a node done at time k+1. But this now holds because condition (2) of Theorem 1.1 does not hold for such subsets by exactly the same argument as used for \mathcal{P}_1 above.

Finally, the result for general residue classes $X \pmod{k}$ closed under multiplication by 2 and 3 follows by taking a set union of decompositions of the minimal clases $X_{a,k}$ contained in X.

7. Concluding remarks. We describe some related work on problems which involve generating functions with integer coefficients associated to 3x + 1 type iterations which are (or sometimes may be) rational functions.

Berg and Meinardus [4] (see also [5]) introduced a different set of generating functions for encoding information about 3x + 1 iterates which are also power series with integer coefficients. They introduced for each fixed $m \ge 1$ and for k = 1 the function

(7.1)
$$g_k^{(m)}(z) := \sum_{n=1}^{\infty} T_k^{\circ m}(n) z^n,$$

which encodes the iteration exactly m times, where the input value varies. One may call these functions mth iterate generating functions. These functions converge on the open unit disk $\{|z| < 1\}$. Berg and Meinardus [4, Theorem 2] showed that for each $m \ge 1$ these functions are rational functions of z, and determined properties of these rational functions: all of their poles fall on the circle $\{|z| = 1\}$, comprise a subset of the 2^m th roots of unity, and are at most double poles. Chamberland [8] extended their results to general $k \equiv \pm 1 \pmod{6}$, and to more general maps $(qx + k \pmod{6})$. He studied the polar part of the singularities of these rational functions in detail as m varies.

Berg and Meinardus [4] also introduced for fixed $n \ge 1$ and k = 1 the forward orbit generating functions

(7.2)
$$h_{k,n}(w) := \sum_{m=0}^{\infty} T_k^{\circ m}(n) w^m,$$

which encode the complete sequence of forward iterates of a fixed integer n. These power series have integer coefficients, but their radii of convergence are not known in general. For given T_k and starting value $n \geq 1$, if the forward orbit of n is eventually periodic then the power series for $h_{k,n}(w)$

will converge on $\{|w| < 1\}$, and $h_{k,m}(w)$ will be a rational function of w. In particular, if the 3x + 1 Conjecture is true, then all $h_{1,n}(w)$ will be rational functions. In the remaining case that the forward orbit $\mathcal{O}_k^+(n)$ is a divergent trajectory, Berg and Meinardus only assert that the radius of the disk on which the series converges must be at least $\frac{2}{3}$. One might expect that $h_{k,n}(w)$ will not be a rational function of w in this case, but justifying this expectation remains an open problem.

Finally, Berg and Meinardus [4] introduced for k=1 the bivariate generating functions

$$F_k(z, w) := \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} T_k^{\circ m}(n) z^n w^m.$$

They gave a system of functional equations which this generating function satisfies (see [4, Theorem 4]). It is not known whether this function is ever a bivariate rational function.

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