Generalized 3x + 1 Mappings: Markov Chains and Ergodic Theory

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ABSTRACT. This paper reviews connections of the 3x + 1 mapping and its generalizations with ergodic theory and Markov chains. The work arose out of efforts to describe the observed limiting frequencies of divergent trajectories in the congruence classes (mod m).

1. Introduction

One of the most tantalizing conjectures in number theory is the so-called 3x+1 conjecture, attributed to Lothar Collatz [6]. Let the Collatz mapping $C : \mathbb{Z} \to \mathbb{Z}$ be defined by

(1)
$$C(x) = \begin{cases} x/2 & \text{if } x \equiv 0 \pmod{2} \\ 3x+1 & \text{if } x \equiv 1 \pmod{2} \end{cases}$$

Collatz conjectured that if $x \ge 1$, then the trajectory

$$x, C(x), C^{2}(x), \dots$$

eventually reaches the cycle 1, 4, 2, 1, also denoted by $\langle 1, 4, 2 \rangle$. If $x \in \mathbb{Z}$, it is also conjectured that the trajectory $\{C^k(x)\}$ eventually reaches this cycle or one of the cycles

(a)
$$\langle -1 \rangle$$
;
(b) $\langle -5, -14, -7, -20, -10 \rangle$;
(c) $\langle -17, -50, -25, -74, -37, -110, -55, -164, -82, -41, -122, -61, -182, -91, -272, -136, -68, -34 \rangle$;

(d)
$$\langle 0 \rangle$$
.

Another version of the problem iterates the 3x + 1 function, T(x), defined by

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

The conjecture here is that a positive integer x has iterates

$$x, T(x), T^2(x), \ldots$$

that eventually reach the cycle $\langle 1, 2 \rangle$.

The Collatz map and the 3x+1 map are both special cases of generalized Collatz mappings, introduced in Section 2, about which conjectural (heuristic) predictions

This contains some small additions and deletions to the book chapter - see footnotes

can be made concerning the behaviour of trajectories. Broadly speaking, there are similar conjectures that can be made about such mappings which seem equally unsolvable and tantalizing.

Since 1981, in a series of papers [26, 27, 25, 20, 4, 22], the author and collaborators were led to connections with ergodic theory and Markov chains. This analysis proceeds by studying the behaviour of the iterates modulo d. This is modelled by a Markov chain, which if irreducible, predicts that most trajectories spend a fixed fraction of time in each congruence class mod d (for a given number of steps). This permits one to compute an asymptotic exponential growth rate of the size of iterates; if it exceeds 1, one predicts most trajectories will diverge; while if it is between 0 and 1, one predicts all trajectories will enter cycles. More generally, one can also analyze the behaviour of iterates modulo m for an arbitrary modulus m (where it simplifies things to require that d divides m). It turns out experimentally that divergent trajectories also possess some regularity of distribution of iterates in congruence classes mod m for arbitrary modulus m.

It is easy to describe the conjectural picture for mappings of relatively prime type, as defined in section 2, a class which include the 3x + 1 mapping. The Markov chains take a fairly simple form in this case. However the Markov chains are more difficult to describe for maps of non-relatively prime type, and this case leads to many open problems.

There are natural generalizations to other rings of interest to number theorists, namely GF(q)[x] and the ring of integers of an algebraic number field. The conjectural picture is not so clear with GF(q)[x]. Also with number fields, it is not just a matter of studying finitely many cycles in the ring of integers. The situation with number fields is also not clear. We illustrate these possibilities with maps in $GF(2)[x], \mathbb{Z}[\sqrt{2}]$ and $\mathbb{Z}[\sqrt{3}]$.

For an account of other work on the 3x + 1 problem, we refer the reader to Lagarias' survey [18], Wirsching's book [33] and Guy's problem book [12, pages 215–218].

2. Generalized 3x + 1 mappings

Let $d \ge 2$ be a positive integer and m_0, \ldots, m_{d-1} be non-zero integers. Also for $i = 0, \ldots, d-1$, let $r_i \in \mathbb{Z}$ satisfy $r_i \equiv im_i \pmod{d}$. Then the formula

(3)
$$T(x) = \frac{m_i x - r_i}{d} \quad \text{if } x \equiv i \pmod{d}$$

defines a mapping $T : \mathbb{Z} \to \mathbb{Z}$ called the generalized Collatz mapping or generalized 3x + 1 mapping. In this definition we allow $gcd(m_i, r_i, d) > 1$, so that the denominator in lowest terms of (3) for a given $x \equiv i \pmod{d}$ may be any divisor of d.

The minimal integer $d = d(T) \ge 1$ such that the mapping is affine on each residue class (mod d) is called the *modulus* of the mapping T.

As examples, the Collatz mapping C(x) in (1) corresponds to parameter choices $d = 2, m_0 = 1 m_1 = 6, r_0 = 0, r_1 = -2$ in (3) while the 3x+1 mapping corresponds to the choices $d = 2, m_0 = 1, m_1 = 3, r_0 = 0, r_1 = -1$.

EQUIVALENT FORM: An equivalent form of (3) is:

(4)
$$T(x) = \left\lfloor \frac{m_i x}{d} \right\rfloor + a_i \qquad if \ x \equiv i \ (mod \ d),$$

where a_0, \ldots, a_{d-1} are any given integers and $\lfloor y \rfloor$ denotes the largest integer no larger than y. (Here $a_i = \frac{s_i - r_i}{d}$ where $0 \le s_i < d$ has $s_i \equiv im_i \pmod{d}$.)

We say that a generalized $3x + 1 \mod T$ is of relatively prime type if all multipliers m_i are relatively prime to d, i.e., $gcd(m_0m_1\cdots m_{d-1}, d) = 1$, and otherwise it is of non-relatively prime type. If no restrictions are put on T, we call it of general type. For example, the $3x + 1 \mod (2)$ is of relatively prime type, and the Collatz map (1) is of non-relatively prime type.

The behaviour of generalized 3x + 1 maps (at least conjecturally) is quite well understood in the relatively prime case, as we shall explain in sections 3 and 4. We describe auxiliary models which appear to make accurate predictions how trajectories behave in the relatively prime case. These models continue to work well for many maps in the non-relatively prime case; however many mysteries remain for maps in this case.

Starting in 1982, Tony Watts and I investigated the frequency of occupation of congruence classes modulo m of trajectories for generalized 3x+1 functions of relatively prime type. Here we consider a general integer modulus m, not necessarily related to d. The distribution of occupation frequencies in the particular case of congruence classes modulo d is directly relevant to the growth in size of its members of a trajectory, since it determines the number of multipliers m_i occurring in the iteration. In effect we construct auxiliary Markov model problems which lead to predictions of when trajectories should enter cycles or divergent trajectories, as given in Conjecture 3.1 below. These models are described in the next section.

In the remainder of this section we state basic formulas for forward and backwards iteration of a generalized Collatz map.

We first give a basic formula on forward iteration of a generalized Collatz map. Let T be a generalized Collatz mapping and let $T^{K}(x)$ represent its K-th iterate. If $T^{K}(x) \equiv i \pmod{d}, \ 0 \leq i < d$, we define $m_{K}(x) = m_{i}, r_{K}(x) = r_{i}$ so that

(5)
$$T^{K+1}(x) = \frac{m_K(x)T^i(x) - r_K(x)}{d}.$$

THEOREM 2.1. Let T be a generalized Collatz mapping, and let $T^{K}(x)$ represent its K-th iterate. Then

(i) There holds

(6)
$$T^{K}(x) = \frac{m_{0}(x) \cdots m_{K-1}(x)}{d^{K}} \left(x - \sum_{i=0}^{K-1} \frac{r_{i}(x)d^{i}}{m_{0}(x) \cdots m_{i}(x)} \right).$$

(ii) If $T^i(x) \neq 0$ for all $i \geq 0$, then

(7)
$$T^{K}(x) = \frac{m_{0} \cdots m_{K-1}(x)}{d^{K}} x \prod_{i=0}^{K-1} \left(1 - \frac{r_{i}(x)}{m_{i}(x)T^{i}(x)} \right).$$

Proof. Both parts follow by induction on K, using equation (5). \Box

The following result gives basic facts on allowable sequences of congruence classes modulo m, which underlies the analysis of backwards iteration.

Let B(j,m) denote the congruence class consisting of integers j modulo m, i.e.,

$$B(j,m) = \{x \in \mathbb{Z} : x \equiv j \pmod{m}\}$$

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THEOREM 2.2. Let T be a generalized Collatz map with modulus d. Let B(j,m) denote the congruence class consisting of integers $x \equiv j \pmod{m}$. Then

(i) The set $T^{-1}(B(j,m))$ is a disjoint union of $N_{j,m} \ge 0$ congruence classes (mod md), where

$$N_{j,m} = \sum_{\substack{i=0\\ \gcd(m_i, m)|j - T(i)}}^{d-1} \gcd(m_i, m),$$

where $T(i) = \frac{m_i i - r_i}{d}$. In particular, in the relatively prime case, where $gcd(m_i, m) = 1$ for i = 0, ..., d - 1, all $N_{j,m} = d$. In the general case it is possible that some $N_{i,m} = 0$.

(ii) In the relatively prime case, the d^{α} cylinders

(8)
$$C(i_0, i_1, \dots, i_{\alpha-1}; d) = B(i_0, d) \cap T^{-1}(B(i_1, d)) \cap \dots \cap T^{-(\alpha-1)}(B(i_{\alpha-1}, d))$$

comprise the complete set of d^{α} congruence classes modulo d^{α} .

(iii) In the relatively prime case, if $A = B(j, d^{\alpha})$ and $B = B(k, d^{\beta})$, then $T^{-K}(A) \cap B$ is a disjoint union of $d^{K-\beta}$ congruence classes mod $d^{K+\alpha}$, if $K \geq \beta$.

Proof. Properties (i) and (ii) are proved in [26]. Property (ii) has been the basis of many papers on the subject. Property (iii) then follows from Property (ii) by expressing A and B as disjoint unions of cylinders. \Box

In 4.2 we associate to this data a Markov matrix $Q_T(m)$.

3. Relatively Prime Case: Growth Rate of Iterates

In this section we treat generalized Collatz maps of relatively prime type. In section 3.1 we formulate a general conjecture on the existence of cycles and divergent trajectories. In section 3.2 we describe proved results supporting this conjecture.

3.1. Conjecture on Cycles and Divergent Trajectories. Matthews and Watts [26] analyzed the relatively prime case and formulated the following conjectures, and supported them with computer evidence.

CONJECTURE 3.1. For generalized Collatz mappings (3) of relatively prime type,

- (i) If $|m_0 \cdots m_{d-1}| < d^d$, then all trajectories $\{T^K(n)\}, n \in \mathbb{Z}$, eventually cycle. In particular there always must be at least one cycle.
- (ii) If $|m_0 \cdots m_{d-1}| > d^d$, then almost all trajectories $\{T^K(n)\}, n \in \mathbb{Z}$ are divergent (that is, $T^K(n) \to \pm \infty$, except for an exceptional set S of integers n satisfying $\#\{n \in S | -X \leq n \leq X\} = o(X)$.) In particular, there must exist at least one divergent trajectory.
- (iii) The number of cycles is finite.
- (iv) If the trajectory $\{T^K(n)\}, n \in \mathbb{Z}$ is not eventually cyclic, then the iterates are uniformly distributed (mod d^{α}) for each $\alpha \geq 1$:

 $\lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \{ K \le N | T^K(n) \equiv j \pmod{d^{\alpha}} \} = \frac{1}{d^{\alpha}},$ for $0 \le j \le d^{\alpha} - 1.$ We note that the equality case

$$(9) |m_0 \cdots m_{d-1}| = d^d$$

which is not covered in (i) and (ii) can never occur due to the relative primality condition $gcd(m_0m_1\cdots m_{d-1}, d) = 1$. Thus Conjecture 3.1 covers all generalized Collatz maps T of relatively prime type.

The first three parts of Conjecture 3.1 are generalizations of earlier conjectures of Möller [28], who studied a special subclass of mappings (3). Also the last part of (i) generalizes a conjecture of Lagarias [19] concerning the existence of at least one cycle.

Note that in these conjectures the prediction of overall cycling or divergence is independent of the remainder values r_i in (3), or equivalently of the integers a_i in (1)). This is a nice feature of relatively prime type mappings; in the non-relatively prime case, for fixed $(d, m_0, m_1, ..., m_{d-1})$ the choice of the integers a_i may affect the cycling or divergence behaviour of trajectories. Another difference with the general case is that the condition (9) may occur for some T of non-relatively prime type.

These conjectures (i)-(iv) all appear intractable for general maps of relatively prime type. However apart from (iv) they can be proved in some very special cases, namely where the map T is strictly increasing (resp. strictly decreasing) on all sufficiently large |n|.

In Section 5 we present various examples of such maps, which give supporting empirical evidence in favor of parts (i)-(iv) of Conjecture 3.1. In the next two subsections we present theorems which also support parts of this conjecture.

3.2. Growth Rate Heuristic for Forward Iteration. It follows from Theorem 2.1 that the size of iterates is determined by the fraction of the time the iterate spends in the class $i \pmod{d}$. Suppose over the first K steps a trajectory spends time f_i in the class $i \pmod{d}$. Then formula Theorem 2.1(2) suggests that

(10)
$$T^{K}(x) \sim \prod_{i=0}^{d-1} \left(\frac{m_{i}}{d}\right)^{f_{i}} x = \frac{1}{d} \left(\prod_{i=0}^{d-1} m_{i}^{f_{i}}\right) x_{i}$$

For mappings of relatively prime type, it turns out that the distribution describing an "average" input is uniform distribution, where all $f_i = \frac{1}{d}$.

Assuming that the $T^{K}(x)$ are uniformly distributed mod d, we would conclude from (10) that the iterates $|T^{K}(x)|$ grow geometrically at some rate (either expanding or contracting). For, on taking logarithms on the right side of Theorem 2.1 (2), we obtain

$$\log|T^{K}(x)| = \sum_{i=0}^{K-1} \log|m_{i}(x)| + \log x - K \log d + \sum_{i=0}^{K-1} \log\left|1 - \frac{r_{i}(x)}{m_{i}(x)T^{i}(x)}\right|.$$

Then as $a_i = r_i(x)/(m_i(x)T^i(x)) \to 0$, we have $b_i = \log|1 - a_i| \to 0$ and hence $\frac{1}{K}(b_0 + \cdots + b_{K-1}) \to 0$. Consequently

$$\frac{1}{K}\log|T^{K}(x)| = \frac{1}{K}\sum_{i=0}^{K-1}\log|m_{i}(x)| - \log d + o(1).$$

Hence if the $T^{K}(x)$ are uniformly distributed mod d, we deduce

$$\frac{1}{K} \log |T^K(x)| \to \frac{1}{d} \sum_{i=0}^{d-1} \log |m_i| - \log d,$$

and hence

$$|T^{K}(x)|^{1/K} \to \frac{(|m_{0}\cdots m_{d-1}|)^{1/d}}{d}.$$

(See [27, Theorem 1.1(b)] for a more general statement.)

This supports parts (i) and (ii) of Conjecture 3.1. One can also see it as justifying part (iii) in the case that the growth rate constant is smaller than one. In this case one expects that the iterates will contract to a finite basin, in which there can be only finitely many periodic orbits.

In fact in the forward iteration approach one can look at the growth of size of iterates, for a fixed number K of steps, averaged over all inputs $-N \leq x \leq N$, as $N \to \infty$, and precisely justify this heuristic in this limiting situation.

THEOREM 3.1. Let T be a generalized Collatz mapping of relatively prime type with modulus d. Then the first K steps of the iteration are periodic for all x (mod d^K), and the values of iterates

$$(x, T(x), T^{2}(x), \cdots, T^{K-1}(x)) \pmod{d}$$

take on all d^K possible values (mod d). That is, the values of the first K classes are uniformly distributed (mod d).

Proof. This follows from Theorem 2.2, part (2).

Theorem 3.1 does not rigorously establish the heuristic, which is concerned with behaviour in a different limiting case, where x is fixed and $K \to \infty$. To switch between the two limiting cases, requires establishing ergodic behaviour, which we discuss further in section 6.

4. Relatively Prime Case: Markov Models and Ergodic Sets

In this section we consider the behaviour modulo m of the iterates of a generalized Collatz map of relatively prime type. We can consider this problem in two ways: one is for a fixed number of iterations, averaging over all inputs, the second is on all iterates of a divergent trajectory.

4.1. Conjecture on Distribution Modulo m. We considered many examples of generalized Collatz maps of relatively prime type which conjecturally have divergent trajectories. Computer experiments indicated that for each m > 1, every divergent trajectory eventually occupies certain congruence classes mod m with positive limiting frequencies, depending on T. We make the following conjecture.

CONJECTURE 4.1. Let T be a generalized Collatz mapping of relatively prime type. Then for each integer $m \ge 2$, and each trajectory viewed modulo m will have a limiting frequency of iterates f_i in each residue class i (mod m), which depends on the initial starting point of the trajectory.

Stated this way, the conjecture is obviously true for any trajectory that enters a periodic orbit; the limiting frequencies are completely determined by the periodic orbit. The interesting case is that of divergent trajectories.

A simple example is given by the 5x + 1 mapping. Here divergent trajectories are not known to exist, but conjecturally most trajectories will be divergent (by Conjecture 3.1), and we can experimentally sample the distribution modulo m of apparently divergent trajectories. Now consider the case of modulus m = 5. One can show that any trajectory starting from a non-zero integer will eventually visit the class 3 (mod 5) and thereafter remain in the T-invariant set $\mathbb{Z} - B(0, 5)$. Here we find experimentally the elements in each divergent trajectory appear to occupy the congruence classes $0, 1, 2, 3, 4 \pmod{5}$ with limiting frequencies $\mathbf{v} = (0, \frac{1}{15}, \frac{2}{15}, \frac{8}{15}, \frac{4}{15})$ respectively.

We explain this conjecture below, using Markov chain models for iteration (mod m). We use such models to formulate a more precise version of this conjecture below, which gives a way to predict the limiting frequencies in any particular case.

For the 5x + 1 problem these rational numbers are the limits

(11)
$$\rho_j = \lim_{K \to \infty} \mu\{B(i,5) \cap T^{-K}(B(j,5))\} / \mu\{B(i,5)\}, \quad 0 \le j \le 4,$$

where ρ_j is independent of *i* and we define $\mu(S) = \frac{r}{m}$ if S is a disjoint union of r congruence classes mod m. (Here μ is a finitely additive measure on \mathbb{Z} .) Also $\mu\{B(i,5)\cap T^{-K}(B(j,5))\}/\mu\{B(i,5)\}$ is the (i,j) element of the K-th power of a Markov matrix $Q_T(5)$ defined by the recipe in section 4.2.

4.2. Markov chains: maps of relatively prime type. Now we describe Markov chain models $Q_T(m)$ for describing the iterates modulo m of a generalized Collatz mapping T of relatively prime type.

It was implicit in the proof of [27, Lemma 2.8] that if B is the cylinder:

$$B = B(i_0, m) \cap T^{-1}(B(i_1, m)) \cap \dots \cap T^{-K}(B(i_K, m)),$$

then

(12)
$$\mu(B) = q_{i_0 i_1}(m) \cdots q_{i_{K-1} i_K}(m) \mu\{B(i_0, m)\},\$$

where

(13)
$$q_{ij}(m) = \mu\{B(i,m) \cap T^{-1}(B(j,m))\} / \mu\{B(i,m)\} \ 0 \le i,j \le m-1, j \le m-1,$$

Then (see [27, Lemma 2.9]), the matrix

$$Q_T(m) = [q_{ij}(m)]$$

is an $m \times m$ Markov matrix, i.e., a matrix whose elements are non-negative and whose rows sum to unity. That is, it is the transition matrix of a finite Markov chain, see [14] or [29]. (Here we are using the transpose of the matrix used in [27].) If d|m, a simple formula exists for $q_{ij}(m)$:

$$q_{ij}(m) = \begin{cases} \frac{1}{d} & \text{if } T(i) \equiv j \pmod{\frac{m}{d}} \\ 0 & \text{otherwise.} \end{cases}$$

If d does not divide m, the formula for $q_{ij}(m)$ becomes more complicated. With $p_{ij}(m) = dq_{ij}(m)$, we have $[p_{ij}(m)]^K = [p_{Kjk}(m)]$, where $p_{Kjk}(m)$ is the number of congruence classes $(\mod md^K)$ that constitute $B(i,m) \cap T^{-K}(B(j,m))$. (See [27, Lemma 2.8]). This result also holds under the more general condition

$$gcd(m_i, d^2) = gcd(m_i, d), \ 0 \le i < d$$

provided d divides m.

Then for example, Theorem 2.2 (3) tells us that with $m = d^{\alpha}$, $\{Q(m)\}^{K} = \frac{1}{d^{\alpha}}H$ if $K \ge \alpha$, where H has all its entries 1.

For information on Markov chains, the reader may consult Grimmett [11] or Kemeny, Snell and Knapp [15].

To introduce Markov chains, we need a probability space, which we take to be the Prüfer ring $\hat{\mathbb{Z}}$. (See [**30**] or [**10**, pages 7–11].) Like the *d*-adic integers, this ring can be defined as a completion of \mathbb{Z} . The congruence class $\{x \in \hat{\mathbb{Z}} | x \equiv j \pmod{m}\}$ is also denoted by B(j, m). Then our finitely additive measure μ on \mathbb{Z} extends to a probability Haar measure on $\hat{\mathbb{Z}}$.

Equation (12) can then be interpreted as showing that the sequence of random set-valued functions $Y_K(x) = B(T^K(x), m), x \in \hat{\mathbb{Z}}$, forms a Markov chain with states $B(0, m), \ldots, B(m-1, m)$, with transition probabilities $q_{ij}(m)$, given by equation (13). For equation (12) can be rewritten as

$$Pr(Y_0(x) = B(i_0, m), \dots, Y_K(x) = B(i_K, m)) = q_{i_0 i_1}(m) \cdots q_{i_{K-1} i_K}(m)/m.$$

Then from an ergodic theorem for Markov chains (Durrett [7, Example 2.2, page 341]) we have the following result:

PROPOSITION 4.1. Let C be a positive recurrent class and for each $B \in C$, let ρ_B be the component of the unique stationary distribution over C.

$$Pr\left(\lim_{K \to \infty} \frac{1}{K+1} \operatorname{card} \left\{n; n \le K, \ Y_n(x) = B\right\} = \rho_B | Y_n(x) \ \operatorname{enters} \, \mathcal{C}\right) = 1.$$

In other words, if S_C is the union of the congruence classes of C,

$$Pr\left(\lim_{K\to\infty}\frac{1}{K+1} \ card\{n; n \le K, \ T^n(x) \in B\} = \rho_B | T^n(x) \ enters \ \mathcal{S}_{\mathcal{C}}\right) = 1.$$

This, together with computer evidence, leads to formulation of the following sharper form of Conjecture 4.1.

CONJECTURE 4.2. Let T be a generalized Collatz mapping of relatively prime type, having a divergent trajectory. Then for each integer $m \ge 2$, this divergent trajectory viewed modulo m will eventually enter some positive recurrent ergodic component $S_{\mathcal{C}}$ of the associated Markov chain $Q_T(m)$, and will occupy each congruence class B of C with positive limiting frequency ρ_B , given by the invariant probability distribution on C.

We mention two other asymptotic density conjectures:

CONJECTURE 4.3. If $\{T^K(n)\}$ is a divergent trajectory starting in \mathcal{S}_C , then

(14)
$$\lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \{ K \le N | T^K(n) \equiv i_0 \pmod{m}, \dots, T^{K+k}(n) \equiv i_k \pmod{m} \} = q_{i_0 i_1}(m) \cdots q_{i_{k-1} i_k}(m) / m.$$

(15)
$$\lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \{ K \le N | T^K(n) \equiv j \pmod{md} \} \\ = \frac{1}{d} \lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \{ K \le N | T^K(n) \equiv j \pmod{m} \}.$$

Now we present an example.

EXAMPLE 4.1. The 3x + 1 mapping with m = 3. Here

$$Q_T(3) = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 1 \\ 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

Then

$$\{Q_T(3)\}^k = \begin{bmatrix} \frac{1}{2^k} & \frac{1}{3}\left(1 + \frac{(-1)^k}{2^{k+1}}\right) - \frac{1}{2^{k+1}} & \frac{1}{3}\left(2 - \frac{(-1)^k}{2^{k+1}}\right) - \frac{1}{2^{k+1}} \\ 0 & \frac{1}{3}\left(1 + \frac{(-1)^k}{2^{k-1}}\right) & \frac{1}{3}\left(2 - \frac{(-1)^k}{2^{k-1}}\right) \\ 0 & \frac{1}{3}\left(1 - \frac{(-1)^k}{2^k}\right) & \frac{1}{3}\left(2 + \frac{(-1)^k}{2^k}\right) \end{bmatrix}$$

Also $\mathcal{C} = \{B(1,3), B(2,3)\}$ and $\{Q_T(3)\}^k \to \begin{bmatrix} 0 & 1/3 & 2/3 \\ 0 & 1/3 & 2/3 \\ 0 & 1/3 & 2/3 \end{bmatrix}$.

We remark that in papers [4, 22, 27], the matrices $Q_T(m)$ and sets $\mathcal{S}_{\mathcal{C}}$ were studied in some detail for mappings T of relatively prime type. The structure of these sets can be quite complicated.

The positive recurrent classes can be determined numerically using an algorithm from [9]. Also see implementation [24].

It seems likely that there are finitely many sets $\mathcal{S}_{\mathcal{C}}$ as *m* varies, if and only if $T(\mathbb{Z}) = \mathbb{Z}$.

5. Relatively Prime Case: Examples

Our first example is a strict generalization of the 3x + 1 problem, usually called the 3x + k problem.

EXAMPLE 5.1.

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

where k is an odd integer.

Here, as with the 3x + 1 problem, Conjecture 3.1 predicts that all trajectories appear to reach one of finitely many cycles. Here we observe empirically that the number of cycles for T_{5^t} appears to strictly increase with t. (See Fig. 1.) On the other hand, in an email to the author in 2001, Willem Maat pointed out that the only cycles for T_{3^t} are exactly 3^t times those of T_1 .

Cycles for the 3x + k problem were studied in Lagarias [19]. He showed that there exist k having an arbitrarily large (finite) number of cycles. He noted that the number of cycles as a function of k empirically appeared to be a complicated function of k, and that numbers k of the form $k = 2^a - 3^b$ for $a \ge 1$ appeared to have an unusually large number of cycles. In fact, as pointed out by Alan S. Jones in 2002, if $k = 2^{2c+1} - 9$, the numbers $2^n + 3, 1 \le n \le c$, generate c different cycles of length 2c+1. Actually the paper of Lagarias [19] studied an equivalent problem, concerning rational cycles of the 3x + 1 problem, and noted that rational cycles with denominator k correspond in a one-to-one fashion with integral cycles of the 3x + k probem.

For k = 371, we believe there are 9 cycles (lengths in parentheses):

0(1), -371(1), 371(2), -1855(3), -6307(11), 25(222), 265(4), 721(29), -563(14).

t	# of cycles for T_{5^t}	max cycle–length
0	5	11
1	10	27
2	13	34
3	17	118
4	19	118
5	21	165
6	23	433

FIGURE 1. Observed number of cycles for T_{5^t} , $0 \le t \le 6$.

We next consider cycles in a further generalization of the 3x + 1 mapping.

Example 5.2.

$$T(x) = \begin{cases} (x+a)/2 & \text{if } x \equiv 0 \pmod{2} \\ (3x+b)/2 & \text{if } x \equiv 1 \pmod{2}, \end{cases}$$

where a is even, b odd.

We expect all iterates to eventually cycle, with finitely many cycles including the following:

(i) $\langle a \rangle$; (ii) $\langle -b \rangle$; (iii) $\langle b + 2a, 2b + 3a \rangle$; (iv) $\langle -5b - 4a, -7b - 6a, -10b - 9a \rangle$; (v) $\langle -17b - 16a, -25b - 24a, -37b - 36a, -55b - 54a, -82b - 81a, -41b - 40a, -61b - 60a, -91b - 90a, -136b - 135a, -68b - 67a, -34b - 33a \rangle$.

The reader is referred to the author's CALC number theory calculator program [23] for a cycle-finding program called cycle.

By choosing m_0, \ldots, m_{d-1} so that their product is close to, but less than d^d in absolute value, one expects some trajectories to take many iterations to reach a cycle and for some cycles to be rather long. For example:

Example 5.3.

 $T(x) = \begin{cases} x/4 & \text{if } x \equiv 0 \pmod{4} \\ (3x-3)/4 & \text{if } x \equiv 1 \pmod{4} \\ (5x-2)/4 & \text{if } x \equiv 2 \pmod{4} \\ (17x-3)/4 & \text{if } x \equiv 3 \pmod{4}. \end{cases}$

Here $1 \cdot 3 \cdot 5 \cdot 17 = 255 = 4^4 - 1 < 4^4$, so this map falls in case (i) of Conjecture 3.1. We have found 17 cycles, starting at values 0, -3, 2, 3, 6, (period 1747), -18, -46, -122, -330, -117, -137, -186, -513 (period 1426), -261, -333, 5127, -5205.

Regarding the divergent trajectory part of conjecture 3.1(ii), the simplest example where things are evident numerically, but defy proof, is the 5x + 1 mapping:

EXAMPLE 5.4. The (5x + 1)/2 Problem.

$$T(x) = \begin{cases} x/2 & \text{if } x \equiv 0 \pmod{2} \\ (5x+1)/2 & \text{if } x \equiv 1 \pmod{2}. \end{cases}$$

Probabilistic models for behaviour of the 5x + 1 problem indicate that most trajectories should be divergent. Some models are detailed at length in Volkov [**32**]. The trajectory $\{T^{K}(7)\}$ appears to be divergent. However T is known to have 5 cycles, with starting values 0, 1, 13, 17, -1, and infinitely many integers have trajectories entering these cycles.

We next consider the original map attributed to Collatz (see [18]), which is a permutation. It first appeared in print in Klamkin [16] in 1963.

EXAMPLE 5.5. (Collatz-Klamkin)

$$T(x) = \begin{cases} 2x/3 & \text{if } x \equiv 0 \pmod{3} \\ (4x-1)/3 & \text{if } x \equiv 1 \pmod{3} \\ (4x+1)/3 & \text{if } x \equiv 2 \pmod{3} \end{cases}$$

The map T is a 1–1 mapping and its inverse is the 4–branched mapping

$$T^{-1}(x) = \begin{cases} 3x/2 & \text{if } x \equiv 0 \pmod{4} \\ (3x+1)/4 & \text{if } x \equiv 1 \pmod{4} \\ 3x/2 & \text{if } x \equiv 2 \pmod{4} \\ (3x-1)/4 & \text{if } x \equiv 3 \pmod{4} \end{cases}$$

The trajectory $\{T^{K}(8)\}$ appears to be divergent. There are 9 known cycles, with starting values: -44, -4, -2, -1, 0, 1, 2, 4, 44.

The set of generalized 3x + 1 mappings is closed under composition: If T_1, T_2 have d_1, d_2 branches respectively, then $T = T_2T_1$ has d_1d_2 branches. For example if we take T_1, T_2 to be the 3x + 1, 5x + 1, mappings, then we obtain the following map.

Example 5.6.

$$T(x) = \begin{cases} x/4 & \text{if } x \equiv 0 \pmod{4} \\ (3x+1)/4 & \text{if } x \equiv 1 \pmod{4} \\ (5x+2)/4 & \text{if } x \equiv 2 \pmod{4} \\ (15x+7)/4 & \text{if } x \equiv 3 \pmod{4}. \end{cases}$$

Here all trajectories appear to enter cycles, with 7 known cycles, having starting values: -749, -2, 0, 1, 7, 10, 514.

Now we consider examples which conjecturally have divergent trajectories, and we consider the behaviour of iterates modulo m for various m.

EXAMPLE 5.7. The (5x+1)/2 mapping with m = 5. The Markov chain formed by states $0, 1, 2, 3, 4 \mod 5$ has transition matrix

$$Q_T(5) = \begin{bmatrix} 1/2 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/2 & 1/2 & 0 \end{bmatrix}.$$

The set of states $C = \{1, 2, 3, 4 \pmod{5}\}$ form a positive recurrent class with limiting probabilities $\mathbf{v} = (\frac{1}{15}, \frac{2}{15}, \frac{8}{15}, \frac{4}{15}).$

EXAMPLE 5.8. The (5x-3)/2 mapping with 3|m. This example, discovered by Tony Watts, was a very interesting one. Empirical data suggested there exist two measures on $\hat{\mathbb{Z}}$ with respect to which T is ergodic and whose values on congruence classes give the observable frequencies of occupation of integer congruence classes. With m = 15, the Markov chain formed by states $0, \ldots, 14 \pmod{15}$ has two positive classes:

 $C_1 = \{1, 2, 4, 7, 8, 11, 13, 14 \pmod{15}\}, \quad C_2 = \{3, 6, 9, 12 \pmod{15}\},\$

with limiting probabilities

$$\mathbf{V}_1 = \left(\frac{4}{15}, \frac{1}{30}, \frac{1}{15}, \frac{1}{30}, \frac{2}{15}, \frac{4}{15}, \frac{2}{15}, \frac{1}{15}\right), \quad \mathbf{V}_2 = \left(\frac{4}{15}, \frac{8}{15}, \frac{2}{15}, \frac{1}{15}\right),$$

respectively.

6. Ergodic Theory

One innovation in Matthews and Watts [26] was the introduction of ergodic theory (see [3]). It uses an extension of mapping T to a mapping of the d-adic integers \mathbb{Z}_d into itself. The d-adic integers \mathbb{Z}_d can be regarded as a completion of \mathbb{Z} , consisting of all formal sums

$$x = \sum_{i=0}^{\infty} a_i d^i, \quad a_i \in \{0, 1, \dots, d-1\},\$$

with addition and multiplication done as with ordinary positive integers, by "carrying the digit". (See [17] or [21].) Here \mathbb{Z}_d is a complete metric space, under the *d*-adic metric

$$d(x,y) = |x - y|_d,$$

in which $|\cdot|_d$ is the *d*-adic norm, given by $|0|_d = 0$ and $|x|_d = d^{-k}$, where $k = \min_{a_j \neq 0}(j)$, if $x \neq 0$. We note that the integers \mathbb{Z} are dense in \mathbb{Z}_d in its metric topology.

THEOREM 6.1. Let $T : \mathbb{Z} \to \mathbb{Z}$ be a generalized Collatz mapping, with modulus d. Then there is a unique continuous extension $\hat{T} : \mathbb{Z}_d \to \mathbb{Z}_d$, where \mathbb{Z}_d denotes the d-adic integers.

Proof. The behaviour of the map $\hat{T}(x)$ for $x \in \mathbb{Z}_d$ is determined by its first *d*-adic digit $x \equiv a_0 \pmod{d}$, which determines its congruence class $a_0 \equiv i \pmod{d}$, and $\hat{T}(x) = \frac{m_i x - r_i}{d}$ is a *d*-adic integer. This defines a continuous map of \mathbb{Z}_d to itself, because the sets $\{\alpha \in \mathbb{Z}_d : \alpha \equiv i \pmod{d}\}$ are both open and closed in the *d*-adic topology. It obviously agrees with the map T on \mathbb{Z} , and since \mathbb{Z} is dense in \mathbb{Z}_d it is unique. \Box

This extension makes sense for an arbitrary generalized Collatz mapping. For such mappings of relatively prime type, one can say much more. The space \mathbb{Z}_d is a compact group under addition, and as such has a canonical Haar measure, which may be normalized to have volume 1. This measure is a (Borel) measure called the *d*-adic measure μ_d , which is completely determined by its values

$$\mu_d(B(j, d^{\alpha}) = \mu_d(\{x \in \mathbb{Z}_d : x \equiv j \pmod{d^{\alpha}}\}) = \frac{1}{d^{\alpha}}.$$

Here we note that the cylinders $B(j, d^{\alpha})$, originally defined on \mathbb{Z} , now make sense on \mathbb{Z}_d .

THEOREM 6.2. Let $T : \mathbb{Z} \to \mathbb{Z}$ be a generalized Collatz mapping, with modulus d, that is of relatively prime type, and let $\hat{T} : \mathbb{Z}_d \to \mathbb{Z}_d$ denote its continuous extension to \mathbb{Z}_d .

(1) The mapping \hat{T} is measure-preserving for the d-adic measure. That is,

$$\mu(\hat{T}^{-1}(A)) = \mu(A),$$

where A is a Haar-measurable set in \mathbb{Z}_d .

(2) The mapping \hat{T} is strongly mixing. That is,

$$\lim_{K \to \infty} \mu(\hat{T}^{-K}(A) \cap B) = \mu(A)\mu(B)$$

for all Haar-measurable sets A and B in \mathbb{Z}_d .

(3) The map \hat{T} is ergodic. That is, $\hat{T}^{-1}(A) = A \Rightarrow \mu(A) = 0$ or 1. In particular, there holds

$$\lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \{ K \le N | \hat{T}^K(x) \equiv j \pmod{d^{\alpha}} \} = \frac{1}{d^{\alpha}}$$

for almost all $x \in \mathbb{Z}_d$.

Proof. (1) Let us assume that T is a generalized Collatz mapping of relatively prime type. Then by Theorem 2.2, Property (ii), the inverse image of a congruence class mod d^{α} is the disjoint union of d classes mod $d^{\alpha+1}$. This gives the measurepreserving property on cylinders, i.e., $\hat{T}^{-1}(B(j, d^{\alpha}))$ has μ_d -measure equal to $\frac{1}{d^{\alpha}}$. The measure preserving property holds in general since the cylinders generate the Borel sets.

(2) Theorem 2.2, Property (iii) implies the strongly mixing property on cylinders $B(j, d^{\alpha})$, whence it holds for general measurable sets.

(3) The strong mixing property for a measure-preserving map implies ergodicity of \hat{T} . Now the Ergodic Theorem [3, page 12] applied to the measurable set $B(j, d^{\alpha})$ gives the required property

$$\lim_{N \to \infty} \frac{1}{N+1} \operatorname{card} \left\{ K \le N | \hat{T}^K(x) \equiv j \pmod{d^{\alpha}} \right\} = \frac{1}{d^{\alpha}},$$

for almost all $x \in \mathbb{Z}_d$. \Box

For a map of relatively prime type, applying the ergodic theorem to the cylinder (8) gives a similar result for the d-adic integers x which satisfy

$$\hat{T}^{K}(x) \equiv i_0 \pmod{d}, \dots, \hat{T}^{K+\alpha-1}(x) \equiv i_{\alpha-1} \pmod{d},$$

namely, for almost all $x \in \mathbb{Z}_d$ these have a limiting density $\frac{1}{d^{\alpha}}$.

Theorem 6.2 implies that, on the level of ergodic theory, for generalized Collatz maps of relatively prime type, the predictions of limiting densities of iterates (mod d^{α}) of trajectories are correct, if one takes a generic input $x \in \mathbb{Z}_d$.

A much stronger ergodic property can be proved for some generalized Collatz maps of relatively prime type.

THEOREM 6.3. Let T be the 3x + 1 map. There is a 3x + 1 conjugacy map $C_T : \mathbb{Z}_2 \to \mathbb{Z}_2$, which is an automorphism such that

$$C_T \circ \hat{T} = \hat{S}_2 \circ C_T,$$

where \hat{S}_2 is the 2-adic shift map

$$S_2(x) = \frac{x - a_0}{2}, \text{ for } x \equiv a_0 \pmod{2}.$$

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Here the 2-adic shift mapping simply chops off the first 2-adic digit and shifts the 2-adic expansion one unit to the right; it has the maximal amount of mixing possible. This result is proved in Lagarias [18] and is studied further in Bernstein [1] and Bernstein and Lagarias [2]. The 3x + 1 conjecture can be encoded in properties of this conjugacy map. An analogous result should hold for all generalized Collatz mappings of relatively prime type (by a similar proof): they are conjugate to the *d*-adic shift map.

Finally we note another nice feature of the d-adic extension for maps of relatively prime type.

THEOREM 6.4. (Möller) Let T be a generalized Collatz mapping of relatively prime type. Then every d-adic integer $x \in \mathbb{Z}_d$ possesses an d-adically convergent series given by:

(16)
$$x = \sum_{i=0}^{\infty} \frac{r_i(x)d^i}{m_0(x)\cdots m_i(x)} \text{ if } x \in \mathbb{Z}_d.$$

Proof. Möller [28, p. 221] proves this result for a related mapping H. Equation (6) holds for d-adic integers and gives

$$m_0(x)\cdots m_{K-1}(x)x \equiv \sum_{i=0}^{K-1} r_i(x)d^i m_{i+1}(x)\cdots m_{K-1}(x) \pmod{d^K}$$

and this is equivalent to (16), as $m_0(x), \ldots, m_{K-1}(x)$ are units in \mathbb{Z}_d .

Theorem 6.4 tells us that the congruence classes mod d occupied by the iterates of $x \in \mathbb{Z}_d$ in fact completely determine x. A corresponding expansion is used to advantage later in Section 8 for a mapping $T : GF(2)[x] \to GF(2)[x]$. (See mapping (27) below.)

What happens from the ergodic theory viewpoint for generalized Collatz maps not of relatively prime type? Here we enter mysterious terrain, which is much more complicated. The first issue is that the *d*-adic measure need not be an invariant measure for the map $T : \mathbb{Z}_d \to \mathbb{Z}_d$. There is the issue of finding an invariant Borel measure for this map. We do not know of a general construction of an invariant measure on \mathbb{Z}_d , although it can be done for special classes of maps. Also, it appears that there are cases where there may be more than one invariant measure that is absolutely continuous with respect to the *d*-adic measure. When an invariant measure is constructed, there then remains the issue of determining ergodicity of the maps for such measures.

7. General Case: Leigh and Venturini Markov chains

In 1983, George Leigh, then a 4th year mathematics student at the University of Queensland, suggested that to predict the frequencies mod m of divergent trajectories for the generalized Collatz mapping (3), we should restrict m to be a multiple of d and allow the states of the Markov chain to be all congruence classes in $\hat{\mathbb{Z}}$ of the form mk, where k divides some power of d. The idea is to keep track of how much information we have on the congruence classes to which an iterate belongs.

Leigh's viewpoint leads to chains with states with the startling feature that the congruence classes for different states may sometimes have one included inside another. For example, in the mapping of Example 8.5 below, which has modulus d = 8, if we start off in state B(4, 8), then we know T(x) is in B(0, 32) (here we keep track only of powers of 2 in the modulus) Then B(0, 32) is all the information we have about where T(x) is located. All the information is in the current state, regardless of the previous states of the trajectory. It turns out that this chain also has a state B(0, 8), which must be kept separate from B(0, 32).

Leigh introduced two related Markov chains, denoted by $\{X_n\}$ and $\{Y_n\}$. We shall consider here only the latter one. (Leigh proved the two chains contain equivalent information.) To define his Markov chain $\{Y_n\}$, we need some definitions: Let $m_i = b_i d_i$, where $b_i \in \mathbb{Z}$, $d_i \in \mathbb{N}$ and $gcd(d, b_i) = 1$, where d_i divides some power of d, $0 \leq i < d$. Let d|m. We define a sequence of random functions on $\hat{\mathbb{Z}} : x \to Y_n(x) \in \mathcal{B}$, where \mathcal{B} is the collection of congruence classes of the form B(j, mk), k dividing some power of d:

(1) The set of states $\{\mathcal{B}\}$ that the chain can reach, are defined recursively by the following recipe:

(a) $Y_0(x) = B(x, m);$ (b) $Y_{n+1}(x) = B(T^{n+1}(x), mk_{n+1}),$ where (17) $k_0 = 1 \text{ and } k_{n+1} = \frac{d_j k_n}{\gcd(d_j k_n, d)},$

and where j is determined by $T^n(x) \equiv j \pmod{d}, \ 0 \le j \le d-1.$

(2) Transition probabilities $q_{BB'}$ are defined for $B, B' \in \mathcal{B}$, as follows: Let B = B(j, mk), B' = B(j', mk'). Then (18)

$$q_{BB'} = \begin{cases} \frac{kd_j}{k'd} = \frac{\gcd(kd_j,d)}{d} & \text{if } k' = \frac{kd_j}{\gcd(kd_j,d)} \text{ and } T(j) \equiv j' \pmod{mkd_j/d}, \\ 0 & \text{otherwise.} \end{cases}$$

Then (see [20, page 133]), the set-valued functions $\{Y_n(x)\}$ form a Markov chain with transition probabilities $q_{BB'}$, by virtue of the equation

$$\Pr\left(Y_0(x) = B_0, \dots, Y_n(x) = B_n\right) = q_{B_0 B_1} q_{B_1 B_2} \cdots q_{B_{n-1} B_n} / m.$$

Leigh gives a recursive scheme for constructing the states reached. This shows that at stage n, there are $d/\gcd(d_jk_n, d)$ possibilities for $Y_{n+1}(x)$ and that all these possibilities arise for suitable initial values x. The scheme depends on the following result:

LEMMA 7.1. If
$$Y_n(x) = B(j, M), 0 \le j < M$$
 and $M' = Md_j/d$, then

(19)
$$Y_{n+1}(x) = B(T(j) + tM', M''),$$

where M'' = lcm(M', m) and $0 \le t < \frac{M''}{M'} = d/ \text{gcd}(d_j k_n, d).$

Conversely if $0 \le t < \frac{M''}{M}$, there exists a y such that (19) holds with x replaced by y.

REMARK 7.1. The converse follows from a fundamental equation of Leigh ([20, (42) p. 132]), which asserts that there exist U, w, with gcd(w, d) = 1, such that for all a

(20)
$$T^{n+1}(x+aU) = T^{n+1}(x) + awM'$$

and the fact that $\frac{M^{''}}{M'}$ divides a power of d. The recursive step is depicted as follows, in Leigh's notation:

$$\begin{split} B(j,M) \xrightarrow{H} B(T(j),M') \xrightarrow{G} B(T(j),M^{''}) \\ \to B(T(j)+M',M^{''}) \\ \cdots \\ \to B(T(j)+(\underline{M''}-1)M',M^{''}) \end{split}$$

Now let \mathcal{C} be a positive recurrent class (assuming that one exists) and for each $B \in \mathcal{C}$, let ρ_B be the corresponding limiting probability. Then from the result of Durrett [7] mentioned earlier, we have

$$Pr\left(\lim_{K \to \infty} \frac{1}{K+1} \operatorname{card} \{n; n \le K, Y_n(x) = B\} = \rho_B | Y_n(x) \text{ enters } C\right) = 1.$$

To find the limiting frequency p_i of occupancy of a particular congruence class B(i,m), we must sum the contributions of each congruence class in C which is contained in B(i,m), obtaining

(21)
$$Pr(f_i = p_i | Y_n(x) \text{ enters } \mathcal{C}) = 1,$$

where

(22)
$$f_j = \lim_{K \to \infty} \frac{1}{K+1} \operatorname{card} \{n; n \le K, \ T^n(x) \equiv j \, (\operatorname{mod} m)\}$$

and

(23)
$$p_j = \sum_{\substack{B \in \mathcal{C} \\ B \subseteq B(j,m)}} \rho_B.$$

(See [**20**, Theorem 5].)

For mappings T of relatively prime type, or when

 $gcd(m_i, d^2) = gcd(m_i, d), \ 0 \le i < d,$

(equivalently $d_i|d$ for all *i*) this Markov chain reduces to the one implicitly studied by Matthews and Watts and formula (18) with $d_j|d, k = k' = 1, B = B(j, m)$ and B' = B(j', m), simplifies to⁸

$$q_{BB'} = \begin{cases} \frac{1}{d} \operatorname{gcd}(m_j, d) & \text{if } T(j) \equiv j' \pmod{\frac{m}{d} \operatorname{gcd}(m_j, d)} \\ 0 & \text{otherwise.} \end{cases}$$

However in the general case the chain can be infinite.

Leigh ([20, equations (15, 23)]) also proved that if

$$p_{nij} = Pr(T^n(x) \equiv j \pmod{m} | x \equiv i \pmod{m}),$$

then

(24)
$$p_{nij} = \sum_{B \subseteq B(j,m)} q_{B(i,m)B}^{(n)}$$

(25)
$$\lim_{N \to \infty} \frac{1}{N} \sum_{n \le N} p_{nij} = \sum_{\mathcal{C}} p_j f_{B(i,m)\mathcal{C}},$$

 $^8 \mathrm{added}$ 4th July 2012

where $f_{B(i,m)\mathcal{C}} = Pr(Y_n(x) \in \mathcal{C} \text{ for some } n | Y_0 = B(i,m)).$

In the case where there is just one positive recurrent class C which is aperiodic and $B(i,m) \in C$, then (25) reduces to

(26)
$$\lim_{N \to \infty} \sum_{n \le N} p_{nij} = p_j.$$

We finish this section with some generalizations of conjectures 3.1 (i),(ii) and (iv) due to Leigh. Here we define $S_{\mathcal{C}}$ to be the union of the states in a positive class \mathcal{C} , i.e.,

$$S_C = \bigcup_{B \in C} B.$$

CONJECTURE 7.1. (Leigh) Suppose that the Markov chain $\{Y_n\}$ above has finitely many states. Then:

(a) Every divergent trajectory will eventually enter some positive class $S_{\mathcal{C}}$ and will occupy each class B of C with limiting frequency ρ_B .

(b) Let C be a positive recurrent class for the Markov chain mod d and let p_i be defined by (23). Then if

$$\prod_{i=0}^{d-1} \left| \frac{m_i}{d} \right|^{p_i} < 1,$$

all trajectories starting in $\mathcal{S}_{\mathcal{C}}$ will eventually cycle.

However if

$$\prod_{i=0}^{d-1} \left| \frac{m_i}{d} \right|^{p_i} > 1,$$

almost all trajectories starting in \mathcal{S}_C diverge.

(c) (Matthews) If a positive recurrent class C is aperiodic, then trajectories starting in S_C will enter finitely many cycles.⁹

8. General Case: Examples

The general case exhibits a much wider variety of behaviours under iteration than the relatively prime case.

We begin with a family of maps including the original form of Collatz version for the 3x + 1 problem.

EXAMPLE 8.1. (Collatz family) For an integer a,

$$C_a(x) = \begin{cases} x/2 & \text{if } x \equiv 0 \pmod{2} \\ 3x + a & \text{if } x \equiv 1 \pmod{2}, \end{cases}$$

The original version of Collatz [6] for the 3x + 1 problem is the case a = 1. The 3x + 1 map is given by

$$T(x) = \begin{cases} C_1(x) = x/2 & \text{if } x \equiv 0 \pmod{2} \\ C_1^2(x) = (3x+1)/2 & \text{if } x \equiv 1 \pmod{2}. \end{cases}$$

so in this case we expect all trajectories of C_1 should enter cycles. However for a = 0 every trajectory of C_0 diverges (except x = 0), for once an iterate becomes odd, it increases in size monotonically. In fact whenever a is an even integer there

⁹added 4th July 2012

are divergent orbits, by similar reasoning. This example illustrates that the value of integers a_i in (1) matter in determining the behaviour of orbits in the general case.

EXAMPLE 8.2.

$$T(x) = \begin{cases} x/3 - 1 & \text{if } x \equiv 0 \pmod{3} \\ (x+5)/3 & \text{if } x \equiv 1 \pmod{3} \\ 10x - 5 & \text{if } x \equiv 2 \pmod{3} \end{cases}$$

There appear to be five cycles, with starting values 0, 5, 17, -1, -4. However this example becomes less mysterious if we consider the related mapping

$$T'(x) = \begin{cases} T(x) & \text{if } x \equiv 0 \text{ or } 1 \pmod{3} \\ T^2(x) = (10x - 8)/3 & \text{if } x \equiv 2 \pmod{3}. \end{cases}$$

For T' is a mapping of relatively prime type and Conjecture 3.1 predicts that all trajectories eventually cycle.

Our next example contains provably divergent trajectories.

EXAMPLE 8.3.

$$T(x) = \begin{cases} 2x & \text{if } x \equiv 0 \pmod{3} \\ (7x+2)/3 & \text{if } x \equiv 1 \pmod{3} \\ (x-2)/3 & \text{if } x \equiv 2 \pmod{3} \end{cases}$$

Using an abbreviated notation, the transition probabilities scheme is:

The states are B(0,3), B(1,3) and B(2,3) with

$$Q_T(3) = \begin{bmatrix} 1 & 0 & 0\\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3}\\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}.$$

There is one positive recurrent class $C_1 = \{B(0,3)\}$ and transient states B(1,3) and B(2,3).

Here 3|x implies 3|T(x); so once a trajectory enters the zero residue class mod 3, it remains there and diverges. Experimental evidence strikingly suggests that if a trajectory takes values $T^k(x) \equiv \pm 1 \pmod{3}$ for all $k \ge 0$, then the trajectory must eventually enter one of the cycles -1, -1 or -2, -4, -2. The author offers a \$100 (Australian) prize for a proof. This problem seems just as intractable as the 3x + 1 problem and is a simple example of the more general Conjecture (4.2) on divergent trajectories.

EXAMPLE 8.4.

$$T(x) = \begin{cases} 12x - 1 & \text{if } x \equiv 0 \pmod{4} \\ 20x & \text{if } x \equiv 1 \pmod{4} \\ (3x - 6)/4 & \text{if } x \equiv 2 \pmod{4} \\ (x - 3)/4 & \text{if } x \equiv 3 \pmod{4}. \end{cases}$$

To predict the frequency distribution mod 4 of divergent trajectories, we find there are 8 states in the Markov chain:

 $S = \{B(0,4), B(1,4), B(2,4), B(3,4), B(15,16), B(4,16), B(47,64), B(11,16)\}$ with corresponding transition probability scheme and matrix Q(4):

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$$\begin{aligned} B(0,4) &\to B(15,16) \to B(15,16) \\ B(1,4) &\to B(4,16) \to B(4,16) \\ B(2,4) &\to B(0,1) \to B(0,1;2;3,4) \\ B(3,4) \to B(0,1) \to B(0;1;2;3,4) \\ B(15,16) \to B(3,4) \to B(3,4) \\ B(4,16) \to B(47,64) \to B(47,64) \\ B(47,64) \to B(11,16) \to B(11,16) \\ B(11,16) \to B(2,4) \to B(2,4) \end{aligned}$$

The Markov matrix is primitive (its 8th power is positive) and the limiting probabilities are $(\frac{1}{10}, \frac{1}{10}, \frac{2}{10}, \frac{2}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10})$ To find the predicted frequency p_0 for the congruence class 0 (mod 4), we must sum the contributions arising from the states B(0, 4) and B(4, 16), namely $p_0 = \frac{1}{10} + \frac{1}{10} = \frac{2}{10}$. Similarly the other frequencies are $p_1 = \frac{1}{10}, p_2 = \frac{2}{10}, p_3 = \frac{2}{10} + \frac{1}{10} + \frac{1}{10} + \frac{1}{10} = \frac{5}{10}$. Then as $12^{2/10}20^{1/10}(\frac{3}{4})^{2/10}(\frac{1}{4})^{5/10} > 1$,

we expect most trajectories to be divergent. The trajectory starting with 21 appears to be divergent.

We have found 6 cycles, with starting values -1, 5, -19, -4, -6, 19133.

EXAMPLE 8.5. (Leigh [**20**, page 140])

$$T(x) = \begin{cases} x/4 & \text{if } x \equiv 0 \pmod{8} \\ (x+1)/2 & \text{if } x \equiv 1 \pmod{8} \\ 20x - 40 & \text{if } x \equiv 2 \pmod{8} \\ (x-3)/8 & \text{if } x \equiv 3 \pmod{8} \\ 20x + 48 & \text{if } x \equiv 4 \pmod{8} \\ (3x-13)/2 & \text{if } x \equiv 5 \pmod{8} \\ (11x-2)/4 & \text{if } x \equiv 6 \pmod{8} \\ (x+1)/8 & \text{if } x \equiv 7 \pmod{8} \end{cases}$$

We find there are 9 states in the Markov chain mod 8: B(0,8), B(1,8), B(2,8), B(3,8), B(4,8), B(5,8), B(6,8), B(7,8), B(0,32),with corresponding transition probability scheme:

The corresponding transition matrix is

There are two positive recurrent classes: $C_1 = \{B(1,8), B(5,8)\}$ and

$$C_2 = \{B(0,8), B(0,32), B(2,8), B(4,8), B(6,8)\}$$

with transient states B(3,8) and B(7,8).

The limiting probabilities are $\mathbf{v}_1 = (\frac{1}{2}, \frac{1}{2})$ and $\mathbf{v}_2 = (\frac{3}{8}, \frac{1}{4}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8})$, respectively. We have $p_1 = p_5 = \frac{1}{2}$ and as

$$\left(\frac{1}{2}\right)^{1/2} \left(\frac{3}{2}\right)^{1/2} < 1$$

we expect every trajectory starting in $\mathcal{S}_{\mathcal{C}_1} = B(1,8) \cup B(5,8)$ to cycle. Also $p_0 = \frac{3}{8} + \frac{1}{4} = \frac{5}{8}$ and $p_2 = p_4 = p_6 = \frac{1}{8}$. Then as

$$\left(\frac{1}{4}\right)^{5/8} 20^{1/8} 20^{1/8} \left(\frac{11}{4}\right)^{1/8} > 1,$$

we expect most trajectories starting in $S_{C_2} = B(0, 2)$ to diverge, displaying frequencies $\mathbf{v} = (\frac{5}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ in the respective component congruence classes. (Leigh uses another Markov chain $\{X_n\}$ and arrives at $\mathbf{v} = (\frac{4}{7}, \frac{1}{7}, \frac{1}{7}, \frac{1}{7})$, which is erroneous, as one discovers on observing the apparently divergent trajectory starting with 46.)

We have found 13 cycles, with starting values

 $\{0, 1, 10, 13, 61, 158, 205, 3292, 4244, -2, -11, -12, -18\}.$

G. Venturini (see [**31**]) further expanded on Leigh's ideas and gave many interesting examples. One spectacular example is worth mentioning.

EXAMPLE 8.6. (Venturini)

$$T(x) = \begin{cases} 2500x/6 + 1 & \text{if } x \equiv 0 \pmod{6} \\ (21x - 9)/6 & \text{if } x \equiv 1 \pmod{6} \\ (x + 16)/6 & \text{if } x \equiv 2 \pmod{6} \\ (21x - 51)/6 & \text{if } x \equiv 3 \pmod{6} \\ (21x - 72)/6 & \text{if } x \equiv 4 \pmod{6} \\ (x + 13)/6 & \text{if } x \equiv 5 \pmod{6}. \end{cases}$$

There are 9 states in the Markov chain mod 6:

B(0,6), B(1,6), B(2,6), B(3,6), B(4,6), B(5,6), B(1,12), B(5,12), B(9,12).These form a recurrent class with limiting probabilities

$$\mathbf{v} = \left(\frac{18}{202}, \frac{20}{202}, \frac{53}{202}, \frac{20}{202}, \frac{18}{202}, \frac{55}{202}, \frac{6}{202}, \frac{6}{202}, \frac{6}{202}\right).$$

Noting that $B(1, 12) \subseteq B(1, 6), B(5, 12) \subseteq B(5, 6), B(9, 12) \subseteq B(3, 6)$, we get
 $p_0 = \frac{9}{101}, p_1 = \frac{20}{202} + \frac{6}{202} = \frac{13}{101}, p_2 = \frac{53}{202},$

$$p_{3} = \frac{101}{202} + \frac{6}{202} = \frac{13}{101}, p_{4} = \frac{9}{101}, p_{5} = \frac{202}{502} + \frac{6}{202} = \frac{61}{202}.$$

Then $\left(\frac{2500}{6}\right)^{9/101} \left(\frac{21}{6}\right)^{13/101} \left(\frac{1}{6}\right)^{53/202} \left(\frac{21}{6}\right)^{13/101} \left(\frac{21}{6}\right)^{9/101} \left(\frac{1}{6}\right)^{61/202} < 1$ and we expect all trajectories to eventually cycle. in fact, there appear to be two cycles, with starting values 2 and 6.

EXAMPLE 8.7.

$$T(x) = \begin{cases} 2x - 2 & \text{if } x \equiv 0 \pmod{6} \\ (x - 3)/2 & \text{if } x \equiv 1 \pmod{6} \\ (2x - 1)/3 & \text{if } x \equiv 2 \pmod{6} \\ 7x/3 & \text{if } x \equiv 3 \pmod{6} \\ (5x - 2)/6 & \text{if } x \equiv 4 \pmod{6} \\ 9x & \text{if } x \equiv 5 \pmod{6} \end{cases}$$

There are 14 Markov states, with two periodic positive recurrent classes:

$$\mathcal{C}_1 = \{ B(5,6), B(45,54), B(15,18) \}, \\ \mathcal{C}_2 = \{ B(5,12), B(45,108), B(33,36) \},$$

where $S_{C_2} \subseteq S_{C_1}$ and corresponding limiting probabilities $\mathbf{v}_1 = \mathbf{v}_2 = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. We also have transient states

B(0,6), B(1,6), B(2,6), B(3,6), B(4,6), B(10,12), B(1,12), B(9,12).

For both C_1 and C_2 , we have $p_3 = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$, $p_5 = \frac{1}{3}$. Also $(\frac{7}{3})^{2/3}9^{1/3} > 1$. Hence we expect most trajectories starting in S_{C_1} and S_{C_2} to diverge.

The trajectories $\{T^k(-1)\}$ and $\{T^k(5)\}$ apparently diverge. Experimentally, $\{T^k(-1)\}$ meets each of B(11, 12), B(99, 108), B(15, 36) with limiting frequencies 1/3 and does not meet $S_{\mathcal{C}_2}$; $\{T^k(5)\}$ meets each of B(5, 12), B(45, 108), B(33, 36) with limiting frequencies 1/3. Also $B(11, 12) \cup B(99, 108) \cup B(15, 36) = S_{\mathcal{C}_1} - S_{\mathcal{C}_2}$ is *T*-invariant. There appears to be one cycle $\langle -2 \rangle$.

Venturini gave a sufficient condition for the $\{X_n\}$ chain to be finite. Here is a corresponding condition for the $\{Y_n\}$ chain to be finite. (Proof not yet constructed!)

THEOREM 8.1. ([31, Theorem 7, p. 196]). Assume m = d. Let $D_n(x) = d_{j_0} \cdots d_{j_{n-1}}$, where $T^i(x) \equiv j_i \pmod{d}$ for $0 \leq i \leq n-1$. Suppose $D_{\nu}(x)$ divides d^{ν} for all $x, 0 \leq x < d^{\nu}$. Then $Y_n(x) = mk_n(x)$, where $k_n(x)$ divides $d^{\nu+1}$ for all $n \geq 0$.

We finish this section with an example where there are infinitely many states in the Markov chain. The example was suggested by Chris Smyth in 1993.

EXAMPLE 8.8.

$$T(x) = \begin{cases} \lfloor 3x/2 \rfloor & \text{if } x \equiv 0 \pmod{2} \\ \lfloor 2x/3 \rfloor & \text{if } x \equiv 1 \pmod{2}. \end{cases}$$

This can be regarded as a 6-branched mapping. The integer trajectories are much simpler to describe than the Markov chain: Non-zero even integers are successively multiplied by 3/2 until one gets an odd integer: if k is even, say $k = 2^r(2c+1), r \ge 1$, then k eventually reaches $3^{r+2}(2c+1) = 6k'+3$. Also $6k+1 \rightarrow 4k \rightarrow 6k \rightarrow 9k \rightarrow 6k$, while $6k+3 \rightarrow 4k+2 \rightarrow 6k+3$.

Finally $6k + 5 \rightarrow 4k + 3$ and unless we encounter 0 or -1 (fixed points), we must eventually reach B(1,6) or B(3,6).

With m = 6, $Y_n(0) = B(0, 2 \cdot 3^{n+1})$ for $n \ge 0$.

9. Other rings: Finite fields

It is natural to investigate analogous mappings T for rings other than \mathbb{Z} , where division is meaningful, namely the ring of integers of a global field. Here global fields are algebraic number fields or function fields in one variable over a finite field, cf. Cassels and Fröhlich [5, Chapter 2].

The author and George Leigh experimented with the ring GF(2)[x] of polynomials over the field with two elements. Here the conjectural picture for trajectories is not so clear. In [25] we examined the following mapping:

EXAMPLE 9.1. (Matthews and Leigh [25]) Over GF(2)[x],

(27)
$$T(f) = \begin{cases} \frac{f}{x} & \text{if } f \equiv 0 \pmod{x} \\ \frac{(x^2+1)f+1}{x} & \text{if } f \equiv 1 \pmod{x} \end{cases}$$

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FIGURE 2. The first 37 iterates for Example 9.1.

This is an example of relatively prime type and $|m_0 \cdots m_{|d|-1}| = |d|^{|d|}$, where $|f| = 2^{\deg f}$. Most trajectories appear to cycle. However the trajectory starting from $1 + x + x^3$ exhibits a regularity which enabled its divergence to be proved (see Figure 2). If $L_n = 5(2^n - 1)$, then

$$T^{L_n}(1+x+x^3) = \frac{1+x^{3\cdot 2^n+1}+x^{3\cdot 2^n+2}}{1+x+x^2}.$$

Figure 2 shows the first 37 iterates.

There are infinitely many cycles. In particular, the trajectories starting with $g_n = (1+x^{2^n-1})/(1+x)$ are purely periodic, with period–length 2^n . Figure 3 shows the cycle printout for g_4 .

EXAMPLE 9.2. (Hicks, Mullen, Yucas and Zavislak [13]) Over GF(2)[x],

(28)
$$T(f) = \begin{cases} \frac{f}{x} & \text{if } f \equiv 0 \pmod{x} \\ \frac{(x+1)f+1}{x} & \text{if } f \equiv 1 \pmod{x} \end{cases}$$

The paper [13] shows that all orbits converge to one of the fixed points 0, 1.

10. Other rings: algebraic number fields

Let d be a non–unit in the ring O_K of integers of an algebraic number field K. Again, the conjectural picture for trajectories is not entirely clear. Here are three examples.

111111111111111
100000000000011
01000000000001111
100000000001111
01000000000110011
100000000110011
01000000011111111
1000000011111111
01000001100000011
1000001100000011
01000111100001111
1000111100001111
01011001100110011
1011001100110011
001111111111111111
0111111111111111
111111111111111

FIGURE 3. Cycle g_4 .

EXAMPLE 10.1. $T: \mathbb{Z}[\sqrt{2}] \to \mathbb{Z}[\sqrt{2}]$ be defined by

$$T(\alpha) = \begin{cases} \alpha/\sqrt{2} & \text{if } \alpha \equiv 0 \pmod{\sqrt{2}} \\ (3\alpha + 1)/\sqrt{2} & \text{if } \alpha \equiv 1 \pmod{\sqrt{2}}. \end{cases}$$

Writing $\alpha = x + y\sqrt{2}$, where $x, y \in \mathbb{Z}$, we have equivalently

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

There appear to be finitely many cycles with starting values

$$\{0, 1, -1, -5, -17, -2 - 3\sqrt{2}, -3 - 2\sqrt{2}, 9 + 10\sqrt{2}\}.$$

An interesting feature is the presence of at least three one-dimensional T-invariant sets S_1 , S_2 , S_3 in $\mathbb{Z} \times \mathbb{Z}$:

$$S_1: x = 0 \text{ or } y = 0, S_2: 2x + y + 1 = 0 \text{ or } x + 4y + 1 = 0,$$

 $S_3: x + y + 1 = 0 \text{ or } x + 2y + 1 = 0 \text{ or } x + 2y + 2 = 0.$

Trajectories starting in S_1 or S_2 oscillate from one line to the other, while those starting in S_3 oscillate between the first and either of the second and third. Trajectories starting in S_1 will cycle, as $T^2(x,0) = (C(x),0)$, where C denotes the 3x + 1 mapping.

Most divergent trajectories appear to be evenly distributed mod $(\sqrt{2})^{\alpha}$. However divergent trajectories starting in S_2 or S_3 present what at first sight appear to be anomalous frequency distributions mod 2. By considering T^2 , these are explicable in terms of the predicted "one-dimensional" uniform distribution. For example, if 2x + y + 1 = 0, then

$$T^{2}(x, y) = \begin{cases} \left(\frac{3x}{2}, -3x - 1\right) & \text{if } x \equiv 0 \pmod{2} \\ \left(\frac{9x + 3}{2}, -9x - 4\right) & \text{if } x \equiv 1 \pmod{2}. \end{cases}$$

EXAMPLE 10.2. $T: \mathbb{Z}[\sqrt{3}] \to \mathbb{Z}[\sqrt{3}]$ is defined by

$$T(x) = \begin{cases} x/\sqrt{3} & \text{if } x \equiv 0 \pmod{\sqrt{3}} \\ (x-1)/\sqrt{3} & \text{if } x \equiv 1 \pmod{\sqrt{3}} \\ (4x+1)/\sqrt{3} & \text{if } x \equiv 2 \pmod{\sqrt{3}} \end{cases}$$

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We have found 103 cycles. The trajectory starting with $-1 + 7\sqrt{3}$ appears to be divergent. Divergent trajectories produce limiting frequencies approximating ($\cdot 27, \cdot 32, \cdot 40$) in the residue classes $0, 1, 2 \pmod{\sqrt{3}}$.

Finally it should be pointed out that divergent trajectories need not tend to infinity in absolute value:

EXAMPLE 10.3. $T: \mathbb{Z}[\sqrt{2}] \to \mathbb{Z}[\sqrt{2}]$ be defined by

$$T(\alpha) = \begin{cases} (1 - \sqrt{2})\alpha/\sqrt{2} & \text{if } \alpha \equiv 0 \pmod{\sqrt{2}} \\ (3\alpha + 1)/\sqrt{2} & \text{if } \alpha \equiv 1 \pmod{\sqrt{2}}. \end{cases}$$

If $\{T^K(x)\}$ is a divergent trajectory and $T^K(x) = x_K + y_K \sqrt{2}, x_K, y_K \in \mathbb{Z}$, then apparently $x_K/y_K \to -\sqrt{2}$ and $T^K(x) \to 0$.

11. Concluding Remarks

This paper is intended to draw attention to the Markov chains that arise from generalized Collatz maps $T : \mathbb{Z} \to \mathbb{Z}$. When the number of states is finite, these chains give confident predictions regarding cycling and almost everywhere divergence of trajectories, as well as predicting the frequencies of occupation of certain congruence classes by divergent trajectories.

In the non-relatively prime case, the question of when there are only finitely many cycles remains open.

The conjectural situation for rings other than \mathbb{Z} also invites systematic investigation.

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