Averaging Structure in the 3x+1 Problem

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1 Introduction

The 3x+1 problem concerns iterates of the function $T : \mathbb{Z}^+ \to \mathbb{Z}^+$ defined as

$$T(n) = \begin{cases} n/2, & n \text{ even}, \\ (3n+1)/2, & n \text{ odd}. \end{cases}$$

The (still) open conjecture is that for each $n \in \mathbb{Z}^+$ there exists a k such that $T^{(k)}(n) = 1$, that is, the k^{th} iterate of n equals one. Despite its simplicity, this beguiling problem has withstood many challenges, including over 300 related papers which have barely made a dent into a resolution. A comprehensive resource [7] contains articles, surveys, and an annotated bibliography.

One of the main challenges of the 3x+1 problem is the apparent lack of structure of the iterates. While the process is deterministic, broad mixing patterns are witnessed experimentally, which agree with stochastic models for this problem; see Kontorovich and Lagarias[5]. Lagarias [7, p.21] noted that the pseudorandomness of the 3x+1 problem make it extremely resistant to analysis. Moreover, he states: “If one could rigorously show a sufficient amount of mixing is guaranteed to occur, in a controlled number of iterations in terms of the input size n, then one could settle part of the 3x+1 conjecture, namely prove the non-existence of divergent trajectories. Here we have the fundamental difficulty of proving in effect that the iterations actually do have an explicit pseudo-random property.” The averaging properties reported in this paper offer evidence towards this goal.

An intriguing approach to the 3x+1 problem started by Berg and Meinardus[1, 2] uses generating functions

$$f_n(x) = \sum_{k=1}^{\infty} T^{(n)}(k)x^k.$$

They develop a formula which connects f_n to f_{n+1} (which we generalize in Theorem 3.2) and a statement concerning a functional equation which is equivalent to the 3x+1 problem. If the 3x+1 map behaves as expected, then the two sequences $\{f_{2n}(x)\}$ and $\{f_{2n+1}(x)\}$ should each converge in coefficient space. The pseudorandomness of this process suggests that the functions f_n or averages over its coefficients can offer insightful structure. However, the erratic behavior of the orbits of T means the tail of the generating functions is difficult to analyze.

This paper finds new properties of these generating functions (Section 2) which leads to new averaging structure concerning the function T (Sections 3 and 4). We work with a broader class of functions $T_{q,r}$ defined as

$$T_{q,r}(n) = \begin{cases} n/2, & n \text{ even} \\ (qn+r)/2, & n \text{ odd} \end{cases}$$

where q and r are odd numbers, and we study the generating functions

$$f_{n,q,r}(x) = \sum_{k=1}^{\infty} T_{q,r}^{(n)}(k)x^k.$$

Usually the values of q and r will be generic, so unless special values are called for, the subscripts will be omitted so that the long calculations will be less dense.

2 The Generating Functions

Before building and examining the generating functions, a general property of T will be developed. This requires the auxiliary function $O_{q,r}^{(n)}(k)$ defined as the number of odd terms in the set $\{k, T_{q,r}^{(1)}(k), T_{q,r}^{(2)}(k), \ldots, T_{q,r}^{(n-1)}(k)\}$. The first result generalizes a well-known fact for the 3x+1 case; see Terras[8] or Lagarias[6].

Theorem 2.1 *For fixed odd (q,r) and for all $n,k,j \geq 0$ there holds*

$$T_{q,r}^{(n)}\left(2^n k+j\right)=q^{O_{q,r}^{(n)}(j)}k+T_{q,r}^{(n)}(j).$$

Proof: The proof follows by induction on n. The $n=0$ case is trivial since each side equals $k+j$. Using the inductive hypothesis, one sees that

$$\begin{aligned}
T^{(n+1)}(2^{n+1}k+j) &= \begin{cases} \frac{qT^{(n)}(2^{n+1}k+j)+r}{2}, & , \quad T^{(n)}(2^{n+1}k+j) \text{ odd,} \\ \frac{T^{(n)}(2^{n+1}k+j)}{2}, & , \quad T^{(n)}(2^{n+1}k+j) \text{ even} \end{cases} \\
&= \begin{cases} \frac{q(q^{O^{(n)}(j)}2k+T^{(n)}(j))+r}{2}, & T^{(n)}(j) \text{ odd} \\ \frac{q^{O^{(n)}(j)}2k+T^{(n)}(j)}{2}, & T^{(n)}(j) \text{ even} \end{cases} \\
&= \begin{cases} q^{O^{(n)}(j)+1}k+\frac{qT^{(n)}(j)+r}{2}, & T^{(n)}(j) \text{ odd} \\ q^{O^{(n)}(j)}k+\frac{T^{(n)}(j)}{2}, & T^{(n)}(j) \text{ even} \end{cases} \\
&= q^{O^{(n+1)}(j)}k+T^{(n+1)}(j).
\end{aligned}$$

□

Theorem 2.1 yields a straightforward observation.

Theorem 2.2 *The functions $f_{n,q,r}(x)$ are rational functions which converge on the disc $|x|<1$. They take the form $P_{n,q,r}(x)/(1-x^{2^n})^2$ in which $P_{n,q,r}$ is a polynomial of degree $2^{n+1}-1$ and x divides $P_{n,q,r}(x)$. This polynomial satisfies*

$$f_{n,q,r}(x)=\frac{1}{(1-x^{2^n})^2}\sum_{j=1}^{2^n} q^{O_{q,r}^{(n)}(j)}x^j+\frac{1}{1-x^{2^n}}\sum_{j=1}^{2^n}\left[T_{q,r}^{(n)}(j)-q^{O_{q,r}^{(n)}(j)}\right]x^j. \quad (1)$$

Proof:

We have

$$\begin{aligned}
f_{n,q,r}(x) &= \sum_{k=1}^{\infty} T^{(n)}(k)x^k \\
&= \sum_{m=0}^{\infty}\sum_{j=1}^{2^n} T^{(n)}(2^n m+j)x^{2^n m+j} \\
&= \sum_{m=0}^{\infty}\sum_{j=1}^{2^n}\left(q^{O^{(n)}(j)}m+T^{(n)}(j)\right)x^{2^n m+j}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{x^{2^n}}{(1-x^{2^n})^2}\sum_{j=1}^{2^n} q^{O^{(n)}(j)}x^j + \frac{1}{1-x^{2^n}}\sum_{j=1}^{2^n} T^{(n)}(j)x^j \\
&= \frac{1}{(1-x^{2^n})^2}\sum_{j=1}^{2^n} q^{O^{(n)}(j)}x^j + \frac{1}{1-x^{2^n}}\sum_{j=1}^{2^n}\left[T^{(n)}(j) - q^{O^{(n)}(j)}\right]x^j.
\end{aligned}
$$

□

The first four functions for 3x+1 case are

$$
\begin{aligned}
f_{0,3,1}(x) &= \frac{x}{(1-x)^2}, \\
f_{1,3,1}(x) &= \frac{x\left(x^2+x+2\right)}{(1-x^2)^2}, \\
f_{2,3,1}(x) &= \frac{x\left(x^6+x^5+2\,x^4+x^3+8\,x^2+2\,x+1\right)}{(1-x^4)^2}, \\
f_{3,3,1}(x) &= \frac{x\left(x^{14}+x^{13}+x^{12}+x^{11}+5x^{10}+2x^9+7x^8+x^7+26x^6+8x^5+2x^4+2x^3+4x^2+x+2\right)}{(1-x^8)^2}.
\end{aligned}
$$

Theorem 2.2 implies that the poles of $f_{n,q,r}$ are exactly the roots s of $s^{2^n} = 1$. In an attempt to find structure in $f_{n,q,r}$, a contour integral of $f_{n,q,r}$ around the curve $|x| = 2$ (which contains all the poles) was performed. Amazingly, for the 3x+1 problem, numerical integration suggested

$$
\oint_{|x|=2} f_{n,3,1}(x)dx = 2\pi i \tag{2}
$$

for all n. To generalize and prove this observation, it is easier to work in the *exterior* of the contour. To this end, we establish a result which connects two different generating functions on two different domains. This paper will usually only consider the function $T_{q,r}(x)$, but an extra wrinkle will be helpful. Let $T_{+,q,r}(x) = T_{q,r}(x)$, while $T_{-,q,r}(x) = T_{+,q,-r}$. Studying $T_{+,q,r}$ on the negative integers is equivalent to studying $T_{-,q,r}$ on the positive integers since $T^{(n)}_{+,q,r}(-j) = -T^{(n)}_{-,q,r}(j)$. A related observation is $O^{(n)}_{+,q,r}(-j) = O^{(n)}_{-,q,r}(j)$. Both $T_{+,q,r}$ and $T_{-,q,r}$ can be combined in another interesting way.

Theorem 2.3 *For each $n \in \mathbb{Z}^+$ there holds the equality of rational functions*

$$
f_{n,q,r}(x) = f_{n,q,-r}\left(\frac{1}{x}\right).
$$

Proof:

$$\begin{aligned}
f_n(x) &= \sum_{k=1}^{\infty} T_+^{(n)}(k)x^k \\
&= \frac{x^{2^n}}{(1-x^{2^n})^2}\sum_{j=1}^{2^n} q^{O_+^{(n)}(j)}x^j + \frac{1}{1-x^{2^n}}\sum_{j=1}^{2^n} T_+^{(n)}(j)x^j \\
&= \frac{1}{\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=1}^{2^n} q^{O_+^{(n)}(j)}x^{j-2^n} - \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=1}^{2^n} T_+^{(n)}(j)x^{j-2^n} \\
&= \frac{1}{\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=0}^{2^n-1} q^{O_+^{(n)}(2^n-j)}x^{-j} - \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=0}^{2^n-1} T_+^{(n)}(2^n-j)x^{-j} \\
&= \frac{1}{\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=0}^{2^n-1} q^{O_+^{(n)}(-j)}x^{-j} - \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=0}^{2^n-1} \left(q^{O_+^{(n)}(-j)} + T_+^{(n)}(-j)\right)x^{-j} \\
&= \frac{1}{x^{2^n}\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=0}^{2^n-1} q^{O_+^{(n)}(-j)}x^{-j} - \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=0}^{2^n-1} T_+^{(n)}(-j)x^{-j} \\
&= \frac{1}{x^{2^n}\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=1}^{2^n} q^{O_+^{(n)}(-j)}x^{-j} - \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=1}^{2^n} T_+^{(n)}(-j)x^{-j} \\
&= \frac{1}{x^{2^n}\left(1-\frac{1}{x^{2^n}}\right)^2}\sum_{j=1}^{2^n} q^{O_-^{(n)}(j)}x^{-j} + \frac{1}{1-\frac{1}{x^{2^n}}}\sum_{j=1}^{2^n} T_-^{(n)}(j)x^{-j} \\
&= \sum_{k=1}^{\infty} T_-^{(n)}(k)\frac{1}{x^k}.
\end{aligned}$$

□

Berg and Meinardus [1] claim that this result (in the 3x+1 case) follows from a general theorem; see [4, p.205]. Theorem 2.3 shows that only one generating function is needed to represent both the qx+r and the qx-r problems. However, as $n \to \infty$, the set of poles of $f_{n,q,r}(x)$ becomes dense on the unit circle, in effect separating the function's domain into two components.

We now can prove a generalization of the contour result conjectured earlier.

Theorem 2.4 *For fixed odd* (q, r) *and each* $m, n \geq 1$ *we have*

$$\oint_{|x|=2} f_{n,q,r}(x)x^{m-1}dx = 2\pi i T_{-,q,r}^{(n)}(m). \tag{3}$$

Proof:

We simply use Theorem 2.3:

$$\begin{aligned}\oint_{|x|=2} f_n(x)x^{m-1}dx &= -\oint_{|y|=1/2} f_n\left(\frac{1}{y}\right) y^{1-m}\left(\frac{-1}{y^2}\right) dy \\ &= \oint_{|y|=1/2} \sum_{k=1}^{\infty} T_{-}^{(n)}(k) y^k y^{-1-m} dy \\ &= 2\pi i T_{-}^{(n)}(m).\end{aligned}$$

□

Equation (2) follows as a special case of Equation (3) with $m = 1$ since $T_{-,3,1}^{(n)}(1) = 1$ for all n.

3 Interpolating Polynomials $A_{n,q,r}(s)$ and $B_{n,q,r}(s)$

In this section we derive a new formula for the rational functions $f_{n,q,r}(x)$ which displays more of their properties as rational functions of x.

This formula is based on explicitly calculating the polar singularities of $f_{n,q,r}$ which are at most double poles at the 2^n-roots of unity. One can use it to give another derivation of Equation (3) without using Theorem 2.3. This approach requires more work but reveals another representation for $f_{n,q,r}$. The following theorem gives a partial fractions decomposition of the rational functional $f_{n,q,r}(x)$.

Theorem 3.1 *For fixed odd (q, r) we have for each $n \geq 1$*

$$f_{n,q,r}(x) = \sum_{s^{2^n}=1} \left[\frac{s^2}{(x-s)^2} B_{n,q,r}(s) + \frac{s}{x-s}\left(A_{n,q,r}(s) + B_{n,q,r}(s)\right)\right] \tag{4}$$

in which for a 2^n-th root of unity s we have the constants

$$A_{n,q,r}(s) = -\frac{1}{2^n}\sum_{j=1}^{2^n} T_{q,r}^{(n)}(j)s^j + \frac{1}{4^n}\sum_{j=1}^{2^n} q^{O_{q,r}^{(n)}(j)} j s^j$$

and

$$B_{n,q,r}(s) = \frac{1}{4^n} \sum_{j=1}^{2^n} q^{O_{q,r}^{(n)}(j)} s^j.$$

The expression $A_{n,q,r}(s)$ is the residue term while $B_{n,q,r}$ is the double pole contribution at the 2^n-th root of unity s.

Proof:

Suppose $s^{2^n} = 1$. An asymptotic expansion around $x = s$ produces

$$\frac{x-s}{1-x^{2^n}} = -\frac{s}{2^n} + \frac{1}{2}\left(1 - \frac{1}{2^n}\right)(x-s) + O\left((x-s)^2\right).$$

Expanding near the singularity $x = s$ generates

$$\begin{aligned}
f_n(x) &= \frac{x^{2^n}}{(1-x^{2^n})^2} \sum_{j=1}^{2^n} q^{O^{(n)}(j)} x^j + \frac{1}{1-x^{2^n}} \sum_{j=1}^{2^n} T^{(n)}(j) x^j \\
&= \left[-\frac{s}{2^n}\frac{1}{x-s} + \frac{1}{2}\left(1-\frac{1}{2^n}\right)\right]^2 \cdot \left[1 + \frac{2^n}{s}(x-s)\right] \cdot \left[\sum_{j=1}^{2^n} q^{O^{(n)}(j)} s^j + \frac{x-s}{s}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} j s^j\right] \\
&\quad + \left[-\frac{s}{2^n}\frac{1}{x-s} + \frac{1}{2}\left(1-\frac{1}{2^n}\right)\right] \cdot \left[\sum_{j=1}^{2^n} T^{(n)}(j) s^j\right] + O(1) \\
&= \frac{1}{(x-s)^2}\frac{s^2}{4^n}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} s^j + \frac{1}{x-s}\left\{-\frac{s}{2^n}\left(1-\frac{1}{2^n}\right)\sum_{j=1}^{2^n} q^{O^{(n)}(j)} s^j\right. \\
&\quad \left. + \frac{s^2}{4^n}\frac{2^n}{s}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} s^j + \frac{s^2}{4^n}\frac{1}{s}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} j s^j - \frac{s}{2^n}\sum_{j=1}^{2^n} T^{(n)}(j) s^j\right\} + O(1) \\
&= \frac{1}{(x-s)^2}\frac{s^2}{4^n}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} s^j + \frac{1}{x-s}\left\{\frac{s}{4^n}\sum_{j=1}^{2^n} q^{O^{(n)}(j)} (j+1) s^j - \frac{s}{2^n}\sum_{j=1}^{2^n} T^{(n)}(j) s^j\right\} \\
&\quad + O(1) \\
&= \frac{s^2}{(x-s)^2} B_n(s) + \frac{s}{x-s}\left(A_n(s) + B_n(s)\right) + O(1).
\end{aligned}$$

This implies that $f_n(x)$ takes the form

$$\sum_{s^{2^n}=1} \left[\frac{s^2}{(x-s)^2} B_n(s) + \frac{s}{x-s}\left(A_n(s) + B_n(s)\right)\right] + p_n(x)$$

where $p_n(x)$ is a polynomial for each n. But since $f_n(0) = 0$ and Equation (1) implies

$$\lim_{|x|\to\infty} f_n(x) = T^{(n)}(2^n) - q^{O^{(n)}(2^n)} = 1 - 1 = 0,$$

this forces $p_n(x)$ to be identically zero and we have the desired result.

□

In the hope of eventually gaining more understanding about the functions f_n, we also generalize a main result of Berg and Meinardus.

Theorem 3.2 *Suppose $q > r > 0$ are both odd. Letting $\mu = e^{2\pi i/q}$, we have*

$$f_{n+1,q,r}(x^q) = f_{n,q,r}(x^{2q}) + \frac{1}{qx^r}\sum_{k=0}^{q-1} \mu^{(q-r)k/2} f_{n,q,r}(\mu^k x^2)$$

Proof:

By splitting the generating function into even and odd components, we have

$$\begin{aligned}
f_{n+1}(x^q) &= \sum_{k=1}^{\infty} T^{(n+1)}(k)x^{qk} \\
&= \sum_{k=1}^{\infty} T^{(n+1)}(2k)x^{2qk} + \sum_{k=1}^{\infty} T^{(n+1)}(2k-1)x^{(2k-1)q} \\
&= \sum_{k=1}^{\infty} T^{(n)}(k)x^{2qk} + \sum_{k=1}^{\infty} T^{(n)}\left(qk + \frac{r-q}{2}\right) x^{(2k-1)q} \\
&= f_n(x^{2q}) + \frac{1}{x^r}\sum_{k=1}^{\infty} T^{(n)}\left(qk + \frac{r-q}{2}\right) x^{2(qk+(r-q)/2)} \\
&= f_n(x^{2q}) + \frac{1}{qx^r}\sum_{j=1}^{\infty} T^{(n)}(j)x^{2j}\left[1 + \mu^{(q-r)/2+j} + \mu^{2((q-r)/2+j)} + \cdots + \mu^{(q-1)((q-r)/2+j)}\right] \\
&= f_n(x^{2q}) + \frac{1}{qx^r}\sum_{k=0}^{q-1} \mu^{(q-r)k/2} f_n(\mu^k x^2).
\end{aligned}$$

□

4 Averaging Properties of T

We now study the structure of the polar parts of the double poles of $f_{n,q,r}$ which are given by the residue term $A_{n,q,r}(s)$ and the double pole part $B_{n,q,r}(s)$, where s is the 2^n-th root of unity. We treat s as a fixed 2^N-th root of unity and study how these polar parts change for $n \geq N$.

We saw that Theorem 2.4 was inspired by numerical evidence pointing to an invariance in a contour integral. Equation (4) gives a new representation of the generating functions by calculating the residues at each of the poles. These two theorems hint that there may be some invariance of the residues themselves. That is the finding of the next theorem which gives some sense of the averaging which takes place among the iterates. Note the difference when $q = 3$ versus $q \geq 5$.

Theorem 4.1 *Suppose $s^{2^N} = 1$. Then*

$$B_{n+1,q,r}(s) = \frac{q+1}{4} B_{n,q,r}(s)$$

for all $n \geq N$. If $s \neq 1$, then

$$A_{n+1,q,r}(s) = \frac{q+1}{4} A_{n,q,r}(s)$$

for all $n \geq N$, and

$$A_{n,q,r}(1) = \begin{cases} \frac{r}{3-q}\left(\frac{q+1}{4}\right)^n - \frac{r}{3-q}, & q \neq 3 \\ -\frac{rn}{4}, & q = 3 \end{cases}$$

for all n.

Proof:

We start with the claim for $B_{n,q,r}(s)$. We have

$$\begin{aligned}
4^{n+1} B_{n+1}(s) &= \sum_{j=1}^{2^{n+1}} q^{O^{(n+1)}(j)} s^j \\
&= \sum_{j=1}^{2^n} \left[s^j q^{O^{(n+1)}(j)} + s^{2^n+j} q^{O^{(n+1)}(2^n+j)} \right] \\
&= \sum_{j=1}^{2^n} \left[s^j q^{O^{(n+1)}(j)} + s^{1-j} q^{O^{(n+1)}(2^{n+1}+1-j)} \right] \\
&= \sum_{j=1}^{2^n} \left[s^j \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ even} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ odd} \end{cases} + s^{1-j} \begin{cases} q^{O^{(n)}(2^{n+1}+1-j)}, & T^{(n)}(2^{n+1}+1-j) \text{ even} \\ q^{O^{(n)}(2^{n+1}+1-j)+1}, & T^{(n)}(2^{n+1}+1-j) \text{ odd} \end{cases} \right]
\end{aligned}$$

We then have

$$
\begin{aligned}
4^{n+1}B_{n+1}(s) &= \sum_{j=1}^{2^n}\left[s^j\begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j)\text{ even}\\ q^{O^{(n)}(j)+1}, & T^{(n)}(j)\text{ odd}\end{cases} + s^{1-j}\begin{cases} q^{O^{(n)}(1-j)}, & T^{(n)}(1-j)\text{ even}\\ q^{O^{(n)}(1-j)+1}, & T^{(n)}(1-j)\text{ odd}\end{cases}\right]\\
&= \sum_{j=1}^{2^n}s^j\left[\begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j)\text{ even}\\ q^{O^{(n)}(j)+1}, & T^{(n)}(j)\text{ odd}\end{cases} + \begin{cases} q^{O^{(n)}(j-2^n)}, & T^{(n)}(j-2^n)\text{ even}\\ q^{O^{(n)}(j-2^n)+1}, & T^{(n)}(j-2^n)\text{ odd}\end{cases}\right]\\
&= \sum_{j=1}^{2^n}s^j\left[\begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j)\text{ even}\\ q^{O^{(n)}(j)+1}, & T^{(n)}(j)\text{ odd}\end{cases} + \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j)\text{ odd}\\ q^{O^{(n)}(j)+1}, & T^{(n)}(j)\text{ even}\end{cases}\right]\\
&= (q+1)\sum_{j=1}^{2^n}q^{O^{(n)}(j)}s^j\\
&= (q+1)4^nB_n(s).
\end{aligned}
$$

This yields

$$B_{n+1}(s) = \frac{q+1}{4}B_n(s).$$

In a similar way, an identity for A_n is derived:

$$
\begin{aligned}
4^{n+1}A_n(s) &= \sum_{j=1}^{2^{n+1}}q^{O^{(n+1)}(j)}js^j - 2^{n+1}\sum_{j=1}^{2^{n+1}}T^{(n+1)}(j)s^j\\
&= \sum_{j=1}^{2^n}q^{O^{(n+1)}(j)}js^j + \sum_{j=1}^{2^n}q^{O^{(n+1)}(2^n+j)}(2^n+j)s^j\\
&\quad -2^{n+1}\sum_{j=1}^{2^n}T^{(n+1)}(j)s^j - 2^{n+1}\sum_{j=1}^{2^n}T^{(n+1)}(2^n+j)s^j\\
&= \sum_{j=1}^{2^n}q^{O^{(n+1)}(j)}js^j + \sum_{j=1}^{2^n}q^{O^{(n+1)}(2^{n+1}+1-j)}(2^{n+1}+1-j)s^{1-j}\\
&\quad -2^{n+1}\sum_{j=1}^{2^n}T^{(n+1)}(j)s^j - 2^{n+1}\sum_{j=1}^{2^n}T^{(n+1)}(2^{n+1}+1-j)s^{1-j}\\
&= \sum_{j=1}^{2^n}js^j\begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j)\text{ even}\\ q^{O^{(n)}(j)+1}, & T^{(n)}(j)\text{ odd}\end{cases}\\
&\quad +\sum_{j=1}^{2^n}(2^{n+1}+1-j)s^{1-j}\begin{cases} q^{O^{(n)}(2^{n+1}+1-j)}, & T^{(n)}(1-j)\text{ even}\\ q^{O^{(n)}(2^{n+1}+1-j)+1}, & T^{(n)}(1-j)\text{ odd}\end{cases}\\
&\quad -2^n\sum_{j=1}^{2^n}s^j\begin{cases} T^{(n)}(j), & T^{(n)}(j)\text{ even}\\ qT^{(n)}(j)+r, & T^{(n)}(j)\text{ odd}\end{cases}
\end{aligned}
$$

$$
\begin{aligned}
& -2^{n+1}\sum_{j=1}^{2^n} s^{1-j}\left[q^{O^{(n+1)}(1-j)}+T^{(n+1)}(1-j)\right] \\
= & \sum_{j=1}^{2^n} js^j \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ even} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ odd} \end{cases} + \sum_{j=1}^{2^n}(2^{n+1}+1-j)s^{1-j} \begin{cases} q^{O^{(n)}(1-j)}, & T^{(n)}(1-j) \text{ even} \\ q^{O^{(n)}(1-j)+1}, & T^{(n)}(1-j) \text{ odd} \end{cases} \\
& -2^n \sum_{j=1}^{2^n} s^j \begin{cases} T^{(n)}(j), & T^{(n)}(j) \text{ even} \\ qT^{(n)}(j)+r, & T^{(n)}(j) \text{ even} \end{cases} - 2^{n+1}\sum_{j=1}^{2^n} s^{1-j} \begin{cases} q^{O^{(n)}(1-j)}, & T^{(n)}(1-j) \text{ even} \\ q^{O^{(n)}(1-j)+1}, & T^{(n)}(1-j) \text{ odd} \end{cases} \\
& -2^n \sum_{j=1}^{2^n} s^{1-j} \begin{cases} T^{(n)}(j), & T^{(n)}(j) \text{ even} \\ qT^{(n)}(j)+r, & T^{(n)}(j) \text{ even} \end{cases} \\
= & \sum_{j=1}^{2^n} js^j \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ even} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ odd} \end{cases} + \sum_{j=1}^{2^n}(j-2^n)s^j \begin{cases} q^{O^{(n)}(j-2^n)}, & T^{(n)}(j-2^n) \text{ even} \\ q^{O^{(n)}(j-2^n)+1}, & T^{(n)}(j-2^n) \text{ odd} \end{cases} \\
& -2^n \sum_{j=1}^{2^n} s^j \begin{cases} T^{(n)}(j), & T^{(n)}(j) \text{ even} \\ qT^{(n)}(j)+r, & T^{(n)}(j) \text{ even} \end{cases} \\
& -2^n \sum_{j=1}^{2^n} s^j \begin{cases} T^{(n)}(j-2^n), & T^{(n)}(j-2^n) \text{ even} \\ qT^{(n)}(j-2^n)+r, & T^{(n)}(j-2^n) \text{ even} \end{cases} \\
= & \sum_{j=1}^{2^n} js^j \left[\begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ even} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ odd} \end{cases} + \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ odd} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ even} \end{cases}\right] \\
& -2^n \sum_{j=1}^{2^n} js^j \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ odd} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ even} \end{cases} \\
& -2^n \sum_{j=1}^{2^n} s^j \left[\begin{cases} T^{(n)}(j), & T^{(n)}(j) \text{ even} \\ qT^{(n)}(j)+r, & T^{(n)}(j) \text{ odd} \end{cases} + \begin{cases} T^{(n)}(j), & T^{(n)}(j) \text{ odd} \\ qT^{(n)}(j)+r, & T^{(n)}(j) \text{ even} \end{cases}\right] \\
& +2^n \sum_{j=1}^{2^n} js^j \begin{cases} q^{O^{(n)}(j)}, & T^{(n)}(j) \text{ odd} \\ q^{O^{(n)}(j)+1}, & T^{(n)}(j) \text{ even} \end{cases} \\
= & \sum_{j=1}^{2^n} q^{O^{(n)}(j)} js^j(q+1) - 2^n \sum_{j=1}^{2^n}\left[(q+1)T^{(n)}(j)+r\right] s^j \\
= & (q+1)4^n A_n(s) - 2^n r \sum_{j=1}^{2^n} s^j.
\end{aligned}
$$

If $s \neq 1$, then the last sum equals zero and

$$A_{n+1}(s) = \frac{q+1}{4} A_n(s).$$

If $s = 1$, we have

$$A_{n+1}(1) = \frac{q+1}{4} A_n(1) - \frac{r}{4}.$$

Solving this linear difference equation, coupled with $A_0(1) = 0$ produces

$$A_n(1) = \begin{cases} \frac{r}{3-q}\left(\frac{q+1}{4}\right)^n - \frac{r}{3-q}, & q \neq 3, \\ -\frac{rn}{4}, & q = 3. \end{cases}$$

□

We can use Theorem 4.1 to express the iterates of T in terms of $A_{n,q,r}(s)$ and $B_{n,q,r}(s)$ directly.

Theorem 4.2 *For fixed (q, r) the n^{th} iterate of $T_{q,r}(\cdot)$ at $m \geq 1$ is given by*

$$T_{q,r}^{(n)}(m) = \sum_{s^{2^n}=1} \frac{1}{s^m} \left[m B_{n,q,r}(s) - A_{n,q,r}(s) \right].$$

Proof: For fixed $m \geq 1$, we have

$$\begin{aligned}
\sum_{s^{2^n}=1} \frac{1}{s^m} \left[m B_{n,q,r}(s) - A_{n,q,r}(s) \right] &= \sum_{s^{2^n}=1} \frac{1}{s^m} \sum_{k=1}^{2^n} \left[\frac{m}{4^n} q^{O^{(n)}(k)} s^k + \frac{1}{2^n} T^{(n)}(k) s^k - \frac{1}{4^n} q^{O^{(n)}(k)} k s^k \right] \\
&= \sum_{k=1}^{2^n} \sum_{s^{2^n}=1} \left[\frac{m}{4^n} q^{O^{(n)}(k)} + \frac{1}{2^n} T^{(n)}(k) - \frac{k}{4^n} q^{O^{(n)}(k)} \right] s^{k-m} \\
&= \sum_{s^{2^n}=1} \left[\frac{m}{4^n} q^{O^{(n)}(m)} + \frac{1}{2^n} T^{(n)}(m) - \frac{m}{4^n} q^{O^{(n)}(m)} \right] \\
&= T^{(n)}(m)
\end{aligned}$$

□

In the $q = 3$ case, these theorems can be used to heuristically argue that any orbit is bounded. Theorem 4.1 asserts that if s is a 2^n-th root of unity, then the functions $A_{n,3,r}(s)$ and $B_{n,3,r}(s)$ remain fixed for all higher values of n. Equation (4) then suggests that the family of functions $\{f_{n,3,r}(x),\ n \geq 1\}$ are uniformly bounded on any compact set in the open unit disk. Montel's Theorem[3] then implies that this sequence of functions is normal, that is, there is a subsequence which converges uniformly. This would imply that the coefficients in the generating functions each enter a cycle, and so the T-orbit of every positive integer eventually enters a cycle. This same observation about the functions $A_{n,3,r}(s)$ and $B_{n,3,r}(s)$, coupled with Theorem 4.2, also suggests that the T-orbits of every positive integer are bounded.

If $q \geq 5$, Theorem 4.1 asserts that both $A_{n,3,r}(s)$ and $B_{n,3,r}(s)$ diverge as $n \to \infty$ if they take non-zero values for some choice of n. Equation (4) or Theorem 4.2 suggest that the T-orbits of positive integers diverge. Care must be taken here, however, since some orbits may converge. For example, when $q = 5$ and $r = 1$, there is the cycle $\{1, 3, 8, 4, 2\}$. It is conjectured (see [5]) that the set of points which diverge has density one.

5 The $x + 1$ Problem

We illustrate our theorems with the very special case $q = r = 1$. This case, the $x+1$ problem, is completely understood: for $m \geq 1$, the iterates of $T_{1,1}(m)$ strictly decrease until they reach the fixed point $m = 1$. However, it is instructive to compute the generating functions $A_{n,1,1}(s)$ and $B_{n,1,1}(s)$.

It is not difficult to show that $T_{1,1}^{(n)}(j) = 1$ for all $1 \leq j \leq 2^n$ (thinking in binary helps). Theorem 2.2 is then used to show that

$$f_{n,1,1}(x) = \frac{x}{1-x} \cdot \frac{1}{1-x^{2^n}}.$$

This family of functions is clearly uniformally bounded on any compact subset of the interior of the unit disk. We also have that

$$B_{n,1,1}(s) = 0$$

if $s \neq 1$ is a root of unity and $B_{n,1,1}(1) = 1/2^n$. Moreover,

$$A_{n,1,1}(s) = \frac{s}{s-1} \cdot \frac{1}{2^n}$$

if $s \neq 1$ is a root of unity and $A_{n,1,1}(1) = (2^{-n} - 1)/2$. Equation (4) then gives

$$f_{n,1,1}(x) = \frac{1}{2^n} \cdot \frac{1}{(1-x)^2} + \frac{1}{x-1}\left[\frac{3}{2} \cdot \frac{1}{2^n} - \frac{1}{2}\right] + \sum_{s^{2^n}=1, s\neq 1} \frac{s}{x-s} \cdot \frac{s}{s-1} \cdot \frac{1}{2^n}.$$

The structure of the expressions for $A_{n,1,1}(s)$ and $B_{n,1,1}(s)$ confirm Theorem 4.1. Lastly, Theorem 4.2 yields

$$T_{1,1}^{(n)}(j) = \frac{j}{2^n} + \frac{1}{2}\left(1 - \frac{1}{2^n}\right) - \sum_{s^{2^n}=1, s\neq 1} \frac{1}{s^j}\frac{s}{s-1} \cdot \frac{1}{2^n}.$$

Acknowledgement: The author thanks the anonymous referee for many helpful suggestions.

References

[1] Lothar Berg and Günter Meinardus. *Functional Equations Connected with the Collatz Problem.* Results in Mathematics, 25, (1994), 1–12.

[2] Lothar Berg and Günter Meinardus. *The 3n+1 Collatz Problem and Functional Equations.* Rostock Math. Kolloq., 48, (1995), 11–18.

[3] John B. Conway. *Functions of One Complex Variable.* Springer, New York, 1973

[4] Walter B. Ford. *Studies on Divergent Series and Summability and The Asymptotic Developments of Functions Defined by Maclaurin Series.* Chelsea, New York, 1960

[5] A.V. Kontorovich and J.C. Lagarias, *Stochastic models for the 3x+1 and 5x+1 problems and related problems.* in *The Ultimate Challenge: The 3x+1 Problem*, 131–188, Amer. Math. Soc., Providence, RI, 2010.

[6] Jeffrey C. Lagarias, *The 3x+1 problem and its generalizations.* American Mathematical Monthly, 92, (1985) 3–23.

[7] *The Ultimate Challenge: the 3x+1 problem.* Edited by Jeffrey C. Lagarias. American Mathematical Society, Providence, RI, 2010.

[8] R. Terras. *A Stopping Time Problem on the positive integers.* Acta Arithmetica, 30, (1976) 241–252.