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DÉPARTEMENT DE MATHÉMATIQUES
UNIVERSITÉ DE SAINT-ETIENNE
23, rue du docteur Paul Michelon
F-42023 Saint-Etienne Cedex 2, France

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The set of rational cycles for the $3x+1$ problem

by

JEFFREY C. LAGARIAS (Murray Hill, N.J.)

1. Introduction. The notorious $3x+1$ problem concerns the behavior under iteration of the $3x+1$ function

$$T(n) = \begin{cases} (3n+1)/2, & n \equiv 1 \pmod 2, \\ n/2, & n \equiv 0 \pmod 2. \end{cases} \tag{1.1}$$

The $3x+1$ *Conjecture* is the claim that, starting from any positive integer n the iterates $(n, T(n), T(T(n)), \ldots)$ eventually reach the value 1, and subsequently run through the cycle $\{1, 2\}$ of period 2. The $3x+1$ Conjecture is often attributed to L. Collatz who studied similar iteration problems (but not necessarily this one); it was certainly made by B. Thwaites [15]. The $3x+1$ Conjecture remains unproved; it has however been verified for all $n \leqslant 10^{12}$. The *Finite Cycles Conjecture* asserts that the function T has only finitely many cycles on $\boldsymbol{Z}$; it too remains unproved. The $3x+1$ Conjecture would be disproved by exhibiting a cycle on the positive integers other than $\{1, 2\}$. It is known that T has no cycles in $\boldsymbol{Z}$ of length $< 250{,}000$, except those beginning with $1, 0, -1, -5$ and -17 (see [6], [7]). These results together with much of the previous work on the $3x+1$ problem are surveyed in [10].

This paper studies properties of *rational cycles* of the $3x+1$ problem, which are cycles of the function T considered on the domain $\boldsymbol{Q}[(2)]$ of all rational numbers having an odd denominator (1). The $3x+1$ function T is well defined on $\boldsymbol{Q}[(2)]$ and, more generally, is well defined on the set of 2-adic integers $\boldsymbol{Z}_2$, into which $\boldsymbol{Q}[(2)]$ is canonically embedded (see [10]). Unlike the set of integer cycles of T, which is presumed to be finite, the set $\mathscr{C}$ of all elements of $\boldsymbol{Q}[(2)]$ in cycles of T is large and well-behaved. Cycles of period n can be indexed by the n residue classes (mod 2) of their iterates. In Section 2 we show that every possible such sequence (mod 2) gives rise to an element in a unique rational cycle and conversely. Theorem 2.1 shows that for each $\mathbf{v} = (v_0, \ldots, v_{n-1}) \in \{0, 1\}^n$ there is a unique $x(\mathbf{v}) \in \boldsymbol{Q}[(2)]$ with the property that $x(\mathbf{v})$ is

(1) The ring $\boldsymbol{Q}[(2)]$ is the (local) ring of fractions of $\boldsymbol{Z}$ at the prime ideal (2), so would be denoted $\boldsymbol{Z}_{(2)}$ in the notation of [2], p. 38. To avoid confusion with the 2-adic integers $\boldsymbol{Z}_2$ we adopt the notation $\boldsymbol{Q}[(2)]$.

in a rational cycle of T of period n with $T^{(i)}(x(\mathbf{v})) \equiv v_i \pmod 2$ for $1 \leqslant i \leqslant n$, and in fact

$$(1.2) \qquad x(\mathbf{v}) = \frac{\sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1}+\dots+v_{n-1}}}{2^n - 3^{v_0+\dots+v_{n-1}}}.$$

Such rationals are exactly those of the form

$$(1.3) \qquad \frac{\sum_{j=0}^{k} 3^j 2^{a(j)}}{2^n - 3^{k+1}},$$

with $n > a(0) > a(1) > \dots > a(k) \geqslant 0$. Theorem 2.1 is essentially due to Böhm and Sontacchi [4] (who however only study integer cycles), and is also proved in Gurwood [8]. (See Seifert [12] for a related result.)

The set $\mathscr{C}$ has another interpretation, in terms of the set of all elements in integer cycles of the ensemble of $3x+k$ functions

$$T_k(n) = \begin{cases} (3n+k)/2 & \text{if } n \equiv 1 \pmod 2, \\ n/2 & \text{if } n \equiv 0 \pmod 2, \end{cases}$$

with $k \geqslant 1$ and $k \equiv \pm 1 \pmod 6$. Each rational cycle of T is associated to an integer cycle of a unique such T_k by clearing denominators; all the rationals in a given rational cycle of T have this denominator k when written in lowest terms. An integer cycle of T_k obtained in this way has all integers relatively prime to k; a cycle with this property is called a *primitive cycle* of T_k. Conversely, each primitive cycle of T_k arises from a rational cycle of T, so that the elements of $\mathscr{C}$ are in one-to-one correspondence with the set of elements $\mathscr{C}$ in all primitive cycles of the set of $3x+k$ functions T_k as k varies over all positive integers with $k \equiv 1 \pmod 6$.

The main results of this paper concern how the elements of $\mathscr{C}$ are distributed among the various k. The complexity of this problem arises from the fact that the representation (1.2) for an element in a cycle of period n may not be in lowest terms, and large cancellations of common factors between the numerator and denominator of fractions (1.3) sometimes occur. Let $C_{\text{prim}}(k)$ count the number of primitive cycles of T_k and let $C_{\text{prim}}(k, y)$ count the number of such primitive cycles of period at most y. In Section 3 we give heuristic arguments for the two conjectures that for all $k \equiv \pm 1 \pmod 6$ one has:

(1) $C_{\text{prim}}(k) \geqslant 1$,
(2) $C_{\text{prim}}(k)$ is finite.

These conjectures both seem difficult. We study the more tractable function $C_{\text{prim}}(k, y)$. We show that $C_{\text{prim}}(k, \frac{5}{4}k^{1/3}) = 0$ for infinitely many k (Theorem 3.1). This implies that if $C_{\text{prim}}(k) \geqslant 1$ for such k then huge cancellations between numerator and denominator in (1.2) must occur for the numbers in the associated rational cycle of T (see Theorem 3.2). We show that there is a constant c_0 such that for any $\varepsilon > 0$ one has

$$(1.4) \qquad C_{\text{prim}}(k, (1+\varepsilon)\log k) \geqslant k^{1 - c_0/\log\log k},$$

for infinitely many k (Theorem 3.3). We also show that any positive n_0 that occurs in a primitive cycle for one T_k with $k > 0$ also occurs in a primitive cycle for infinitely many T_k (Theorem 3.4). This holds for $n_0 = 1$ and 5 and is conjectured to hold for all positive $n_0 \equiv \pm 1 \pmod 6$. Then we show that each negative n_0 is in a primitive cycle only for finitely many T_k with $k > 0$ (Theorem 3.5).

Section 4 studies certain average values for the number of primitive cycles. We consider the sums

$$\Phi(x, y) = \sum_{\substack{1 \leqslant k \leqslant x \\ k \equiv \pm 1 \pmod 6}} C_{\text{prim}}(k, y),$$

with $y = \beta \log x$ for a fixed $\beta > 0$. To estimate these sums we study the divisibility properties $(\operatorname{mod} M)$ of the 2^n numerators of the rationals (1.2) associated to all $\mathbf{v} \in \{0, 1\}^n$, i.e. of the set

$$\Sigma_n = \Big\{ \sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1}+\dots+v_{n-1}} : \mathbf{v} \in \{0, 1\}^n \Big\}.$$

Let $F(n, M)$ denote the maximum number of elements of Σ_n in any residue class $(\operatorname{mod} M)$. We prove that

$$F(n, M) < \begin{cases} n+1, & M > 3^n, \\ 2n\, 2^n/M^{\varphi}, & 1 \leqslant M \leqslant 3^n, \end{cases}$$

where $\varphi = (\log_2 3)^{-1} \doteq 0.63093$ (Theorem 4.1). We also prove a stronger estimate valid for $M = 2^{\alpha n}$ with $\alpha \leqslant \alpha_c \doteq 0.04766$:

$$(1.5) \qquad F(n, M) \leqslant 2n^4 2^n/M$$

(Theorem 4.2). This is quite close to the expected value $2^n/M$ which would occur if the elements of Σ_n were uniformly distributed in all residue classes $(\operatorname{mod} M)$. Using these bounds we show that, for any fixed $\beta \geqslant 1$,

$$\Phi(x, \beta \log x) \leqslant 4(\beta \log x)^6 x^{f(\beta) + c_0\beta/\log\log x}, \quad \text{where}$$

$$f(\beta) = \begin{cases} 1 & \text{if } 1 \leqslant \beta \leqslant \beta_c \doteq 1.050005, \\ (1-\varphi)\beta + \varphi & \text{if } \beta > \beta_c, \end{cases}$$

and c_0 is an absolute constant (Theorem 4.3). The same proof shows that

$$C_{\text{prim}}(k, \beta \log k) \leqslant 4(\beta \log k)^6 k^{f(\beta)}.$$

For $\beta \leqslant \beta_c$ this upper bound is quite close to the lower bound (1.4) attained for infinitely many k, e.g. $C_{\text{prim}}(k, 1.01 \log k) < 5k(\log k)^5$. Finally, we conjecture that there is a constant c such that for all n one has

$$F(n, M) \leqslant \begin{cases} n^c, & M \geqslant 2^n, \\ n^c 2^n/M, & 1 \leqslant M \leqslant 2^n. \end{cases}$$

It seems likely that further progress can be made on this conjecture.

I am indebted to Ralph Tamlyn for the computation of Table 3.1.

2. Rational $3x+1$ **cycles.** The $3x+1$ function T defined by (1.1) makes sense on the ring $\boldsymbol{Q}[(2)]$ of all rationals p/q such that q is odd, where one considers such rationals even or odd, according to the parity of their numerator p. Associate to any such rational x its *parity sequence* $\mathbf{b}(x) = (b_0(x), b_1(x), \dots, b_j(x), \dots)$ where

$$b_j(x) \equiv T^{(j)}(x) \pmod 2,$$

and each $b_j(x) = 0$ or 1. Call $b_n(x)$ the *n-th bit* in the parity sequence of x.

The following result shows that every periodic parity sequence corresponds to a unique $x \in \boldsymbol{Q}[(2)]$ in some rational cycle and vice versa; the proof follows that of Böhm and Sontacchi [4], Thm. 5.

THEOREM 2.1. *Given any 0-1 vector* $\mathbf{v} = (v_0, v_1, \dots, v_{n-1})$ *there is a unique* x *in* $\boldsymbol{Q}[(2)]$ *which is periodic of period n under iteration by the* $3x+1$ *function T, and whose parity sequence starts with* $\mathbf{v}$. *It is given by*

$$x = x(\mathbf{v}) = (2^n - 3^{v_0+\dots+v_{n-1}})^{-1} \sum_{j=0}^{n-1} v_j 3^{v_{j+1}+\dots+v_{n-1}} 2^j. \tag{2.1}$$

Proof. Let $U_0(x) = x/2$ and $U_1(x) = (3x+1)/2$. A necessary condition for x to be periodic of period n with parity sequence starting with $\mathbf{v}$ is that

$$x = U_{v_{n-1}}\left(U_{v_{n-2}}\left(\dots\left(U_{v_0}(x)\right)\right)\dots\right). \tag{2.2}$$

Substituting the definition of the $U_i(x)$ yields

$$x = \frac{1}{2^n}\left(3^{v_0+\dots+v_{n-1}} x + \sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1}+\dots+v_{n-1}}\right).$$

The solution $x(\mathbf{v})$ to this linear equation is (2.1), and $x(\mathbf{v})$ clearly is in $\boldsymbol{Q}[(2)]$. This shows that $x(\mathbf{v})$ *is* unique if it exists.

The main assertion of the theorem is that the solution (2.1) actually is never extraneous, i.e. when the function T is applied to $x(\mathbf{v})$ defined by (2.1) the parity sequence of $x(\mathbf{v})$ starts out with $\mathbf{v}$. To see this, note that for $y \in \boldsymbol{Q}[(2)]$ *exactly one* of $U_0(y)$ and $U_1(y)$ is in $\boldsymbol{Q}[(2)]$: if y is even then $U_0(y) \in \boldsymbol{Q}[(2)]$ and if y is odd then $U_1(y) \in \boldsymbol{Q}[(2)]$. Also if a rational $y \notin \boldsymbol{Q}[(2)]$ then both $U_0(y) \notin \boldsymbol{Q}[(2)]$ and $U_1(y) \notin \boldsymbol{Q}[(2)]$. Consequently, given any $y \in \boldsymbol{Q}[(2)]$ there is *exactly one* of the 2^n possible sequences $\mathbf{w}$ of 0-1 vectors with $U_{w_{n-1}}(\dots(U_{w_0}(y))\dots) \in \boldsymbol{Q}[(2)]$.

Now $x(\mathbf{v}) \in \boldsymbol{Q}[(2)]$ so $T^{(n)}(x(\mathbf{v})) \in \boldsymbol{Q}[(2)]$, while

$$U_{v_{n-1}}\left(U_{v_{n-2}}\left(\dots\left(U_{v_0}(x(\mathbf{v}))\right)\right)\right) \in \boldsymbol{Q}[(2)]$$

by (2.2), hence

$$T^{(n)}(x(\mathbf{v})) = U_{v_{n-1}}\left(U_{v_{n-2}}\left(\dots\left(U_0(x(\mathbf{v}))\right)\right)\dots\right) = x(\mathbf{v}),$$

as required. ∎

This result has two interesting corollaries.

COROLLARY 2.1a. *For fixed k, the integers given by*

$$\sum_{i=0}^{k} 2^{a_i} 3^i, \quad a_0 > a_1 > \dots > a_k \geqslant 0, \tag{2.3}$$

are all distinct.

Proof. Suppose not, and that $\sum_{i=0}^{k} 2^{a_i} 3^i = \sum_{i=0}^{k} 2^{b_i} 3^i$. Take $n = \max(a_0, b_0)+1$. Define the parity vectors $\mathbf{v} = (v_0, \dots, v_{n-1})$, $\mathbf{w} = (w_0, \dots, w_{n-1})$ with $v_{a_i} = 1$ and all other $v_j = 0$, $w_{b_i} = 1$ and all other $w_j = 0$. Then

$$x(\mathbf{v}) = (2^n - 3^k)^{-1} \sum_{i=0}^{k} 2^{a_i} 3^i, \quad x(\mathbf{w}) = (2^n - 3^k)^{-1} \sum_{i=0}^{k} 2^{b_i} 3^i,$$

hence $x(\mathbf{v}) = x(\mathbf{w}) = x$, say. The parity sequences of x must start with both $\mathbf{v}$ and $\mathbf{w}$ by Theorem 2.1, so that $\mathbf{v} = \mathbf{w}$, contradicting $(a_0, \dots, a_k) \neq (b_0, \dots, b_k)$. ∎

Corollary 2.1a has a simple direct proof due to Don Coppersmith. If $B = \sum_{i=0}^{k} 2^{a_i} 3^i$ satisfies (2.3) for a fixed k, then 2^{a_k} is the highest power of 2 dividing B. This determines a_k, so one obtains

$$B' = B - 2^{a_k} 3^k = \sum_{i=0}^{k-1} 2^{a_i} 3^i.$$

Now a_{k-1} is determined similarly as the largest power of 2 dividing B', and proceeding recursively one can recover all of the a_i, thus proving uniqueness of the representation (2.3).

The assertion of Corollary 2.1a is no longer true if one allows integers (2.3) with different k, e.g.

$$2^4 + 3 = 2^2 + 2 \cdot 3 + 3^2 = 19.$$

A parity sequence is said to be *aperiodic* if it is not eventually periodic. A trajectory $(x, T(x), \dots, T^{(k)}(x), \dots)$ for the $3x+1$ function on $\boldsymbol{Q}[(2)]$ is *divergent* if $\lim_{k\to\infty} |T^{(k)}(x)| = \infty$. It is easily checked that any trajectory is either eventually periodic or divergent. Several authors have conjectured that no divergent trajectories exist (see [10]).

COROLLARY 2.1b. *Any divergent trajectory must have an aperiodic parity sequence.*

Proof. We use the fact proved in [10] that the mapping from $\boldsymbol{Q}[(2)]$ that sends x to its parity sequence $\mathbf{b}(x)$ is one-to-one. (This was proved more generally for all x in the 2-adic integers $\boldsymbol{Z}_2$.) Suppose the corollary were false, and that y gives a counterexample. By iterating y if necessary we may assume that it has a divergent trajectory with a purely periodic bit sequence. Suppose that this bit sequence has period $\mathbf{v}$. Then $x(\mathbf{v})$ given by Theorem 2.1 has the same bit sequence, and $x(\mathbf{v})$ has a purely periodic trajectory under T so $x(\mathbf{v}) \neq y$. This contradicts the map $\mathbf{b}(\cdot)$ being one-to-one. ∎

It is an easy matter to count the number of cycles of a given length. Call a 0-1 vector $\mathbf{v} = (v_0, \ldots, v_{n-1})$ *reducible* if $\mathbf{v} = \mathbf{w}^j$ for some $j \geqslant 2$, where $\mathbf{w}^j$ denotes the concatenation of j copies of $\mathbf{w}$; otherwise call it *irreducible*. A vector $\mathbf{v}$ is irreducible if and only if its n cyclic permutations $\sigma_k(\mathbf{v}) = (v_k, v_{k+1}, \ldots, v_{n-1}, v_0, \ldots, v_{k-1})$ are all distinct. An *irreducible cycle* of length n corresponds to a set of n cyclic permutations of an irreducible vector $\mathbf{v}$ of length n. Let $I(n)$ denote the number of irreducible cycles of length n. Using the action of the group of cyclic permutations on the set $\{0, 1\}^n$ one has

$$\sum_{d \mid n} d I(d) = 2^n. \tag{2.4}$$

Möbius inversion gives

$$I(n) = \frac{1}{n} \sum_{d \mid n} \mu(d) 2^{n/d}, \tag{2.5}$$

where $\mu(d)$ is the Möbius function. From this formula one easily deduces that

$$I(n) = \frac{1}{n} 2^n + O(2^{n/2}). \tag{2.6}$$

Small values of $I(n)$ are given in Table 2.1.

Table 2.1
Number of irreducible cycles $I(n)$.

n	$I(n)$	n	$I(n)$
1	2	11	186
2	1	12	335
3	2	13	630
4	3	14	1161
5	6	15	2182
6	9	16	4080
7	18	17	7710
8	30	18	14532
9	56	19	27594
10	99	20	52377

Table 2.2 gives the lexicographically largest member $\mathbf{v}$ of each irreducible cycle of length $n \leqslant 6$, and the corresponding values $x(\mathbf{v})$.

Table 2.2
Members of irreducible cycles ($n \leqslant 6$)

	$\mathbf{v}$	$x(\mathbf{v})$		$\mathbf{v}$	$x(\mathbf{v})$
$n=1$:	1	-1	$n=6$:	111110	$-\frac{211}{179}$
	0	0		111100	$-\frac{65}{17}$
				111010	$-\frac{73}{17}$
$n=2$:	10	1		111000	$\frac{19}{37}$
				110100	$\frac{23}{37}$
$n=3$:	110	-5		110010	$\frac{31}{37}$
	100	$\frac{1}{5}$		110000	$\frac{1}{11}$
				101000	$\frac{7}{55}$
$n=4$:	1110	$-\frac{19}{11}$		100000	$\frac{1}{61}$
	1100	$\frac{5}{7}$			
	1000	$\frac{1}{13}$			
$n=5$:	11110	$-\frac{65}{49}$			
	11100	$\frac{19}{5}$			
	11010	$\frac{23}{5}$			
	11000	$\frac{5}{23}$			
	10100	$\frac{7}{23}$			
	10000	$\frac{1}{29}$			

Since the $3x+1$ function T does not change the denominator of any rational $x \in \boldsymbol{Q}[(2)]$ to which it is applied, it is clear that all rationals in a $3x+1$ cycle of period n written in lowest terms have the same denominator, which we call the *denominator* $\delta(\mathbf{v})$ of a cycle including $x(\mathbf{v})$. Clearly

$$\delta(\mathbf{v}) = \frac{D(\mathbf{v})}{(N(\mathbf{v}), D(\mathbf{v}))},$$

where

$$D(\mathbf{v}) = 2^n - 3^{v_0 + \ldots + v_{n-1}}, \tag{2.7a}$$

$$N(\mathbf{v}) = \sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1} + \ldots + v_{n-1}} \tag{2.7b}$$

are the denominator and numerator of the fraction (2.1) before it is reduced to lowest terms. Table 2.2 includes one example $\mathbf{v} = 110000$ having $D(\mathbf{v}) \neq \delta(\mathbf{v})$, with $D(\mathbf{v}) = 55$, $\delta(\mathbf{v}) = 11$.

3. Primitive $3x+k$ cycles. The $3x+k$ function T_k is defined for $k \equiv 1 \pmod 2$ by

$$T_k(n) = \begin{cases} (3n+k)/2, & n \equiv 1 \pmod 2, \\ n/2, & n \equiv 0 \pmod 2. \end{cases} \tag{3.1}$$

A rational cycle for the $3x+1$ problem with denominator k gives rise to an integral cycle for the $3x+k$ function obtained by clearing the denominator k. Since the denominator $D(\mathbf{v})$ of a rational cycle $x(\mathbf{v})$ of T_1 has $(D(\mathbf{v}), 6) = 1$, we always have $k \equiv \pm 1 \pmod 6$ in this correspondence. Conversely, all integral cycles of all $3x+k$ functions with $k \equiv \pm 1 \pmod 6$ arise in this fashion from rational $3x+1$ cycles.

Note that T_{-k} and T_k are essentially the same function because $T_k(n) = T_{-k}(-n)$, so we suppose $k \geqslant 1$ in what follows.

The map T_k sends $\mathbf{Z}$ to $\mathbf{Z}$; more generally define for $d|k$ the set $\mathbf{Z}(d, k) = \{n: (n, k) = d\}$ and observe that T_k maps $\mathbf{Z}(d, k)$ into $\mathbf{Z}(d, k)$. The action of T_k on $\mathbf{Z}(d, k)$ is the same as the action of $T_{k/d}$ on $\mathbf{Z}(1, k/d)$ up to a multiplicative scale factor. For this reason we study the action of T_k on the domain $\mathbf{Z}(1, k)$, which we call the set of *primitive integers* (mod k). A cycle of T_k on $\mathbf{Z}(1, k)$ is called a *primitive cycle* (mod k). (Minimal invariant sets of residue classes (mod N) for a class of functions generalizing T_k are studied by Matthews and Watts [11] and Buttsworth and Matthews [5].)

The discussion so far describes a bijection between the set $\mathscr{C}$ of elements of $\mathbf{Q}[(2)]$ in some cycle of the $3x+1$ function T_1 and the set $\bar{\mathscr{C}}$ of all members of primitive cycles of some T_k with $k > 0$ and $k \equiv \pm 1 \pmod 6$. In the remainder of this section we shall therefore suppose that $k > 0$ and $k \equiv \pm 1 \pmod 6$.

3.1. *Two conjectures about primitive cycles.* Let $C_{\text{prim}}(k)$ count the number of primitive cycles of T_k, and let $C_{\text{prim}}(k, y)$ be the somewhat more tractable function that counts the number of primitive cycles of T_k of period $\leqslant y$. One expects that the behavior of iterates of T_k on $\mathbf{Z}(1, k)$ will be qualitatively similar to that of the $3x+1$ function T_1 on $\mathbf{Z}$. A heuristic argument similar to that in [10], Sec. 2.1, suggests that (averaged over a long series of iterates) $T_k(n)$ is about $(\frac{3}{4})^{1/2} n$. One then expects that no trajectory can diverge to infinity, hence every trajectory becomes eventually periodic. This leads to the following conjecture.

Primitive Cycles Existence Conjecture. *For each* $k \equiv \pm 1 \pmod 6$ *the* $3x+k$ *function* T_k *has a primitive cycle, i.e.* $C_{\text{prim}}(k) \geqslant 1$.

This conjecture seems difficult, if not intractable, for reasons indicated in Section 3.2.

How many primitive cycles are there for a fixed k? The following conjecture is an extension of one made for the $3x+1$ problem.

Finite Primitive Cycles Conjecture. *For each* $k \equiv \pm 1 \pmod 6$, *one has* $C_{\text{prim}}(k) < \infty$.

Some evidence for this conjecture, in the case $k = 1$, is that T_1 has 5 small cycles and no other cycles of length $< 250{,}000$ (see [6], [7], [10]). A heuristic argument supporting this conjecture is described in Section 3.6. At present it also seems an intractably hard problem.

3.2. *Existence of primitive cycles.* To gain insight into the Primitive Cycles Existence Conjecture, we examine numerical evidence. Table 3.1 gives for $k \leqslant 150$ the smallest positive n_0 such that n_0 is in a primitive cycle of T_k, and gives the period length of that cycle. (This need *not* be the shortest primitive cycle of T_k.) Table 3.1 includes a number of examples of cycles $\mathbf{v}$ of T_k of minimal period approximately k, e.g. $k = 85, 107, 139$. The rational $x(\mathbf{v})$ given by (3.1) for such a cycle has a denominator $D(\mathbf{v}) = 2^n - 3^l$ for some l before being reduced to lowest terms, while in lowest terms the denominator $\delta(\mathbf{v}) = k$. It is apparent that the unreduced denominator $D(\mathbf{v})$ must be of size at least the minimum of $|2^n - 3^l|$ for $0 \leqslant l \leqslant n$, and for $n = 85, 107, 139$ this is at least $\frac{1}{3} \cdot 2^n$. Consequently, there must be a cancellation of a huge common factor from the denominator $D(\mathbf{v})$ and numerator $N(\mathbf{v})$ of $x(\mathbf{v})$ in these examples.

Table 3.1

Minimal positive cycles for the $3x+k$ problem ($k \leqslant 150$)

k	n_0	cycle length	k	n_0	cycle length
1	1	2	77	1	38
5	1	3	79	1	44
7	5	4	83	65	24
11	1	6	85	7	100
13	1	4	89	17	17
17	1	7	91	1	48
19	5	11	95	1	72
23	5	5	97	1	18
25	7	16	101	7	14
29	1	5	103	5	21
31	13	23	107	1	106
35	7	3	109	19	52
37	19	6	113	1	29
41	1	20	115	13	27
43	1	11	119	1	75
47	5	18	121	5	44
49	25	38	125	1	7
53	103	29	127	1	37
55	1	12	131	13	26
59	1	28	133	11	36
61	1	6	137	1	14
65	19	24	139	11	136
67	17	30	143	7	140
71	29	10	145	1	10
73	19	60	149	19	59

We show below that in order for the Primitive Cycles Existence Conjecture to be true, the cancellation of huge common factors $(N(\mathbf{v}), D(\mathbf{v}))$ must occur for infinitely many k. It is this property that makes the Primitive Cycles Existence Conjecture appear difficult.

We first show there exist infinitely many k for which T_k has no short primitive cycle.

THEOREM 3.1. *There exist infinitely many* $k \equiv \pm 1 \pmod 6$ *such that* T_k *has no primitive cycle of period* $\leqslant \frac{5}{4}k^{1/3}$, *i.e.* $C_{\text{prim}}(k, \frac{5}{4}k^{1/3}) = 0$.

Proof. If $\mathbf{v}$ is a primitive cycle of period n of T_k then the rational number $x(\mathbf{v})$ expressed in lowest terms has denominator k. Hence k divides $D(\mathbf{v}) = 2^n - 3^l$ where $1 \leqslant l \leqslant n$. Consider

$$S(t) = \prod_{n=1}^{t} \prod_{l=1}^{n} |2^n - 3^l|.$$

It is easy to see that $S(t) \leqslant 3^{t(t+1)(2t+1)/6}$. Now if all T_l for $k_0 \leqslant l \leqslant k$ have a primitive cycle of length $\leqslant t$ then the least common multiple $[k_0, k]$ of k_0 through k must divide $S(t)$. It is well known (and equivalent to the prime number theorem) that

$$\log[1, k] = k + o(k),$$

as $k \to \infty$ ([9], Theorem 434). Also $[k_0, k] \geqslant [1, k]/[1, k_0]$, for any k_0. On choosing $t = \frac{5}{4}k^{1/3}$ one has, using the upper bound for $S(t)$, that for sufficiently large k_0,

$$\log[k_0, k] > 0.99(k - k_0) \geqslant \log S(\tfrac{5}{4}k^{1/3})$$

for $k \geqslant 5k_0$. This contradicts $[k_0, k] | S(\frac{5}{4}k^{1/3})$, and thus proves that there is at least one such k in the interval $[k_0, 5k_0]$ having no primitive cycle of length $\leqslant \frac{5}{4}k^{1/3}$. ∎

One can improve the constant $\frac{5}{4}$ in Theorem 3.1 slightly with a more careful argument.

Now we can show that huge cancellations must sometimes occur, if the Primitive Cycles Existence Conjecture is true.

THEOREM 3.2. *There exist infinitely many* $k \equiv \pm 1 \pmod 6$ *such that either* T_k *has no primitive cycle or else every primitive cycle* $\mathbf{v}$ *of* T_k *has*

$$k = \frac{D(\mathbf{v})}{(N(\mathbf{v}), D(\mathbf{v}))} \leqslant (\log D(\mathbf{v}))^3. \tag{3.2}$$

Proof. We first show $D(\mathbf{v})$ is large for all $\mathbf{v}$. A result of A. Baker and N. I. Fel'dman ([3], Theorem 3.1) on linear forms in logarithms of algebraic numbers implies that there exists an effectively computable constant $c_0 > 0$ such that for all $n \geqslant 2$

$$|n \log 2 - l \log 3| \geqslant n^{-c_0}.$$

From this it is easily shown that there exists an effectively computable constant c_1 such that for $n \geqslant 2$ one has

$$|2^n - 3^l| \geqslant \tfrac{1}{2} n^{-c_1} 2^n. \tag{3.3}$$

Now take a T_k having no primitive cycle of period $\leqslant \frac{5}{4}k^{1/3}$, which exists by Theorem 3.1. Let $\mathbf{v}$ be a primitive cycle of T_k, necessarily of period $n > \frac{5}{4}k^{1/3}$. Now

$$\log_2 D(\mathbf{v}) = \log_2 |2^n - 3^l| \geqslant n - c_1 \log_2 n - 1$$
$$\geqslant \tfrac{5}{4}k^{1/3} - O(\log k) \geqslant k^{1/3},$$

for all $k \geqslant c_2$ for some constant c_2. ∎

3.3. *Large values for* $C_{\text{prim}}(k)$. We show that $C_{\text{prim}}(k)$ takes occasional large values.

THEOREM 3.3. *There is a positive constant* c_0 *such that for any fixed* $\varepsilon' > 0$ *one has*

$$C_{\text{prim}}(k, (1+\varepsilon')\log k) > k^{1 - c_0/\log\log k} \tag{3.4}$$

for infinitely many k.

Proof. Consider the set S_n of 0-1 vectors $\mathbf{v}$ of length $2n$ containing exactly n ones. There are at least $n^{-1}\binom{2n}{n}$ distinct primitive cycles associated to such $\mathbf{v}$ (with period dividing n), and each such cycle has a denominator $\delta(\mathbf{v}) | B_n = 2^{2n} - 3^n$. Now B_n has $d(B_n)$ divisors k, and at least one of them has many primitive cycles. There exists a constant c_0 such that $d(B) \leqslant B^{c_0/\log\log B}$ for all $B > 1$ ([9], Theorem 317). Now let $C^{+}_{\text{prim}}(k, n)$ count the number of primitive cycles of T_k with period *dividing* n. Clearly $C_{\text{prim}}(k, n) \geqslant C^{+}_{\text{prim}}(k, n)$. The argument just given shows that there is some $k | B_n$ such that

$$C^{+}_{\text{prim}}(k, 2n) \geqslant \frac{1}{n}\binom{2n}{n} d(B_n)^{-1} \geqslant 2^{2n - c_0/\log\log n}. \tag{3.5}$$

Let k_n denote the smallest k such that (3.5) holds. We claim that, for any fixed $\varepsilon > 0$, $k_n \geqslant 2^{(1-\varepsilon)2n}$ for all $n \geqslant n_0(\varepsilon)$. Assuming that this claim is proved, the bound (3.4) holds with $1+\varepsilon' = (1-\varepsilon)^{-1}$ for all k_n with $n \geqslant n_0(\varepsilon')$ since $2n < (1+\varepsilon')\log k_n$. Also since $2^{2n} \geqslant k_n \geqslant 2^{(1-\varepsilon)2n}$ there are infinitely many different k_n for which (3.4) holds.

It remains to prove the claim. To do this, we use an estimate to be proved later (Theorem 4.1), which shows that the number of $\mathbf{v} \in \{0, 1\}^n$ with $M | N(\mathbf{v})$ is at most $2n^2 2^n / M^{\varphi}$, where $\varphi = (\log_2 3)^{-1}$. Now suppose $K \leqslant 2^{(1-\varepsilon)2n}$, so that for any $B = 2^{2n} - 3^l$ with $K | B$ one has $M = B/K \geqslant n^{-c_1} 2^{2\varepsilon n}$ using (3.3). Consequently, the number of $\mathbf{v} \in \{0, 1\}^n$ having $M | N(\mathbf{v})$ is at most $2n^{2+c_1} 2^{(1-\varphi\varepsilon)2n}$. Now there are $n+1$ choices of l, hence at most $n+1$ choices of M, so that

$$C^{+}_{\text{prim}}(K, 2n) \leqslant 2n^{3+c_1} 2^{(1-\varphi\varepsilon)2n}.$$

This contradicts (3.5) for all large enough n, so $k_n \nmid K$ and thus $k_n > 2^{(1-\varepsilon)2n}$, proving the claim. ∎

3.4. *Primitive cycles containing a fixed integer.* For fixed $k \equiv \pm 1 \pmod 6$ we may index primitive cycles by their smallest member n_0. This will always be an integer $n_0 \equiv \pm 1 \pmod 6$. For how many k is n_0 a member of some primitive cycle? The simplest case is $n_0 = 1$. Table 3.1 suggests the possibility that 1 is in a cycle for a positive proportion of all T_k with $k \geqslant 1$. This seems hard to prove. However, it is easy to show that 1 is in a cycle for infinitely many k. The vector $\mathbf{v} = 10^m$ has $x(\mathbf{v}) = 1/(2^m - 3)$, hence T_k for $k = 2^m - 3$ has a primitive cycle containing 1. More generally we have the following result.

THEOREM 3.4. *If a positive n_0 is in a primitive cycle for some T_k with $k > 0$, then it is in a primitive cycle for infinitely many T_k with $k > 0$. If in addition $n_0 \equiv \pm 1 \pmod 6$ then it is the smallest element in such a primitive cycle for infinitely many k.*

Proof. By hypothesis there is a 0-1 vector $\mathbf{v} = (v_0, \ldots, v_{n-1})$ such that

$$x(\mathbf{v}) = \frac{N(\mathbf{v})}{D(\mathbf{v})} = \frac{n_0}{k}$$

with $(n_0, k) = 1$ and $x(\mathbf{v}) > 0$. If $l = v_0 + \ldots + v_{n-1}$, then $D(\mathbf{v}) = 2^n - 3^l > 0$. The vectors $\mathbf{w}_m = \mathbf{v}0^m$ have $N(\mathbf{w}_m) = N(\mathbf{v})$, $D(\mathbf{w}_m) > 0$ and

$$x(\mathbf{w}_m) = \frac{N(\mathbf{w}_m)}{D(\mathbf{w}_m)} = \frac{N(\mathbf{v})}{2^{n+m} - 3^l}. \tag{3.7}$$

The rational (3.7) reduces in lowest terms to a rational with numerator n_0 whenever

$$G_m = (N(\mathbf{w}_m), D(\mathbf{w}_m)) = (N(\mathbf{v}), 2^{n+m} - 3^l)$$

has $G_m = G_0$, in which case $x(\mathbf{w}_m) = n_0/k_m$ with $k_m = (2^m - 3^l)/G_0$ and $(n_0, k_m) = 1$. The function G_m is periodic with period $p = \mathrm{ord}_{N(\mathbf{v})}(2)$, i.e. the smallest $p \geqslant 2$ with $2^p \equiv 1 \pmod{N(\mathbf{v})}$. In particular $G_m = G_0$ whenever $m \equiv 0 \pmod p$. This shows that infinitely many k_m exist with n_0 in a primitive cycle of T_{k_m}. Finally, we show that if $n_0 \equiv \pm 1 \pmod 6$ then n_0 is the smallest element in the corresponding cycle of T_{k_m} for all sufficiently large $m \equiv 0 \pmod p$. Since n_0 is odd, the first entry of $\mathbf{v}$ is 1, hence for $m \geqslant 4n$,

$$T_k(n_0) = \frac{3n_0 + k_m}{2} \geqslant \frac{k_m}{2} \geqslant \frac{2^{5n} - 2^n}{3^n - 2^n} > 2^n n_0,$$

since $n_0 \leqslant N(\mathbf{v}) \leqslant 3^n - 2^n$. Consequently

$$T_k^{(j)}(n_0) > n_0, \quad 1 \leqslant j \leqslant n.$$

Since the last m entries of $\mathbf{w}_m = \mathbf{v}0^m$ are zero,

$$T_k^{(j)}(n_0) > T_k^{(n+m)}(n_0) = n_0, \quad n+1 \leqslant j < n+m.$$

Thus n_0 is the smallest element in the cycle. ∎

As an example, $\mathbf{v} = 1^2 0^m$ has $x(\mathbf{v}) = 5/(2^m - 9)$ so $n_0 = 5$ is in a primitive cycle of T_k for $k = 2^m - 9$ provided $m \not\equiv 2 \pmod 4$.

CONJECTURE P. *Every positive $n_0 \equiv \pm 1 \pmod 6$ is in a primitive cycle of infinitely many T_k with $k > 0$ and $k \equiv \pm 1 \pmod 6$.*

Theorem 3.4 shows that to prove this conjecture it suffices to prove that each such n_0 is contained in a primitive cycle for one T_k.

The situation for negative n_0 is entirely different.

THEOREM 3.5. *Any negative n_0 is not in a primitive cycle of T_k for all $k > |n_0|$. In particular, $n_0 = -1$ is in a primitive cycle for T_1 and for no T_k with $k > 1$.*

Proof. Let $\mathbf{v}$ be a 0-1 vector with $x(\mathbf{v}) < 0$. We show

$$x(\mathbf{v}) \leqslant -1, \tag{3.8}$$

with equality if and only if $\mathbf{v} = 1^n$. Indeed, if $x(\mathbf{v}) \leqslant 0$ then $D(\mathbf{v}) = 2^n - 3^l < 0$. Now

$$N(\mathbf{v}) = \sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1} + \ldots + v_{n-1}} = \sum_{i=0}^{l-1} 3^i 2^{a(i)}$$

with $a(0) > a(1) > \ldots > a(l) \geqslant 0$. Hence

$$N(\mathbf{v}) \geqslant \sum_{i=0}^{l-1} 3^i 2^{l-i-1} = 3^l - 2^l \geqslant 3^l - 2^n = |D(\mathbf{v})|. \tag{3.9}$$

Clearly equality occurs only if $l = n$ and $\mathbf{v} = 1^n$. Consequently if $x(\mathbf{v}) = n_0/k$ in lowest terms, with $n_0 < 0$, then (3.8) implies that $1 \leqslant k \leqslant |n_0|$. ∎

In particular, Theorem 3.5 shows that the cycles starting with -1, -5 and -17 of the $3x+1$ function are in some sense "exceptional", when viewed over the set of all T_k with $k > 0$, while the cycle starting from 1 is "non-exceptional". The remaining known cycle $\{0\}$ of T_1 is common to all T_k.

3.5. *Finite Primitive Cycles Conjecture.* We describe a simple heuristic argument suggesting that $C_{\mathrm{prim}}(k) < \infty$ for all k. It is easiest to consider the case $k = 1$.

Let $\Sigma_{n,l} = \{\mathbf{v}\colon \mathbf{v} \in \{0, 1\}^n$ and $\sum_{i=0}^{n-1} v_i = l\}$. All members of $\Sigma_{n,l}$ have the same denominator $D_{n,l} = 2^n - 3^l$.

HEURISTIC HYPOTHESIS. *The numerators $\{N(\mathbf{v})\colon \mathbf{v} \in \Sigma_{n,l}\}$ considered $\pmod{D_{n,l}}$ behave as if they were random variables drawn uniformly and independently from the interval $[0, D_{n,l} - 1]$.*

Now one obtains a $\mathbf{v}$ with $k = \delta(\mathbf{v}) = 1$ if and only if $N(\mathbf{v}) \equiv 0 \pmod{D_{n,l}}$, and the heuristic hypothesis asserts that the probability of this is $|\Sigma_{n,l}|/D_{n,l}$. A key point is that in order to obtain a *primitive* cycle of length n, one must find n distinct $\mathbf{v}$ with $\delta(\mathbf{v})=1$, and using the heuristic hypothesis the probability of this is $(|\Sigma_{n,l}|/D_{n,l})^n$. We divide the set of all pairs (n, l) into two classes:

Case 1: $1 \leqslant l \leqslant \frac{3}{5}n$. In this case $D_{n,l} \geqslant 2^n - 3^{3n/5} \geqslant 2^{n-1}$ while

$$|\Sigma_{n,l}| \leqslant \binom{n}{[\frac{1}{2}n]} \leqslant \frac{1}{\sqrt{n}} 2^n.$$

Hence

$$(|\Sigma_{n,l}|/D_{n,l})^n \leqslant n^{-n/2}\, 2^n.$$

Case 2: $\frac{3}{5}n \leqslant l \leqslant n$. In this case $D_{n,l} \geqslant n^{-c_1} 2^n$ by (3.3) while

$$|\Sigma_{n,l}| \leqslant \binom{n}{[\frac{3}{5}n]} \leqslant (1.98)^n.$$

Hence

$$(|\Sigma_{n,l}|/D_{n,l})^n \leqslant (0.99)^{-n^2}.$$

Now, summing over all pairs (n, l) we see that

$$\sum_{n=1}^{\infty} \sum_{l=1}^{n} (|\Sigma_{n,l}|/D_{n,l})^n \tag{3.10}$$

converges extremely rapidly. It is this fact that suggests $C_{\mathrm{prim}}(1) < \infty$. Similar heuristic arguments suggest that $C_{\mathrm{prim}}(k) < \infty$ for all k.

How convincing is this heuristic argument? In its precise details, not very. The heuristic hypothesis is certainly false because the denominators $\delta(\mathbf{v})$ of elements in a cycle are correlated. However, the extreme rapidity of convergence of (3.10) suggests that $C_{\mathrm{prim}}(1) < \infty$ would follow from a much weaker heuristic hypothesis concerning the distribution of $\{N(\mathbf{v})\colon \mathbf{v} \in \Sigma_{n,l}\}$ (mod $D_{n,l}$). The next section gives general results on the distribution of $\{N(\mathbf{v})\colon \mathbf{v} \in \{0, 1\}^n\}$ (mod M) for artibrary moduli M, which show that the distribution is nearly uniform for $M < 2^{0.047n}$, and cannot be too non-uniform for all M.

4. Upper bounds for the number of primitive $3x+k$ **cycles.** We obtain upper bounds for the sums

$$\Phi(x, y) = \sum_{\substack{1 \leqslant k \leqslant x \\ k \equiv \pm 1 \ (\mathrm{mod}\ 6)}} C_{\mathrm{prim}}(k, y), \tag{4.1}$$

where $y = \beta \log x$ for some constant β.

The general approach to obtaining such upper bounds is to show that for most $\mathbf{v}$ the quantity $(N(\mathbf{v}), D(\mathbf{v}))$ cannot be very large. To do this we study the distribution of $\Sigma_n = \{N(\mathbf{v})\colon \mathbf{v} \in \{0, 1\}^n\}$ (mod M) for an arbitrary modulus M.

4.1. *Distribution of numerators* (mod M). We study the sets

$$\Sigma_{n,l} = \Big\{\sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1}+\dots+v_{n-1}}\colon \mathbf{v} \in \{0, 1\}^n,\ \sum_{i=0}^{n-1} v_i = l\Big\},$$

and their union

$$\Sigma_n = \bigcup_{l=0}^{n} \Sigma_{n,l} = \Big\{\sum_{j=0}^{n-1} v_j 2^j 3^{v_{j+1}+\dots+v_{n-1}}\colon \mathbf{v} \in \{0, 1\}^n\Big\}.$$

Let $F(n, M)$ count the maximum number of elements of Σ_n that occur in any congruence class (mod M). Note that the elements in each $\Sigma_{n,l}$ are all distinct by Corollary 2.1a, but those in Σ_n need not always be distinct, and in the definition of $F(n, M)$ they are to be counted with multiplicity.

How big ought $F(n, M)$ to be? If the elements of Σ_n were uniformly distributed (mod M) then about $2^n/M$ elements of Σ_n would fall in each residue class (mod M). We propose the following conjecture.

Equidistribution Conjecture. *There exists an absolute constant c such that if* $(M, 6) = 1$ *then*

$$F(n, M) \leqslant \begin{cases} n^c, & M > 2^n, \quad (4.2a)\\ n^c 2^n/M, & M \leqslant 2^n. \quad (4.2b)\end{cases}$$

We will show the conjecture is true for "large" $M > 3^n$, which is rather trivial, and also for all "small" $M < 2^{0.047n}$ (Theorem 4.2 below).

We begin with an upper bound for $F(n, M)$ valid for all M.

Theorem 4.1. *Given* M *with* $(M, 3) = 1$. *Define* α *by* $M = 2^{\alpha n}$. *Then*

$$F(n, M) \leqslant \begin{cases} n+1, & \alpha > \log_2 3, \quad (4.3a)\\ 2n\, 2^{(1-\varphi\alpha)n}, & 0 < \alpha \leqslant \log_2 3, \quad (4.3b)\end{cases}$$

where $\varphi = (\log_2 3)^{-1} \doteq 0.63093$.

Proof. We first consider the easy case where $\alpha > \log_2 3$, i.e. $M > 3^n$. The maximum element of Σ_n is

$$\sum_{j=0}^{n-1} 2^j 3^{n-j} = 3^n - 2^n, \tag{4.4}$$

so any two elements of Σ_n in a congruence class (mod M) necessarily are equal. Now for any $M \in [0, 3^n - 1]$ there can be at most one element of value M in $\Sigma_{n,l}$ for $0 \leqslant M \leqslant n$ by Corollary 2.1a, hence the value M is taken at most $n+1$ times.

Now consider the more interesting case $0 < \alpha \leqslant \log_2 3$. Given $\mathbf{v} \in \{0, 1\}^n$ write $\mathbf{v} = \mathbf{w}\bar{\mathbf{w}}$ where $\mathbf{w}$ is of length m and $\bar{\mathbf{w}}$ is of length $n-m$. Set $\langle \mathbf{w}, \mathbf{w} \rangle = \sum_{i=1}^{m} w_i^2 = \sum_{i=1}^{m} w_i$ and let $|\mathbf{w}|$ denote the length m of $\mathbf{w}$.

Then

$$(4.5)\quad N(\mathbf{v}) = \Big(\sum_{j=0}^{m-1} v_j 2^j 3^{v_{j+1}+\ldots+v_{m-1}}\Big)3^{\langle\bar{\mathbf{w}},\bar{\mathbf{w}}\rangle} + \Big(\sum_{j=0}^{n-m-1} v_{m+j} 2^j 3^{v_{m+j+1}+\ldots+v_{n-1}}\Big)2^m$$
$$= N(\mathbf{w})3^{\langle\bar{\mathbf{w}},\bar{\mathbf{w}}\rangle} + N(\bar{\mathbf{w}})2^m.$$

Consider the set of 2^m vectors $\mathbf{v}\in\{0, 1\}^n$ having a fixed vector $\bar{\mathbf{w}}$, and choose $m = \lfloor \varphi\alpha n \rfloor$. We claim that for any fixed residue class $r \pmod M$ at most m choices of $\mathbf{w}\in\Sigma_m$ will yield $\mathbf{v} = \mathbf{w}\bar{\mathbf{w}}$ with $N(\mathbf{v}) \equiv r \pmod M$. To prove the claim, we prove that there is at most one choice of $\mathbf{w}$ having $\langle \mathbf{w}, \mathbf{w}\rangle = l$ with $0 \leqslant l \leqslant m$ and $N(\mathbf{w}\bar{\mathbf{w}}) = r$. Suppose not. If there were two different choices $\mathbf{w}^{(1)}$ and $\mathbf{w}^{(2)}$, giving the residue class $r \pmod M$, then (4.5) would give

$$3^{\langle\bar{\mathbf{w}},\bar{\mathbf{w}}\rangle}(N(\mathbf{w}^{(1)}) - N(\mathbf{w}^{(2)})) \equiv 0 \pmod M.$$

Since $(M, 3) = 1$ this gives

$$(4.6)\qquad N(\mathbf{w}^{(1)}) - N(\mathbf{w}^{(2)}) \equiv 0 \pmod M.$$

However, the choice of $m = \lfloor \varphi\alpha n \rfloor$ guarantees that $0 \leqslant N(\mathbf{w}^{(i)}) < 3^m \leqslant M$, so (4.6) forces $N(\mathbf{w}^{(1)}) = N(\mathbf{w}^{(2)})$. Now since $\langle \mathbf{w}^{(1)}, \mathbf{w}^{(1)}\rangle = \langle \mathbf{w}^{(2)}, \mathbf{w}^{(2)}\rangle = l$, by Corollary 2.1a one has $\mathbf{w}^{(1)} = \mathbf{w}^{(2)}$, a contradiction proving the claim. The claim shows that

$$F(n, M) \leqslant m2^{n-m} \leqslant 2n\, 2^{(1-\varphi\alpha)n}. \ \blacksquare$$

We are able to give a much sharper estimate for $F(n, M)$ valid for "small" M.

THEOREM 4.2. *Let M be given satisfying $(M, 6) = 1$. If $M = 2^{n\alpha}$, with*

$$\alpha \leqslant \alpha_c = \frac{1-H(\varphi)}{2-H(\varphi)} \doteq 0.04766,$$

then

$$(4.7)\qquad F(n, M) \leqslant 2n^4\, 2^{(1-\alpha)n}.$$

Here $H(x) = -x\log_2 x - (1-x)\log_2(1-x)$ and $\varphi = (\log_2 3)^{-1}$.

Proof. We start with the decomposition $\mathbf{v}\in\{0, 1\}^n$ as $\mathbf{v} = \mathbf{w}\bar{\mathbf{w}}\bar{\bar{\mathbf{w}}}$, where $\bar{\mathbf{w}}$ is an arbitrarily placed "window" of m bits, which gives

$$(4.8)\qquad N(\mathbf{v}) = 3^{\langle\bar{\mathbf{w}},\bar{\mathbf{w}}\rangle+\langle\bar{\bar{\mathbf{w}}},\bar{\bar{\mathbf{w}}}\rangle} N(\mathbf{w}) + 2^{|\mathbf{w}|}3^{\langle\bar{\bar{\mathbf{w}}},\bar{\bar{\mathbf{w}}}\rangle}N(\bar{\mathbf{w}}) + 2^{|\mathbf{w}|+|\bar{\mathbf{w}}|}N(\bar{\bar{\mathbf{w}}}).$$

We will choose $m = \lfloor \alpha n - 2\log_2 n - 1 \rfloor$, so that $M = 2^{\alpha n} > 2n^2 2^m$.

Now we divide the vectors $\bar{\mathbf{w}}\in\{0, 1\}^m$ into two sets, the *normal set* are those with $N(\bar{\mathbf{w}}) \leqslant M$ and the *oversize set* are those with $N(\bar{\mathbf{w}}) > M$. We claim that for any residue class $r \pmod M$ and any fixed choice of vectors $\mathbf{w}$, $\bar{\bar{\mathbf{w}}}$ there are at most m vectors $\bar{\mathbf{w}}$ in the normal set such that $\mathbf{v} = \mathbf{w}\bar{\mathbf{w}}\bar{\bar{\mathbf{w}}}$. This claim is proved the same way as in Theorem 4.1. Hence for a fixed window location, say with $|\mathbf{w}| = l$ and $0 \leqslant l \leqslant n-m$, at most $(n-m+1)2^{n-m}$ vectors $\mathbf{v} = \mathbf{w}\bar{\mathbf{w}}\bar{\bar{\mathbf{w}}}$ with $\bar{\mathbf{w}}$ normal have $N(\mathbf{v}) \equiv r \pmod M$. Now we let the window location vary, by varying l, and conclude that at most $(n-m)(m)2^{n-m}$ vectors $\mathbf{v}$ occur such that

(i) $N(\mathbf{v}) \equiv r \pmod M$,

(ii) $\mathbf{v}$ contains some window vector $\mathbf{w}$ of length m that is normal.

It remains to count the number E of exceptional vectors $\mathbf{v}$ such that $N(\mathbf{v}) \equiv r \pmod M$ and all window vectors $\mathbf{w}$ of size m inside $\mathbf{v}$ are oversize. We bound these by the size $|\Omega|$ of the set Ω consisting of those vectors $\mathbf{v}$ in $\{0, 1\}^n$ all of whose window vectors $\mathbf{w}$ of length m are oversize. Suppose $\mathbf{v}\in\Omega$. Let $\{\bar{\mathbf{w}}^{(l)}\colon 0 \leqslant l \leqslant n-m-1\}$ denote the $n-m$ possible window vectors of $\mathbf{v}$ of length m. If $B(j) = v_{j+1} + \ldots + v_{n-1}$ then (4.8) gives

$$(4.9)\qquad N(\mathbf{v}) \geqslant 2^l 3^{B(l+m)} N(\bar{\mathbf{w}}^{(l)}).$$

Now $\mathbf{v}\in\Omega$ implies $N(\bar{\mathbf{w}}^{(l)}) \geqslant M$ for all l. Summing (4.9) over l yields

$$(4.10)\qquad (n-m)N(\mathbf{v}) \geqslant \sum_{l=0}^{n-m-1} 2^l 3^{B(l+m)} N(\bar{\mathbf{w}}^{(l)}) \geqslant 2^{-m}M\Big(\sum_{l=0}^{n-m-1} 2^{l+m}3^{B(l+m)}\Big)$$
$$\geqslant 2n^2\Big(\sum_{l=0}^{n-m-1} 2^{l+m}3^{B(l+m)}\Big).$$

Now $N(\mathbf{v}) = \sum_{l=0}^{n-1} v_l 2^l 3^{B(l)}$, so this inequality yields

$$n\sum_{l=0}^{m-1} v_l 2^l 3^{B(l)} \geqslant (2n^2-n)\Big(\sum_{l=0}^{n-m-1} 2^{l+m}3^{B(l+m)}\Big) \geqslant (n^2-n)2^n.$$

In particular, there exists some l with $0 \leqslant l \leqslant m$ and $2^l 3^{B(l)} \geqslant 2^n$. This shows that $B(l) \geqslant \varphi(n-l)$, which says that the vector $\mathbf{v}\in\Omega$ has at least $\varphi(n-l)$ ones in its last $n-l$ positions, where $l \leqslant m \leqslant \alpha n$. This restriction on $\mathbf{v}\in\Omega$ yields the bound

$$|\Omega| \leqslant \sum_{l=0}^{m} 2^l\Big(\sum_{j>\varphi(n-l)}\binom{n-l}{j}\Big).$$

To simplify this inequality, we use a bound ([1], Lemma 4.7.2) for the tail of the binomial distribution:

$$\sum_{j>\alpha k}\binom{k}{j} \leqslant 2^{H(\alpha)k},$$

valid for $\alpha \geqslant \frac{1}{2}$, where $H(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the binary entropy function. This yields

$$|\Omega| \leqslant \sum_{l=0}^{m} 2^l 2^{H(\varphi)(n-l)} \leqslant m2^m 2^{H(\varphi)(n-m)} \leqslant n2^{\alpha n}2^{H(\varphi)(1-\alpha)n},$$

where $H(\varphi) \doteq 0.949955$.

Thus for $(M, 6) = 1$ we obtain the bound

$$F(n, M) \leqslant (n-m)(m)2^{n-m} + |\Omega| \leqslant n(n-1)4n^2 2^{(1-\alpha)n} + n2^{\alpha n + H(\varphi)(1-\alpha)n}.$$

This yields

$$F(n, M) \leqslant 4n^4 2^{(1-\alpha)n}$$

whenever $(1-\alpha)n \geqslant \alpha n + H(\varphi)(1-\alpha)n$, and this condition simplifies to

$$\alpha \leqslant \alpha_c \equiv \frac{1-H(\varphi)}{2-H(\varphi)} \cong 0.0476598. \blacksquare$$

The upper bounds for $n^{-1}\log F(n, 2^{\alpha n})$ obtained in Theorems 4.1 and 4.2 are graphed in Fig. 4.1 by the heavy line. The flat segment between α_c and 1 is proved by a modification of the proof of Theorem 4.2 that we omit: one chooses $m = \lfloor \alpha_c n - 2\log_2 n - 1 \rfloor$ for $\alpha_c \leqslant \alpha \leqslant (\log_2 3)\alpha_c$. The dotted line in Fig. 4.1 indicates the upper bound for $n^{-1}\log F(n, 2^{\alpha n})$ asserted by the Equidistribution Conjecture.

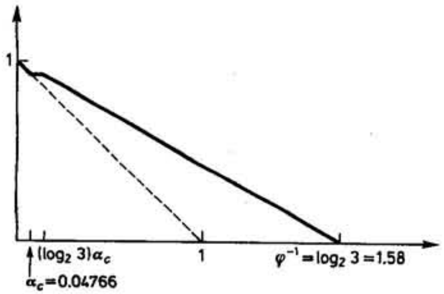

Fig. 4.1. Upper bounds for $n^{-1}\log_2 F(n, 2^{\alpha n})$ (dotted line indicates Equidistribution Conjecture)

It is a peculiar fact that the argument of Theorem 4.2 completely loses its strength at the critical value α_c. To obtain improved bounds for $\alpha > \alpha_c$ by this approach apparently requires improved bounds either for the number of elements in the exceptional set E or for $|\Omega|$.

4.2. *Upper bounds for $\Phi(x, y)$ and $C_{\text{prim}}(k, \beta\log k)$.* We study

$$\Phi(x, y) = \sum_{\substack{1 \leqslant k \leqslant x \\ k \equiv \pm 1 \pmod 6}} C_{\text{prim}}(k, y) \tag{4.11}$$

for $y = \beta\log x$ as $x \to \infty$ with β held constant. The count of all primitive cycles of length $\leqslant \beta\log x$ is the "trivial" upper bound for this sum:

$$\Phi(x, \beta\log x) = \sum_{n=1}^{[\beta\log x]} I(n), \tag{4.12}$$

and this yields

$$\Phi(x, \beta\log x) \leqslant \sum_{n=1}^{[\beta\log x]} \frac{1}{n} 2^n + O(2^{[\beta\log x]/2}) \tag{4.13}$$

$$\leqslant \frac{2x^\beta}{\log_2 x} + O(x^{\beta/2}).$$

The bound (4.12) is exact for $0 < \beta \leqslant \varphi$, and it is still quite sharp for $\varphi < \beta \leqslant 1$, because essentially all denominators $D(\mathbf{v})$ of cycles of length $\leqslant \beta\log x$ are less than x for β in this range. For example, for $\beta = 1$ one can show that

$$\Phi(x, \log x) \geqslant \sum_{n=1}^{[\log x]} I(n) - 2x^{H(\varphi)}, \tag{4.14}$$

where $H(\varphi) \doteq 0.949955$. (To prove this, one excludes all $\mathbf{v}$ with $D(\mathbf{v}) = |2^n - 3^k| > 2^{[\log x]}$, arguing as in [10], Theorem D.)

The results of the previous section enable one to show that for $\beta > 1$ the "trivial" upper bound (4.13) can be improved.

Theorem 4.3. *For $\beta > 1$ one has*

$$\Phi(x, \beta\log x) \leqslant 4(\beta\log x)^6 x^{f(\beta) + c_0\beta/\log\log x}, \quad \textit{where} \tag{4.15}$$

$$f(\beta) = \begin{cases} 1 & \text{if } 1 \leqslant \beta \leqslant \beta_c = 1/(1-\alpha_c) \doteq 1.050005, \\ (1-\varphi)\beta + \varphi & \text{if } \beta > \beta_c, \end{cases} \tag{4.16}$$

with $\varphi = (\log_2 3)^{-1} \doteq 0.63093$, and c_0 is an absolute constant.

Proof. Let $n = \log x$, and consider all 0-1 vectors $\mathbf{v}$ of length $\lfloor \beta n \rfloor$. For simplicity in what follows we treat βn as an integer; the proof works with $\lfloor \beta n \rfloor$ replacing βn throughout. How many of these $\mathbf{v}$ can produce an $x(\mathbf{v})$ which in lowest terms has a denominator $\delta(\mathbf{v}) < x$? To begin with, the unreduced denominator

$$D(\mathbf{v}) = 2^{\beta n} - 3^l$$

takes $\beta n + 1$ possible values. For each one of these values it has at most $2^{c_0\beta n/\log\log n}$ possible divisors M, for an absolute constant c_0. Using (3.3) one has

$$|D(\mathbf{v})| \geqslant (\beta n)^{-c_1} 2^{\beta n} \geqslant x^\beta/(\beta\log x)^{c_1},$$

and this implies that in order to have $|D(\mathbf{v})/M| \leqslant x$ one must have

$$M \geqslant (\beta\log x)^{-c_1} x^{\beta-1} = (\beta n)^{-c_1} 2^{(\beta-1)n}. \tag{4.17}$$

Now for any fixed divisor M let $F_0(n, M) = \#\{\mathbf{v} \in \{0,1\}^n \colon M \mid N(\mathbf{v})\}$. Since $F_0(n, M) \leqslant F(n, M)$ Theorems 4.1 and 4.2 can be used to bound the number of such M. They give

$$F_0(\beta n, M) \leqslant 2\beta n 2^{\beta n}/M^\varphi \quad \text{if } M \leqslant 3^{\beta n},$$

$$F_0(\beta n, M) \leqslant (\beta n)^4 2^{\beta n}/M \quad \text{if } M \leqslant 2^{\alpha_c\beta n}.$$

Now (4.17) gives $M \geqslant 2^{\alpha_0 \beta n}$ with

$$\alpha_0 = 1 - \frac{1}{\beta} - c_1 \frac{\log \beta n}{\beta n}.$$

Hence the number $G(n, \beta n)$ of $\mathbf{v}$ of length βn yielding a cycle with $\delta(\mathbf{v}) \leqslant 2^n$ is bounded by

$$(4.18) \qquad G(n, \beta n) \leqslant \sum_{l=0}^{n} \sum_{\substack{M \mid 2^{\beta n} - 3^l \\ M \geqslant 2^{\alpha_0 \beta n}}} F_0(\beta n, M)$$
$$\leqslant (\beta \log x + 1)\, x^{c_0 \beta / \log\log x} \left(2 (\beta \log x)^4 x^{f(\beta)}\right)$$

where $f(\beta)$ is given by (4.16). Since the right side of (4.18) is a monotone increasing function of β, we have

$$\Phi(x, \beta \log x) \leqslant \sum_{j=1}^{\beta n} G(n, j) \leqslant \beta n G(n, \beta n) \leqslant 4 (\beta \log x)^6 x^{f(\beta) + c_0 \beta / \log\log x}. \ \blacksquare$$

Remarks. (1) The proof gave away a few powers of logarithms more than necessary for $\beta > \beta_c$.

(2) It is known that for any $\varepsilon > 0$ one has $d(B) \leqslant B^{(1+\varepsilon)/\log\log B}$ for all sufficiently large $B \geqslant B_0(\varepsilon)$. Hence any $c_0 > 1$ can be used in (4.15) provided that a suitable multiplicative constant is added.

(3) The Equidistribution Conjecture implies that

$$\Phi(x, \beta \log x) \leqslant C(\beta, \varepsilon) x^{1+\varepsilon}$$

holds for all x, where $C(\beta, \varepsilon)$ is a constant depending on β and ε.

(4) A similar proof gives the upper bound

$$(4.19) \qquad C_{\mathrm{prim}}(k, \beta \log k) \leqslant \sum_{m=1}^{\beta \log k} \sum_{l=0}^{m} \frac{1}{m} F_0\left(m, \frac{2^m - 3^l}{k}\right)$$
$$\leqslant 4 (\beta \log k)^5 k^{f(\beta)},$$

valid for $\beta \geqslant 1$, where $f(\beta)$ is given by (4.16). This upper bound is close to the occasional large values of $C_{\mathrm{prim}}(k)$ given by Theorem 3.3, for $\beta < \beta_c$.

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AT&T BELL LABORATORIES
600 Mountain Avenue
Murray Hill, New Jersey 07974-2070, USA

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