The search for self-contained numbers: k-special 3-smooth representations and the Collatz conjecture

The search for self-contained numbers: k-special 3-smooth representations and the Collatz conjecture

By Alun Stokes

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AUTHOR: Alun Stokes (McMaster University)
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Abstract

The Collatz conjecture is a deceptively simply problem that straddles the line between number theory and dynamical systems. It asks: if we iterate the function that sends some even n to $\frac{n}{2}$ and odd n to $3n+1$, will this converge to 1 for every natural number? This problem has long stood unsolved despite attempts in many mathematical disciplines – in large part due to the difficulty of predicting the multiplicative structure of a number under addition. In this project, we provide a derivation of the most standard algebraic reformulation of the non-trivial cycles subproblem. This results in an infinite family of exponential Diophantine equations which correspond to k-special 3-smooth representations of integers. By imposing conditions on the exponents in these representations, we rewrite it in a multiplicative form that admits iterative solving for parameters of the representation. Doing so while enforcing a maximum value on the largest power of 2 in the representation, we derive a sufficient condition for no non-trivial cycles existing in this process. We show that a self-contained number, w, is exactly one which has an odd element of its orbit modularly equivalent to $-3^{-1} \bmod w$. We then show that non-cyclicity of any self-contained number greater than 5 is sufficient to show that no cycles exist in the Collatz process. This differs from previous modularity-based results, and experimental results suggest that self-contained numbers are relatively rare. We show that exactly 7 such numbers exist less than 10^{15} – improving on the previously known bound of 10^{11}.

Keywords: Collatz conjecture; self-contained numbers; k-special 3-smooth representations; computational number theory; exponential Diophantine equations

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Further, I would like to thank Compute Canada for the use of their distributed computing network, which allowed me to derive the primary contribution in this thesis.

Contents

List of Figures

List of Tables

Declaration of Authorship

I, Alun Stokes, declare that this thesis titled, “The search for self-contained numbers: k-special 3-smooth representations and the Collatz conjecture” and the work presented in it are my own.

Chapter 1

Introduction

The Collatz conjecture is a problem that teases you. In working through this problem, one unravels, layer by layer, subproblem after subproblem, all along the way feeling the excitement of progress - with the idea in mind that this is all going somewhere. Almost universally and unwaveringly, this progress and unravelling eventually ends in the realization that some condition derived or equation formulated is, in essence, the conjecture in its entirety. Sometimes, if you are particularly unlucky, you actually find yourself something harder than what you started with. The Collatz conjecture shields itself fiercely from any elementary attack you may throw at it - and when you have exhausted all that you can, it sits smugly back, revelling in the knowledge that you have come away knowing little more than you went in with. It is for this reason that mathematicians are enchanted by it. It is a problem so simple to state that a child could understand it; so basic in the computation that, given a classroom of sufficiently motivated fifth-graders, one could begin to verify this case-by-case, with little effort. But to say anything about the process in generality is a distinctly difficult task that boils down to one long-standing open question: what happens to the multiplicative structure of an integer under addition?

In this thesis, we specifically focus on the subproblem of determining the existence of non-trivial cycles in the Collatz process. We approach this from an algebraic perspective, reproducing an algebraic reformulation first proposed by Böhm and Santacchi [6]. This reformulation consists of an infinite family of exponential Diophantine equations that amount to representing a particular difference of powers by a special integer representation, referred to as a k-special 3-smooth representation. We investigate some elementary properties of these representations, and numbers for which such a representation exists. We present a method by which a representation (and its existence) can be determined iteratively, and use this to derive a necessary condition for cyclicity. By examining a relaxation of this condition, we characterize a conjecturally sparse set of numbers, termed self-contained numbers, that are shown to be candidates for cyclic numbers. In fact, any cyclic number must be self-contained. Only 7 such numbers are known. By employing distributed computing strategies, we improve the known upper-bound for which no further self-contained numbers exist from 10^{11} to 10^{15}, and propose further refinements to the search strategy such that a greater proportion of numbers may be sieved. We present several properties of self-contained numbers, and partially characterize their relationship to the Collatz process and possible cycles. In each of the last two sections, we take a brief foray into some empirical and experimental results related to k-special representations and self-contained numbers.

We begin with a short literature review on some large results on the conjecture in general - including Tao's recent breakthrough on bounding the maximum element of an orbit [24] - and then some more specific results on the non-trivial cycles subproblem. The totality of literature on k-special 3-smooth numbers is reviewed, and we go on to present the first known results on self-contained numbers outside of OEIS (Online Encyclopedia of Integer Sequences) entry A005184 [12]. Aside from the general review, the literature for particular topics are presented in their relevant sections. For the rest of this section, we will formally present the Collatz conjecture, denote some commonly used notation, explain certain conventions, and introduce some basic concepts that will be broadly applicable throughout the paper. Topic-specific nomenclature and notation will be introduced when it becomes pertinent.

1.1 The Collatz conjecture

The Collatz Conjecture was originally formulated for the Collatz map, C, given

$$C(n) = \begin{cases} 3x+1 & : x \equiv 1 \pmod 2 \\ \dfrac{x}{2} & : x \equiv 0 \pmod 2 \end{cases} \tag{1.1}$$

It asks: will the repeated self-composition of C reach 1 for every positive natural number? The problem can be equivalently stated in terms of two subproblems. First, **SP1**, is to show that for all natural numbers, the Collatz orbit will not have a cycle other than the trivial. We also refer to this as the non-trivial cycles subproblem. The second, **SP2**, is to show that no orbit tends to infinity with continued iteration. Formally,

$$\mathbf{SP1} := \forall n \in \mathbb{N}^+, n \geq 5 \colon \forall m \in \mathbb{N}^+ \colon C^{(m)}(n) \neq n$$

$$\mathbf{SP2} := \forall n \in \mathbb{N}^+, n \geq 2 \colon \exists M \in \mathbb{N}^+ \colon \forall m \in \mathbb{N}^+ \colon C^{(m)}(n) < M$$

Resolutions to **SP1** and **SP2** would resolve the conjecture entirely. Unfortunately, both of these remain undetermined.

Although the conjecture was originally formulated for the map C as given above, we generally use alternate but equivalent maps in actual study of the problem. These are:

$$T(n) = \begin{cases} \dfrac{3x+1}{2} & : x \equiv 1 \pmod 2 \\ \dfrac{x}{2} & : x \equiv 0 \pmod 2 \end{cases} \tag{1.2}$$

and

$$P(n) = \begin{cases} \dfrac{3x+1}{2^{\nu_2(3x+1)}} & : x \equiv 1 \pmod 2 \\ \dfrac{x}{2^{\nu_2(x)}} & : x \equiv 0 \pmod 2 \end{cases} \tag{1.3}$$

for ν_2 the 2-adic valuation function. That is,

$$\nu_2(n) = \begin{cases} \max_{m \in \mathbb{N}} \{2^m | n\} & : n \neq 0 \\ \infty & : n = 0 \end{cases}$$

These are referred to as accelerated maps (given they reduce the orbit length), and principally, they allow us to ignore steps in the Collatz sequences that do not matter. Specifically, P is called the Syracuse map. According to Lagarias [16], the use of 'Syracuse' in the context of this problem was proposed by mathematician Helmut Hasse during a visit to Syracuse University. It is not known to the author whether this visit was also the inception of the Syracuse map.

1.2 Some Terminology

In the study of this problem, various authors have used a fair bit of different standard notation and nomenclature, and sometimes even come up with their own. Here, we outline some of the relevant terms and notation we use that is not specific to a particular section. Also note that throughout this paper, we use the convention that the natural numbers are the non-negative integers, notated $\mathbb{N}$, and write the positive natural numbers as $\mathbb{N}^+$.

We notate the m-th application of some Collatz map, M, to the starting value of x by $M^{(m)}(x)$. Note, this obeys the following equivalence:

$$M^{(m)}(x) = M^{(m-k)}(M^{(k)}(x)) \tag{1.4}$$

An *orbit* is the sequence of numbers arising from the repeated iteration of a Collatz map from some starting point, either terminating in 1 or having infinite length. We denote the orbit of n under some Collatz map, M, by $\text{orb}_M(n)$ For example, the orbit of 5 under C is $\text{orb}_C(5) = (5, 16, 8, 4, 2, 1)$. Orbits are map-dependent, as exemplified by the previous starting value under T, which is $\text{orb}_T(5) = (5, 8, 4, 2, 1)$. Under P it is the shortest, given by $\text{orb}_P(5) = (5, 1)$. The number of elements in an orbit under M is given by the *height function*, $h_M(n)$. If an orbit is non-finite we say that $h_m(n) = \infty$. Since an orbit terminates at the first occurrence of 1, an orbit is infinite only if it does not contain 1. Thus, both non-trivial cycles and diverging sequences are infinite orbits.

The *stopping time* of some $n \in \mathbb{N}^+$ is the smallest $k \in \mathbb{N}^+$ such that for some Collatz map, M, we have $M^{(k)}(n) < n$. We write this $\sigma(n) = k$. The *total stopping time*, written $\sigma_\infty(n)$ is the smallest $k \in \mathbb{N}$ such that $M^{(k)}(n) = 1$. Clearly, $\sigma(n) \leq \sigma_\infty(n)$, with equality only if $n \leq 2$. Similarly to orbits, these are dependent on the choice of Collatz map.

Chapter 2

A Short Literature Review

2.1 Some General Results

First, we start by discussing some of the more general results on the conjecture. These are neither specific to **SP1** or **SP2**. So far, there have only been results that suggest the truth of the conjecture, with little in the way of concrete proofs of significant portions of the problem.

2.1.1 Computation and Established Bounds on Cycle Length

With the abundance of computational power available to us, it is natural to exploit these resources to search for potential counter-examples to the conjecture. Unfortunately, but perhaps unsurprisingly, we still have yet to find one. As of this review being written, all natural numbers up to 2^{68} have been tested [3]. This computation is more useful, however, than just identifying which values hold for the conjecture. It can also tell us something about the minimum length of a cycle, if one exists. Recall $\sigma(n)$ is the smallest k such that $T^{(k)}(n) < n$ for $n \in \mathbb{N}^+$. Terras [26] introduced the *coefficient* stopping time, $\kappa(n)$, for $\kappa(n)$ the least k with $T^{(k)}(n) = \alpha(n)n + \beta(n)$ with $\alpha(n) < 1$ for $\alpha(n) = \frac{3^{a(n)}}{2^n}$, where $a(n)$ is the number of odd iterates up to k-th in the orbit. Evidently, the upper bound on $\kappa(n)$ gives us a lower bound on the cycle length. Terras conjectured that $\kappa(n) = \sigma(n)$ for all $n \geq 2$ - a statement that can be proved up to some bound using the convergents of $\log_2(3)$ and the upper bound on known converging starting points for the Collatz sequence. He proved that this conjecture holds for $\kappa(n) < 2593$. Later, Garner [9] used the improved known bound on tested numbers of $2 \cdot 10^9$ to show that this holds for $\kappa(n) < 10^6$.

The importance of this method is in showing that no *short* cycles exist. Since Garner in 1981, with the bound of 2^{68} being tested, we can show that $\kappa(n) < 6586818670$. Another interesting result on the lengths of cycles was given by Eliahou [8] - which gave an explicit form of the period for a cycle. Specifically, considering the map T, we have that the period $p = (301994)A + (17087915)B + (85137581)C$ for $A, B, C \in \mathbb{N}$, $B \geq 1$, and one of A, C equal to 0. This was done by use of the continued fraction expansion of $\log_2(3)$ and the truth of the conjecture for $n < 2^{40}$. Halbeisen and Hungerbühler

[11] later improved on Eliahou by showing that a lower bound on the truth of Collatz is required for the derived bound on cycle length.

Beyond these facts, not terribly much is known about constraints on cycle length. While unfortunate, this seems partially due to the non-constructive nature of arguments about cycle length, as they are unlikely to resolve in a proof of the conjecture. Much like further verification of the truth of the conjecture for all $n < N$, these only act as heuristic and probabilistic arguments for the conjecture, rather than proof. As a result of these methods, we know that any cycle must be quite large, and as our computations continue to grow, we can easily use further convergents of $\log_2(3)$ to refine our lower bound on cycle length. Having an explicit form for cycle period is also quite interesting, although it has yet to be used for any other purpose than bounding cycle length.

2.1.2 Density of Convergence on an Interval

Given some interval of natural numbers, $[1, x]$ for $x \in \mathbb{N}^+$, we wonder what proportion of of $n \in [1, x]$ hold under the Collatz conjecture? We denote by $\pi_1(x)$ the number of starting values $n < x$ such that n converges to 1 under the Collatz map. Here, the principal study is of the inequality $\pi_1(x) > x^\gamma$, and finding lower bounds for $\gamma \in (0, 1]$. Of course, ideally we could show $\gamma = 1$. This was first investigated by Crandall [7], who pioneered some methods that would be later employed by Applegate, Krasikov, Lagarias, and Sander. Crandall, using Stirling's formula and an asymptotic expansion of certain error functions, shows that, for sufficiently large x, we have $\pi_1(x) > x^\gamma$ for some $\gamma \in (0, 1]$. While he does not compute γ, his proof implies $\gamma \geq 0.05$. While quite a small bound, his methods were quickly extended. Sander [20] improves this bound by directly building on Crandall's argument, achieving a bound of $\gamma \geq \frac{3}{10}$.

Krasikov further improved on this bound, though using an new argument involving (what are now called) Krasikov inequalities. These are a parameterized set of recurrence inequalities on functions of the cardinality of induced subgraphs of an infinite graph representing the Collatz process. The vertices of this graph are the natural numbers, and edges are between each node and where it is sent by the Collatz map. These subgraphs consist of all nodes that eventually map to some node v, and stay under some bound x. This set of inequalities is parameterized by $k \geq 2$, and Krasikov shows the case where $k = 2$, leading to a bound of $\gamma > \frac{3}{7}$. For larger k, the lower bound for γ will be improved. This is exactly what Applegate and Lagarias show, and is later improved upon by Krasikov and Lagarias. Applegate and Lagarias [1] show that Krasikov inequalities can be used to construct a non-linear programming problem of about 2000 variables which yields lower bounds for γ. Using a computer-intensive proof, they show that $\gamma \geq 0.81$. This proof was for the case $k = 9$. Using a similar method, Krasikov and Lagarias [14] prove the case for $k = 11$, giving the best known bound of $\gamma \geq 0.84$.

Since the bound of 0.84, there haven't been further refinements along this line of reasoning. Much like the results in section 2.1.1, these facts provide a body of evidence in support of the conjecture, but they are approximate solutions, and only give us an idea of what to expect *in general.* That is not to say these are unimpressive or useless by any means, and these conclusions are the accumulation of years of progress from many authors. But in the case of Crandall's original method, one would need to prove the case for the limit of $k \to \infty$ to ensure that the density of convergent starting points approaches 1. Given the difficulty of proving this for any given k, and the steeply increasing difficulty as k increases, this appears to be a currently intractable method. However, nearly two decades later, Tao went on to prove a much stronger property of the density of convergence using a completely different approach.

2.1.3 Tao's Result on Boundedness of Orbits

Without a doubt, the most significant result of the past few decades was synthesized by Tao in 2019. The following explanation uses both Tao's original paper [24] and a blog post he wrote on the topic [25]. Although his result is not a proof of the conjecture, it comes tantalisingly close - and makes the possibility that it is not true seem less probable than ever. Denote by $C_{\min}(n)$ the minimum element of the collatz orbit of n. His result is essentially, given any function $f\colon \mathbb{N}^+ \to \mathbb{R}$ with $\lim_{n\to\infty} f(n) = +\infty$, we have $C_{\min}(n) < f(n)$ for *almost* all $n \in \mathbb{N}^+$. We know that if every natural number's orbit contains a number less than itself, then the Collatz conjecture is true, since we can recursively show that every number must converge. Thus, if we could remove that *almost*, we would have the whole conjecture. As such, this result is enormously impressive, and the machinery behind its proof perhaps even more so.

To speak to the significance of this result, we note that one could take, for example, $f(n) = \log\log\log\log n$; a function which would require n on the order of $10^{1656520}$ to reach a value more than 1. And in fact, for any large bound you desire, one could devise a function that ensures its orbit contains an element that is arbitrarily small. The crux of the problem is then this qualification of *almost*, which is used in the sense of logarithmic density. What principally differentiates the result of Tao from previous results is the idea of local vs global control on the dynamics of the Collatz system. Korec [13] showed that the set $M = \{n \in \mathbb{N}^+ \colon C_{\min}(n) < n^{\theta}\}$ has asymptotic density 1 for $\theta = \frac{\log 3}{\log 4}$. What this means is that, if one is to choose some $n \in [1, x]$, then in most cases, it will eventually be mapped by C into $[1, x^{\theta}]$. What this does not assure us, however, is that it will eventually be mapped further into $[1, x^{\theta^2}]$ - the reason being that the uniform measure on $[1, x]$ required for this result is not preserved under the Collatz map.

Thus, Tao improves the result by coming up with a measure that is *more* invariant under C than the uniform measure. Without getting into the details of how this is done, Tao devises the Syracuse random variable (so named for the accelerated map P), upon which a measure can be constructed. This measure is only constructible if the geometric random variables of the Syracuse random variable stabilize as their parameter tends to infinity - which Tao shows that they do. By manipulating the explicit formulation of the Syracuse variable, it can be written as a conditional sum of independent random variables, allowing its characteristic function to be expressed as an averaged Riesz product. This lets him establish an upper bound on the expected value of a function of the Syracuse random variable, which completes the proof.

It is difficult to believe that there are more useful proofs that say something about *most* numbers than this one. Given the astounding degree of control one has with their choice of f, with the only restriction of tending to infinity, one could ask for little more. That said, Tao himself conceded that his is a problem where the difference between *almost* and *all* is far from easily surmountable [25] - and given the nature of this proof, the potential for it to be extended to a stronger result seems unlikely.

2.2 On the Existence of Cycles

Here, we discuss a few results on the existence and size of cycles, should they exist. We only discuss this through the lens of k-cycles, as these methods have been some of the most fruitful in their study.

2.2.1 Background and Some (More) Terminology

Before getting into results, we first introduce some concepts and terminology used in the study of cycles. In the traditional Collatz conjecture, using the map C over the positive natural numbers, we are only aware of 1 cycle. This is referred to as the $1, 4, 2$ or $4, 2, 1$-cycle, or the trivial cycle. The central problem of **SP1** is determining if there exist any cycles *besides* the trivial cycle. This is the cycle that all tested starting numbers are known to terminate in. When the problem is attacked using another map, such as T or P, this becomes the $1, 2$-cycle or 1-cycle, respectively. These are all equivalent in their respective formulations, and for simplicity, it is referred to as the trivial cycle almost universally.

The k-cycle is a way of characterizing cycles originally used by Steiner [23]. A cycle is assigned a k given by half the number of contiguous subsequences when a cycle is partitioned into increasing sequences of odd numbers and decreasing sequences of even numbers. For example, supposing the partial orbit $(5, 10, 20, 14, 7, 5)$ existed, it would be a 1-cycle. Any cycle in the Collatz must be a k-cycle for some k, and this can just be thought of as the number of "ups and downs" in a cycle.

2.2.2 Some Heuristics

Before getting into specific results on cycles and their existence, we will speak to a few proposed heuristics that gives us a general idea of what we *may* expect to be true. These are non-rigorous, and only speak to what it *seems* may be the case, given some simplified way of approaching the problem. This problem in particular is rife with these sorts of propositions, perhaps given the difficulty of determining meaningful properties in a more rigorous manner.

One of the simplest pieces of evidence in favour of the conjecture is that we haven't yet found a non-terminating starting point through extensive calculation. Though far from a proof, in several of the variants of the conjecture - including $3n + 1$ over the integers [15], $5n+1$ [19], and a ceiling function based $bn+1$ [18] - there do exist non-trivial cycles. In all of these problems, the non-trivial cycles occur for quite small values of starting points, which *may* suggest that we are unlikely to find cycles for very large values. As well, no large cycles (in these variants) are known, and we do know that any cycle in the Collatz process must be quite large given currently computed lower bounds on cycle length. One interesting observation respecting the $5n+1$ problem (which has several non-trivial cycles) is that any proof of Collatz must distinguish some difference between 3 and 5, given that the change in scalar in the odd step changes the problem.

Next, we go back to the original results of Crandall [7]. Though he goes on to prove the result discussed earlier, he begins his paper with probabilistic heuristic on why iterates of C should decrease at an exponential rate. This was a random-walk argument, based on the assumption that $\log \frac{C(n)}{n}$ behaves as a pseudo-random variable for sufficiently large n. Then, we have that $\log \frac{C(n)}{n}$ is approximated by $\log 3 - k \log 2$ with probability 2^{-k}, giving us the expected value:

$$\mathbb{E} \log \frac{C(n)}{n} = -\log \frac{4}{3} \tag{2.1}$$

This then indicates that $C(m)$ tends to be less than m. Imagining the iteration of C induces a random walk along the real line, an estimate of $h_C(n)$ is given

$$h_C(n) \sim \frac{\log n}{\log \frac{4}{3}} \tag{2.2}$$

Crandall contends that this suggests that the number of cycles are strongly likely to be finite, and most starting points will converge eventually.

One must of course be careful of becoming *too* convinced by these arguments. What is true for almost all integers is not necessarily true for all, and only a single counterexample is needed for the conjecture to fail. We have no assurance that a counterexample should occur for a small integer either, so knowing that the first 2^{68} natural numbers converge may not be terribly convincing evidence. Still, these types of informal arguments are a good place to find a footing on what results we may expect, and in what directions we should try to find more concrete results.

2.2.3 Results on k-Cycles

Many of the results on cycles come through the perspective of k-cycles, as this has been the most fruitful method of framing the problem by which results can be derived. Unfortunately, as with so many things, as k increases, the complexity of these cycles (and proving things about them) increases non-linearly. As was mentioned, these were first formally studied by Steiner [23], who managed to prove that there is no 1-cycle, other than the trivial cycle. His proof went by showing that the ratio between the number of even and odd numbers in a 1-cycle must be a convergent to $\log_2(3)$, and using a theorem of Baker (not Baker's theorem) on linear forms in 2 logarithms, was able to derive an upper bound for odd steps. He similarly devised a lower bound for the partial quotient of the convergent of any possible solution, and then concluded that the trivial cycle was the only such cycle satisfying these conditions. Lagarias later commented that this result was quite weak, considering the invocation of Baker's results in transcendental number theory [16].

Nearly 3 decades later, Simons [21] directly extended Steiner's methods to prove that no 2-cycles exist. His derivation is thus remarkably similar, and only differs in that the ratio is between the sums of odd steps and even steps for all $2k$ subsequences, and he invokes a theorem from Laurent et al. [17] on linear forms in 2 logarithms to put an upper bound on the number of odd steps. Amusingly, Simons remarked that Lagarias's comments on the weakness of the result still apply here - but he also proves that this method fails for any $k > 2$. Thus, stronger methods need to be devised to show larger k-cycles cannot exist.

Just a year later, Simons and de Weger do so [22]. This method is still heavily based on the original method by Steiner, but generalized in a few ways. Instead of looking at the ratio between the total number of odd steps, M, and even steps, L, they examine $(M+L)\log 2 - K\log 3$, and look for upper and lower bounds for this in terms of M and L. The upper bound is shown to be exponential in M and the lower subexponential in L. Then, using similar methods as in [21], and some amount of brute-force computation on the lower bound, they show that no k-cycles exist for $k \leq 68$. This is a good bit stronger than previous results, although it is of course still limited to a small subset of all possible cycles. What's interesting about this approach is that, for any $k > 68$, it provides upper bounds for which some element in a k-cycle must be less than. What this allows for is the increasing removal of possible k as larger starting points are tested. In fact, it is now known that this is true for $k \leq 75$, since the starting points we have checked have surpassed the minimum elements for k-cycles with k up to 75.

Chapter 3

An Algebraic Formulation of Non-Trivial Cycles Subproblem

Böhm and Sontacchi [6] were the first to come up with an algebraic formulation of **SP1**. They start by generally considering a function that evaluates on one of two linear functions based on some condition as a function of the input. This is a pretty general form of an iterative linear function, of which the Collatz maps are examples. They derive an expression for the output of such a map after b iterations. This is of course entirely dependant on the truth value of the condition that determines which linear function is evaluated at each step. In the case of Collatz, this condition is the parity of the input. Then, restricting to the specific case of the map T, they derive a general form after b iterates:

$$T^{(b)}(n) = \frac{3^a n + \sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k}}{2^b} \tag{3.1}$$

where

$$v_i = (i-1) + \sum_{j=1}^{i} m_j$$

for $(m_1, m_2, \ldots, m_a) \subset \mathbb{N}$.

Unfortunately, this is where Böhm and Sontacchi leave us. The above can easily be turned into a Diophantine equation whose solutions represent cycles, as well as one whose solutions determine convergence to 1. Before taking a look at these, we will take a step back, and provide a derivation for the above - which was taken for granted in their original paper - and give a little bit more insight into the meaning of the sequence of integers, v.

3.1 Deriving the Explicit Map

The proof of the aforementioned explicitization of $T^{(b)}(n)$ was skipped for good reason: it is quite simple. That said, the result on its own is not particularly elucidative for understanding the structure of the summation that appears, and how this relates to our choices of b and n. With that in mind, consider the following theorem.

Theorem 3.1.1. Let $n, b \in \mathbb{N}^+$. Let $v(b,n) = (k\colon T^{(k)}(n) \equiv 1 \pmod 2, 0 \leq k < b)$ be the sequence denoting the zero-indexed indices of the iterates for which $T^{(k)}(n)$ is odd. Denote by a the length of $v(b,n)$, and denote by v_i the i-th element of $v(b,n)$. Then,

$$T^{(b)}(n) = \frac{3^a n + \sum_{k=0}^{a-1} 3^{a-k-1} \cdot 2^{v_k}}{2^b}$$

Proof. For b iterates, we express $T^{(b)}(n)$:

$$T^{(b)}(n) = \frac{3 \cdot \cfrac{\vdots}{3 \cdot \ldots \cdot \cfrac{3 \cdot \cfrac{3 \cdot \cfrac{n}{2^{v_1}} + 1}{2^{v_2 - v_1}} + 1}{} + \ldots + 1}{2^{v_a - v_{a-1}}} + 1}{2^{b - v_a}}$$

Notice that we must have $v_a \leq b - 1$ given that $2^{b-v_a} \geq 2$ in our lowest denominator. Simplifying, we get

$$T^{(b)}(n) = \frac{3^a n}{2^b} + \frac{3^{a-1}}{2^{b-v_1}} + \frac{3^{a-2}}{2^{b-v_2}} + \ldots + \frac{3^0}{2^{b-v_a}}$$
$$T^{(b)}(n) = \frac{3^a n + 2^{v_1} \cdot 3^{a-1} + 2^{v_2} \cdot 3^{a-2} + \ldots + 2^{v_a} \cdot 3^0}{2^b}$$
$$T^{(b)}(n) = \frac{3^a n + \sum_{k=1}^{a} 3^{a-k} 2^{v_k}}{2^b}$$

□

What we see is that our sequence, $v(b,n)$, encodes the steps at which our input into T is odd. This is perhaps unsurprising, as this clearly characterizes the entire sequence; we take all other steps to be acting on even inputs, and we have the whole thing. We also see that $v(b,n)$ must be a strictly increasing sequence, with a minimum difference of 1 between adjacent elements. Thus, we can equivalently encode this by the sequence of differences, $(m_1, m_2, \ldots, m_a) \subset \mathbb{N}$, where $v(b,a)$ is then given

$$v_i = (i-1) + \sum_{j=1}^{i} m_j$$

as we see above.

3.2 An Equation for Cycles

Now, we want to use this fact to generate our Diophantine equation whose solutions determine cycles.

Theorem 3.2.1. Let $w \in \mathbb{N}^+$. Then, w is in a cycle under the Collatz process if there exist $a, b \in \mathbb{N}^+$, $(m_i)_{1\leq i\leq a} \subset \mathbb{N}$ such that

$$w(2^b - 3^a) = \sum_{k=1}^{a} 3^{a-k} 2^{v_k} \tag{3.2}$$

for $v_i = (i-1) + \sum_{j=1}^{i} m_j$ and $v_a \leq b-1$.

Proof. Consider $w = T^{(b)}(w)$ for some $b \in \mathbb{N}^+$. Then

$$\begin{aligned} w &= \frac{3^a w + \sum_{k=1}^{a} 3^{a-k} 2^{v_k}}{2^b} \\ 2^b w - 3^a w &= \sum_{k=1}^{a} 3^{a-k} 2^{v_k} \\ w(2^b - 3^a) &= \sum_{k=1}^{a} 3^{a-k} 2^{v_k} \end{aligned}$$

simply by rearrangement. By Theorem 3.1.1, when we have that when $v_a \leq b-1$, this represents a partial orbit in the Collatz process. Thus, such a solution gives us an orbit that contains the same element twice - and thus a cycle. □

3.2.1 Known Solutions

We will now present the two known solutions to Equation 3.2, and an example of how we can use this to filter out some non-solutions in special cases.

Lemma 3.2.1. Let $w = 1$, $a \in \mathbb{N}^+$, and $b = 2a$. Then Equation 3.2 is satisfied by $v(b, w) = (0, 2, 4, \ldots, b-2)$. Further, this corresponds to the $1, 2$-cycle, with 1 being mapped to 1.

Lemma 3.2.2. Let $w = 2$, $a \in \mathbb{N}^+$, and $b = 2a$. Then Equation 3.2 is satisfied by $v(b, w) = (1, 3, 5, \ldots, b-1)$. Further, this corresponds to the $1, 2$-cycle, with 2 being mapped to 2.

For the time being, we will not provide a derivation of these solutions, as that will hinge upon a different form of Equation 3.2 we introduce in the next chapter. Of course, it suffices to substitute these solutions into the equation to convince ourselves that they truly do represent cycles. A very trivial fact, though one that perhaps bears mentioning, is the following.

Lemma 3.2.3. Let $w = 2^m$ for $m \geq 1$. Then there is no solution, $a, b, v(b, w)$ satisfying Equation 3.2.

Proof. Considering that all powers of 2 trivially converge to 1, and thus are not in a cycle (outside of 1 and 2), this holds. However, we can show this in terms of our equation. We know that for $w = 1$, $v(b, 1) = (0, 2, \ldots, b - 2)$. Under multiplication by 2^m, it is clear simply by the form of our summation that $v(b, 2^m) = (m, m + 2, \ldots, b - 2 + m)$. Since we require that the largest element of $v(b, n)$ does not exceed $b - 1$, we must have that $m \leq 1$. □

In general, we would like to make arguments similar to this for multiplication under arbitrary integers - that is, to transform $v(b, n)$ into $v(b, mn)$ for some $m \in \mathbb{N}^+$. However, little is known about how these sequences behave under multiplication or even addition for arbitrary elements. Later, we will see some empirical examples of this.

3.3 An Equation for Convergence

As we have formulated Equation 3.2, its solutions tell us about cycles in the Collatz process. We can also very easily use Theorem 3.1.1 to derive an equation of a similar form that tells us which numbers converge under T.

Theorem 3.3.1. Let $w \in \mathbb{N}^+$. Then, w converges to 1 under the Collatz process if there exist $a, b \in \mathbb{N}^+$, $(m_i)_{1 \leq i \leq a} \subset \mathbb{N}^+$ such that

$$2^b - 3^a w = \sum_{k=1}^{a} 3^{a-k} 2^{v_k} \tag{3.3}$$

for $v_i = (i - 1) + \sum_{j=1}^{i} m_j$ and $v_a \leq b - 1$.

Proof. The proof follows exactly that of Theorem 3.2.1, except we set $T^{(b)}(w) = 1$. □

This is clearly a very similar problem to our cyclic equation in the previous section, except that we are no longer scaling the difference of the powers of 2 and 3 - just the power of 3. Whether this makes the problem more or less difficult is hard to say. For now, we will discuss integers of the form given by our summation of products of powers of 2 and 3.

Chapter 4

On k-special 3-smooth Representations of Integers

A p-smooth number, for p (generally) a prime, is a number whose prime factors do not exceed p. Smooth numbers have been an object of study for hundreds of years - though they have only been known by the term since the 20th century. Thus, a number, n is said to be 3-smooth if it can be written

$$n = 2^p \cdot 3^q$$

for $p, q \in \mathbb{N}$. We say that a number has a 3-smooth representation if it can be written as the sum of 3-smooth numbers. Such a number, n, can then be written

$$n = \sum_{j=1}^{k} 2^{p_j} \cdot 3^{q_j}$$

for $p_j, q_j \in \mathbb{N}$. Such a representation is called *primitive* if no summand divides another. This can only happen if $p_1 > p_2 > \ldots > p_k \geq 0$ and $0 \leq q_1 < q_2 < \ldots < q_j$ [4]. Further, such a representation is called k-special if it consists of k summands, and $q_1 = 0$, $q_2 = 1$,..., $q_k = k - 1$. It is known that every positive natural number has a primitive 3-smooth representation [5, 4], but not every number has a k-special primitive 3-smooth representation [4, 10, 2]. For the simplest case, just notice that any number divisible by 3 cannot have such a representation. Of course, we see that the sum of interest in Equation 3.2 is an a-special representation of some integer.

4.1 A Bit of Notation

We begin by defining a few sets that will be useful to have a shorthand for, followed by some functions that associate k-special representations and the numbers they represent.

Notation 4.1.1. Let $\mathbb{A}$ denote the set of all strictly monotone increasing sequences of finitely-many elements with entries in $\mathbb{N}$. That is

$$\mathbb{A} = \{(A_i)_{1 \le i \le n} \colon n \in \mathbb{N}^+, A_i < A_{i+1}\}$$

Notation 4.1.2. Let $\mathbb{A}_n$ denote the subset of $\mathbb{A}$ with sequences of length n.

$$\mathbb{A}_n = \{A \in \mathbb{A} \colon |A| = n\}$$

Definition 4.1.1. Let $R \colon \mathbb{A} \to \mathbb{N}$ be the function that maps sequences of monotone increasing natural numbers to the ($|A|$)-special number they represent. Explicitly,

$$R \colon A \mapsto \sum_{k=1}^{|A|} 3^{|A|-k} \cdot 2^{A_j}$$

Definition 4.1.2. Let $R_n \colon \mathbb{A}_n \to \mathbb{N}$ be the function that maps sequences of monotone increasing natural numbers of length n to the n-special number they represent. Explicitly,

$$R_n \colon A \mapsto \sum_{k=1}^{n} 3^{n-k} \cdot 2^{A_j}$$

Remark 4.1.1. Often throughout this paper, we will refer to a number having a k-special representation, or simply having a representation. In any case except those where it is made clear, we are referring to k-special primitive 3-smooth representations. The full descriptor is dropped for the sake of brevity.

4.2 What is Known?

In general, a good bit more is known about 3-smooth representations than k-special 3-smooth representations - and even then, only a few paper exist that present results about them. For example, it has been shown that every $n \in \mathbb{N}^+$ has a 3-smooth representation - and in fact, most of them have quite a few [5, 2]. In fact, for sufficiently large n, we can construct representations that do not include arbitrarily large small terms [4]. Conversely, many numbers do not have a k-special representation for any k, and for those that do, the representation is unique for a given k [10, 4]. We also prove this later. It is also relatively obvious that every number has a representation for at most finitely-many k. As we have seen, there are also parameterized expressions that have a representation for every k. While we do know some facts about these numbers in general, it is much more difficult to speak about them with specificity. For example, it is not well-characterised what happens to a representation of n under multiplication. It is also not known what the density of numbers with a k-special representation is. Given such (seemingly) basic facts about these numbers are unknown, there is a great deal of potential for further research on these representations.

4.3 Some Basic Facts

Here we prove some cursory facts pertaining to R and R_n. We first derive upper and lower bounds on the images of R and R_n, given some maximum on the elements of A.

Proposition 4.3.1. Let $A \in \mathbb{A}$ with $\max A < b$. Then,

$$1 \leq R(A) \leq 3^b - 2^b$$

Proof. Since no term of the sum in $R(A)$ can be negative, and the shortest sequence is of length 1, it is clear that the minimum value is 1, given by $R((0)) = 1$. Similarly, it is apparent that the maximum value is given by the longest A with final entry not exceeding $b-1$, which is $A = (0, 1, \ldots, b-1)$. Then the sum is written

$$\sum_{k=1}^{b} 3^{b-k} \cdot 2^{k-1} = 3^b - 2^b$$

□

Proposition 4.3.2. Let $n \in \mathbb{N}^+$, $A \in \mathbb{A}_n$ with $\max A < b$. Then,

$$3^n - 2^n \leq R_n(A) \leq 2^{b-n}(3^n - 2^n)$$

Proof. Given the length of A is known, it is clear that the smallest value for $R_n(A)$ is achieved when A has the smallest elements it can. This is given by $A = (0, 1, \ldots, n-1)$. Then, the sum is written

$$\sum_{k=1}^{n} 3^{n-k} \cdot 2^{k-1} = 3^n - 2^n$$

Similarly, we can find the maximum value by considering the A with the maximal elements, $A = (b-n, b-n+1, \ldots, b-2, b-1)$ Then the sum is written

$$\sum_{k=1}^{n} 3^{n-k} \cdot 2^{b-n+k-1} = 2^{b-n}(3^n - 2^n)$$

□

Remark 4.3.1. Due to how we could represent the exponents in our sum in Equation 3.2 by either $v(b, n)$ or $(m_i)_{1 \leq i \leq a}$, we can represent our sum as a telescoping product. Given some $A \in \mathbb{A}_n$ for $n \in \mathbb{N}^+$, let $m = (m_i)_{1 \leq i \leq n}$ such that $A_i = (i-1) + \sum_{j=1}^{i} m_j$.

Then, we have

$$\sum_{k=1}^{a} 3^{a-k}2^{A_k} = 2^{m_1}(2^{m_2}(\ldots(2^{m_a}+3)+3^2)+\ldots+3^{a-1})$$

This is easily observed by repeatedly factoring out the largest possible power of 2 that divides all terms, and iterating until we are left with only $2^{m_a}+3$.

It is very clear that R is not surjective. Any multiple of 3, for example, does not have a k-special representation for any $k \in \mathbb{N}^+$. The next natural question is whether R is injective. Perhaps unfortunately, it is not. However, R_n is injective for every $n \in \mathbb{N}^+$.

Lemma 4.3.1. R_n is injective for all $n \in \mathbb{N}^+$.

Proof. Let $w \in \mathbb{N}^+$ such that there exists $n \in \mathbb{N}^+, A \in \mathbb{A}_n$ with $w = R_n(A)$. Let $p = (p_i)_{1\le i\le n}$ such that $A_i = (i-1)+\sum_{j=1}^{i} p_j$. Suppose there exists $B \in \mathbb{A}_n$ with $R_n(A) = R_n(B)$, and similarly let $q = (q_i)_{1\le i\le n}$ such that $B_i = (i-1)+\sum_{j=1}^{i} q_j$. Then, we have

$$R(A) = R(B)$$
$$\sum_{k=1}^{n} 3^{n-k}2^{A_k} = \sum_{k=1}^{n} 3^{n-k}2^{B_k}$$
$$2^{p_1}(2^{p_2}(\ldots(2^{p_n}+3)+3^2)+\ldots+3^{n-1}) = 2^{q_1}(2^{q_2}(\ldots(2^{q_n}+3)+3^2)+\ldots+3^{n-1})$$

Suppose $p_i \neq q_i$ for some $1 \le i \le n$. Then, we have

$$2^{p_i}(2^{p_{i+1}}(\ldots(2^{p_n}+3)+3^2)+\ldots+3^{n-i}) = 2^{q_i}(2^{q_{i+1}}(\ldots(2^{q_n}+3)+3^2)+\ldots+3^{n-i})$$

Without loss of generality, assume $p_i > q_i$. Then, dividing both sides by 2^{q_i}, we get

$$2^{p_i-q_i}(2^{p_{i+1}}(\ldots(2^{p_n}+3)+3^2)+\ldots+3^{n-i}) = 2^{q_{i+1}}(\ldots(2^{q_n}+3)+3^2)+\ldots+3^{n-i-1})+3^{n-i}$$

But clearly the left hand side is even, and the right hand side odd, since $q_k \ge 1$ for all $1 \le k \le n$ - so this is a contradiction. Thus, $p_i = q_i$ for all i, and thus $A_i = B_i$, so $A = B$. □

Remark 4.3.2. An alternative proof of Lemma 4.3.1 is given by Lagarias [15] in Corollary 2.1a.

Remark 4.3.3. Since R_n is injective, it has a left inverse. This will prove useful later, and we define it explicitly using a similar process as in the proof of the injectivity of R_n.

Proposition 4.3.3. Given $w \in \mathbb{N}^+$ for which w has an a-special representation, $m = (m_1, \ldots, m_a) \subset \mathbb{N}^+$, that representation is given by

$$m_i = \nu_2(w - \sum_{j=1}^{i-1} 3^{a-j} 2^{m_j})$$

for each $1 \leq i \leq a$,

Proof. This is stated without proof, as it is determined to be self-evident. □

Lemma 4.3.2. Given $a, b \in \mathbb{N}^+$. Then $2^b - 3^a$ has an a-special representation if and only if $b = 2a$.

Proof. The backward direction is obvious, since we have previously derived the representation for $w(2^b - 3^a)$ for $w = 1$, $b = 2a$. Suppose $2^b - 3^a$ has a k-special representation, and assume that $b \neq 2a$. We show this cannot happen by iteratively solving for the representation. If $b < 2a$, then eventually we derive

$$2^{b - \sum_{k=1}^{l} m_k} - 3^{a-l} = 2^{m_{l+1}}(\ldots(2^m_a + 3) + \ldots + 3^{a-l-1})$$

with $b - \sum_{k=1}^{l} m_k < 2$. Then, we get that

$$2^{b - \sum_{k=1}^{l} m_k} - 3^{a-l} < 0$$

which is impossible, so we get a contradiction. If $b > 2a$, then similarly we derive

$$2^{b - \sum_{k=1}^{a-1} m_k} - 3 = 2^{m_a}$$

so we need that $b - \sum_{k=1}^{a-1} m_k = 2$, since this is the only solution to $2^p - 3 = 2^q$. Since $m_k = 2$ for all $k \neq 1$, we have $b - \sum_{k=1}^{a-1} m_k = b - (2a - 2) > 2$ since $b > 2a$. This is a contradiction. Thus, $b = 2a$. □

Unfortunately, the picture is not so simple when $b \neq 2a$, or $w \neq 1$. As we will see in the next section, the k-special representation of $w(2^b - 3^a)$ depends mostly on the behaviour of w under P. This means that certain w will have a predictable representation, and others will not. In particular - and perhaps predictably - we will see that the w that converge very quickly under P can be assuredly excluded from candidacy for cyclicity. Take the following, for example:

Proposition 4.3.4. Suppose $w \in \mathbb{N}^+$ not equal to 1 with $3w + 1 = 2^n$ for $n \in \mathbb{N}^+$. Then, if $w(2^b - 3^a)$ has an a-special representation, we have $v_a > b - 1$. That is, w is not cyclic.

Proof. This is immediately true given any power of 2 trivially converges to 1, and w maps to 2^n under C. However, consider the following argument in terms of Equation 3.2, and the telescoping product from earlier.

Since $3w + 1 = 2^n$, we have that $w = \frac{4^k-1}{3}$ for some $k \in \mathbb{N}^+$. Consider

$$w \cdot 2^b - w \cdot 3^a = 2^{m_1}(\cdot \ldots \cdot (2^{m_a} + 3) + \ldots + 3^{a-1})$$

We have $m_1 = 0$ since w and $2^b - 3^a$ are odd. Then,

$$w \cdot 2^b - w \cdot 3^a - 3^{a-1} = 2^{m_2}(\cdot \ldots \cdot (2^{m_a} + 3) + \ldots + 3^{a-2})$$
$$w \cdot 2^b - 3^{a-1}(3w + 1) = 2^{m_2}(\cdot \ldots \cdot (2^{m_a} + 3) + \ldots + 3^{a-2})$$

Clearly, $\nu_2(3w + 1) = k$, so if $k \geq b$, we are done. So, assume $k < b$. Then $m_2 = k$. We get

$$w \cdot 2^{b-k} - 3^{a-2}(3 + 1) = 2^{m_3}(\cdot \ldots \cdot (2^{m_a} + 3) + \ldots + 3^{a-3})$$

Which clearly gives $m_3 = 2$ if $b - k > 2$. If we get that $b - k \leq 2$, then we are done. Repeating this process, we get $m_j = 2$ for all $j < a$ while $b - k - \sum_{i=1}^{j-1} m_i > 2$. Thus, if $b < k + 2m$ for some $m < a - 1$, get that $v_a \geq b$. We assume $b - k - \sum_{i=1}^{a-1} m_i > 2$, and denote this quantity by l. We eventually get

$$w \cdot 2^l - 3(3 + 1) = 2^{m_a}$$

We get $m_a = 2 + \nu_2(w \cdot 2^{l-2} - 3)$, and of course have that $w \cdot 2^{l-2} - 3$ is a power of 2 since $w(2^b - 3^a)$ has an a-special representation. The only solutions to this are for $w = 1$ or $w = 5$, and $l = 4$ or $l = 2$. In the first case, get that $m_a = 2$, so $v_a = b - l + m_a = b - 2$. In the second case, $m_a = 3$, so $v_a = b + 1$. Thus, for any w such that $3w + 1 = 2^n$, we get that $v_a > b - 1$ unless $w = 1$. ☐

Much like the above proposition, a good deal of what we will show is not novel in terms of the result - that is, it has been argued before through different means - but it is more an examination of how these facts present in light of this algebraic formulation and k-special representations. Ultimately, it is hoped that by better understanding these integer representations, more deep results can be determined - but for now we will splash around the surface a bit for the sake of familiarizing ourselves these equations.

4.4 k-special Representations and Collatz

With this in mind, we can now recontextualize our discussion of Equation 3.2.

Lemma 4.4.1. Given $w \in \mathbb{N}^+$, we have that w is cyclic if and only if there exist $a, b \in \mathbb{N}^+$ such that $w(2^b - 3^a)$ has an a-special representation with $v_a \leq b - 1$.

Proof. This follows directly from Theorem 3.2.1 ☐

This motivates the discussion of what k-special representations act like under multiplication and addition. Unfortunately, this is far from a simple question to answer for arbitrary multiplication and addition. For example, we know that image(R_n) is not closed under either operation. Further, the coefficients in the representation are unpredictable under these operations. We are truly only interested in the largest power of 2 in the representation of a given integer, and specifically integers of the form $w(2^b - 3^a)$. While one would hope this makes the situation easier, this is only vaguely true. That said, we can exploit the form of the expression, along with our iterative method of solving for a k-special representation, to derive the conditions under which the largest power of 2 does not exceed $b - 1$. We get the following.

Lemma 4.4.2. Let $w \in \mathbb{N}^+$ such that $w(2^b - 3^a)$ has an a-special representation, for $a, b \in \mathbb{N}^+$. Then, the exponent on the largest power of 2 in the a-special representation, v, does not exceed $b - 1$ if and only if there exists $n \in \mathbb{N}^+$ such that

$$2^n w = 1 + 3P^{(a)}(w)$$

Further, $v_a = b - n$.

Proof. In some ways, this is almost self-evident when one considers that for a number, w, to be mapped to itself by C, it must first be mapped to some power of 2 times w. A number may only be mapped to a number larger than itself under C by an odd operation, and the value of every element in $\text{orb}_P(w)$ is odd. Thus, for w to be cyclic, its P-orbit must have an element that, when multiplied by 3 and having 1 added to it, becomes $2^n w$. We also provide a computational derivation using our telescoping product form of a k-special representation.

Consider the process of finding $R_a^{-1}(w(2^b - 3^a))$ as follows:

$$2^b w - 3^a w = 2^{m_1}(2^{m_2}(\dots(2^{m_a} + 3) + 3^2) + \dots + 3^{a-1})$$

Immediately, we get $m_1 = \nu_2(2^b w - 3^a w)$. We assume $m_1 \leq b - 1$. Let $w_1 = \frac{w}{2^{m_1}} = P(w)$. Then, rearranging, we get

$$2^b w - 3^a w_1 - 3^{a-1} = 2^{m_2}(2^{m_3}(\dots(2^{m_a} + 3) + 3^2) + \dots + 3^{a-2})$$
$$2^b w - 3^{a-1}(3w_1 + 1) = 2^{m_2}(2^{m_3}(\dots(2^{m_a} + 3) + 3^2) + \dots + 3^{a-2})$$

Clearly, m_2 is bounded below by $\min\{b - 1, \nu_2(3w_1 + 1)\}$, with equality to $\nu_2(3w_2 + 1)$ if $\nu_2(3w_2 + 1) < b$. If $m_1 + \nu_2(3w + 1) \geq b - 1$, then we have that this solution isn't of interest to us. Thus, we assume $m_1 + \nu_2(3w_1 + 1) < b - 1$. We have $m_2 = \nu_2(3w_1 + 1)$. Let $w_2 = \frac{3w_1+1}{2^{m_2}} = P(3w_1 + 1)$. We continue the procedure as above, each time assuming that $1 + \sum_{k=1}^{q} m_k < b$, as otherwise, we would have that this solution could be discarded. Thus, we get

$$2^{b - \sum_{k=1}^{q} m_k} w - 3^{a-q} w_{q+1} = 2^{m_{q+2}}(\dots) + 3^{a-q-1}$$

for $w_{q+1} = P^{q+1}(w)$. Since the sum of m_k is less than $b-1$ for all $1 \leq q \leq a$, we eventually derive

$$2^{b-\sum_{k=1}^{a} m_k} w - 3w_a = 1$$

Let $n := b - \sum_{k=1}^{a} m_k$. The above is then rewritten:

$$2^n w = 1 + 3w_a \tag{4.1}$$

We now have that any number of the form $w(2^b - 3^a)$ with an a-special representation with the exponent on the largest power of 2 not exceeding b, there must exist a solution to Equation 4.1 for which $n \in \mathbb{N}^+$, and $w_a = P^a(w)$. □

The immediate question is then: which w satisfy Equation 4.1? The unfortunate answer is that this is difficult to determine. We haven't exactly stepped outside of the Collatz process, as we still need to predict the elements of $\text{orb}_P(w)$. If we relax the condition that $w_a = P^{(a)}(w)$, and just check for odd w_a that satisfy this, we get an infinite family of solutions, S_w, of the form:

$$S_w = \begin{cases} \dfrac{4^k w - 1}{3} & : w \equiv 1 \pmod 3 \\ \dfrac{4^k w - 2}{6} & : w \equiv 2 \pmod 3 \end{cases}$$

for some $k \in \mathbb{N}^+$. We use the parameter k here, transformed from n by $k = 2n$ if n is even and $k = 2n-1$ if n is odd. Notice that we do not consider any w which is a multiple of 3, as these cause $w(2^b - 3^a)$ to never have an a-special representation trivially. What we then want is the set of w for which $\text{orb}_P(w) \cap S_w \neq \emptyset$.

In order to reduce the set of possible such w, we notice that $s \equiv -3^{-1} \pmod w$ for any $s \in S_w$. Clearly, there are $x \in \mathbb{N}^+$ with $x \equiv -3^{-1} \pmod w$ and $x \notin S_w$, but for now we will investigate the set of w whose P-orbit contains such an element. For any w that is cyclic, it is a necessary condition that some element of its orbit is equivalent to $-3^{-1} \mod w$. So what is this set? We consider $w \geq 5$, as we trivially have that 1, 2, and 4 are cyclic, and 3 converges. Then, we get that the set of such w is given

$$\{31, 62, 83, 166, 293, 586, 347, 694, 671, 1342, 2684, 19151, 38302, 2025797, 4051594\}$$

for $w \leq 10^7$. Note that every number in this set is either odd, or a power of 2 times an odd element of the set. The question remains: what is this set of numbers, and how are they related? As we will see later on, these are the self-contained numbers.

4.5 A Foray into Empiricism

In this section, we present some empirical results, and make less rigorous observations about some properties that we tend to notice in the study of k-special integer representations. Much of what is written here is conjectural, and derived from observation of a limited set of data. That said, we contend that there may be use in including this section so as to give more insight into the stalled directions research took, and get a better look at some of the problems we would otherwise have little to say about.

4.5.1 Behaviour under multiplication

Here we investigate when the property of having a k-special representation is preserved under multiplication - and what it looks like when it is preserved. In particular, we look at this for numbers of the form $2^b - 3^a$, and further try to characterize when some multiple of a number of this form has a representation - even when $2^b - 3^a$ does not. From Lemma 4.3.2 we know that $2^b - 3^a$ only has a k-special representation when $b = 2a$, but there are $w \in \mathbb{N}^+$ such that $w(2^b - 3^a)$ has a representation for $b \neq 2a$. First, we will investigate the w such that $w(2^{2a} - 3^a)$ has a representation, then more generally, such that $w(2^b - 3^a)$ has one.

The case when $b = 2a$

Denote by $W(a, b)$ the set of $w \in \mathbb{N}^+$ such that $w(2^b - 3^a)$ has an a-special representation, for w odd. Note that we only need to consider odd w, as any power of 2 times such a w will also ensure this has a representation. See Table 4.1 for some values of $W(a, 2a)$. Clearly, $W(a, 2a)$ is dependent on our choice of a - and the size of the set increases with a. We also notice an approximate sequential inclusion between $W(a, 2a)$ and $W(a+1, 2(a+1))$. For small a, this is true inclusion - but as a increases, the number of elements in $W(a, 2a)$ not in $W(a+1, 2(a+1))$ increases. However, if we place an upper bound on the elements in $W(a, 2a)$, we notice that as a increases, the inclusion approaches being complete. That is, if we take the elements of $W(a, 2a)$ and $W(a + 1, 2(a + 1))$ no greater than M, as a gets larger, more elements of $W(a, 2a)$ tend to appear in $W(a + 1, 2(a + 1))$. As an example of a number that does not follow this inclusion, take 547, which first appears for $a = 6$ - but then is not there for $a = 7$. What is interesting is that 547 goes on to be in $W(a, 2a)$ for any $a \geq 11$. So, sometimes numbers appear and then continue to appear for all subsequent a, and other times the will appear once, skip a few a, and then always appear after some other a. This begs the question: do any only show up once, and then never again? Do some show up only a finite number of times? The answer seems to be yes to both of these. For example, both 725 and 821 appear when $a = 7$, do not appear again for any tested a, up to $a = 10^4$. An example for the second point is 8945, which shows up only for $a = 10$ and $a = 12$, and not again (at least up to 10^4). All this paints a bit of a messy picture of the situation, so we will observe this from another perspective to try to understand what is going on.

TABLE 4.1: The sets $W(a, 2a)$ for $1 \leq a \leq 7$, for $w < 3^a$.

a	$W(a, 2a)$
1	{ 1 }
2	{ 1, 5 }
3	{ 1, 5 }
4	{ 1, 5, 53 }
5	{ 1, 5, 11, 53, 85 }
6	{ 1, 5, 11, 53, 85, 151, 341, 547, 565 }
7	{ 1, 5, 11, 19, 53, 85, 151, 325, 341, 565, 725, 821, 2071, 2161 }
8	{ 1, 5, 11, 19, 53, 85, 149, 151, 341, 397, 565, 1477, 1613, 2285, 2801 }

The following may seem a bit unorthodox at first blush, but we end up seeing something interesting. What we do is, for some $x \in W(a, 2a)$ such that $x \in W(a+k, 2(a+k))$ for all $k \geq 1$, we calculate the representation, $v(2a, w)$, of $w(2^{2a} - 3^a)$ for increasing a, as well as the representation, $v(2a, 1)$, for $2^{2a} - 3^a$. Then, we take the component-wise difference of these as vectors, denoted $v(2a, w) - v(2a, 1)$. See Table 4.2 for an example of this with $w = 5$. For an example with $w = 341$, see Table 4.3. Looking at the difference sequences, we see a clear pattern in the examples presented here. For the first a for which some w causes $w(2^{2a} - 3^a)$ to have a representation, we get some difference sequence that doesn't look like the following ones. Then, for every a after that, there is a clear pattern that can be partitioned by a leading sequence, trailing sequence, and repeating digit between them. In the case of $a = 5$, the leading sequence is (0), the trailing is (3), and the repeating digit is 2. For $w = 341$, these are (0), $(10, 9, 8, 7)$, and 8 respectively. Immediately, there are several questions: how do we predict the parameters of this pattern? How do we come up with the term proceeding the first, given the first term? What about the w for which the a such that $w(2^{2a} - 3^a)$ has a representation are not sequential? For now, we can only give observational answers to these most of questions - but we can actually formalize some of these patterns on a case-by-case basis.

We try to generalize what was observed above with respect to a leading sequence, trailing sequence, and repeating digit. Consider the case when $w = 85$. Then, we want $v(2a, 85(2^{2a} - 3^a))$, the a-special representation of $85(2^{2a} - 3^a)$. We will work backwards from the known representation, which is given $(v_k)_{1 \leq k \leq a} = (0, 8, 10, \ldots, 2a - 2, 2a + 1, 2a + 3, 2a + 4)$. In terms of the difference sequences, this has leading sequence (0), trailing sequence $(7, 7, 6)$, and repeating digit 6. We then have

$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 3^{a-1} \cdot 2^0 + 3^2 \cdot 2^{2a+1} + 3^1 \cdot 2^{2a+3} + 3^0 \cdot 2^{2a+4} + \sum_{k=3}^{a-2} 3^k 2^{2(a-k)+4}$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 3^{a-1} \cdot 2^0 + 3^2 \cdot 2^{2a+1} + 3^1 \cdot 2^{2a+3} + 3^0 \cdot 2^{2a+4} + 2^{2(a+2)} \cdot \sum_{k=3}^{a-2} (\frac{3}{4})^k$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 3^{a-1} \cdot 2^0 + 3^2 \cdot 2^{2a+1} + 3^1 \cdot 2^{2a+3} + 3^0 \cdot 2^{2a+4} + 2^{2(a+2)} \cdot (\frac{3^3}{4^2} - \frac{3^{a-1}}{4^{a-2}})$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 3^{a-1} 2^0 + 3^2 \cdot 2^{2a+1} + 3^1 \cdot 2^{2a+3} + 3^0 \cdot 2^{2a+4} + 3^3 \cdot 2^{2a} - 3^{a-1} \cdot 2^8$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 4^a(2^4 + 3 \cdot 2^3 + 3^2 \cdot 2 + 3^3) - 3^{a-1}(2^8 - 1)$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 4^a \cdot 81 - 3^a \cdot 81$$
$$\sum_{k=1}^{a} 3^{a-k} \cdot 2^{v_k} = 81(4^a - 3^a \cdot)$$

Denote the length of the leading sequence by l, the length of the trailing sequence by t, and the repeating digit by s. We can generalize a few things from this example. In the new sum we get once we break out the non-repeating terms, the bounds now go from $k = t$ to $a - (l + 1)$. The power of 2 we pull out from this sum is $2^{2(a-1)+s}$. Using this, when we factor into a difference of a multiple of 4^a and 3^{a-l}, we have that the coefficient on 4^a, which we denote r_1, has the form of a $(t+1)$-special number. Further, the coefficient on 3^{a-l} is $2^{s+2l} - r_2$, for r_2 a l-special number. Finally, the power of 2 on the largest power of 3 in r_1 is 2^{s-2t}. All of this can be shown to generalize for any sequence with this leading, trailing, and repeating form - except for r_1 being $(t + 1)$-special. In many cases it is, but note that $s - 2t$ can be bigger than the exponent on the power of 2 preceding the largest power of 3 term in the representation. Take, for example, when $w = 4835$. Here, $r_1 = 2^{11} + 3 \cdot 2^9 + 3^2 \cdot 2^6 + 3^3 \cdot 2^2 + 3^4 + 3^5 \cdot 2$. Of course, $r_1 = 4835$ - but this is not the $(t + 1)$-special representation of 4835; that is given by $(0, 4, 5, 7, 8, 9)$. What is not clear then is whether we need that r_1 have a $(t+1)$-special representation, even though r_1 is not necessarily of that form. In every tested case, it has been the case that such a representation exists - but this is not known in general. This is unfortunate, as this is the part of this process that is critically important to us - that is, the largest power of 2 in r_1 tells us how much more than $2a$ the largest power of 2 in the a-special representation of $w(2^b - 3^a)$ is. In the case where r_1 matches its $(t + 1)$-special representation, this allows us to say definitively that $v_a > 2a - 2$, but when it does not, the picture is a bit fuzzier. Without dwelling too long here, we will now discuss some of the other patterns observed when the a for which $w(2^{2a} - 3^a)$ had an a-special representation are not sequential.

TABLE 4.2: The a-special representations of $2^{2a} - 3^a$ and $w(2^{2a} - 3^a)$, as well as their difference, for $2 \le a \le 8$ and $w = 5$.

a	$v(2a, 1)$	$v(2a, 5)$	$v(2a, 5) - v(2a, 1)$
2	(0, 2)	(0, 5)	(0, 3)
3	(0, 2, 4)	(0, 4, 7)	(0, 2, 3)
4	(0, 2, 4, 6)	(0, 4, 6, 9)	(0, 2, 2, 3)
5	(0, 2, 4, 6, 8)	(0, 4, 6, 8, 11)	(0, 2, 2, 2, 3)
6	(0, 2, 4, 6, 8, 10)	(0, 4, 6, 8, 10, 13)	(0, 2, 2, 2, 2, 3)
7	(0, 2, 4, 6, 8, 10, 12)	(0, 4, 6, 8, 10, 12, 15)	(0, 2, 2, 2, 2, 2, 3)
8	(0, 2, 4, 6, 8, 10, 12, 14)	(0, 4, 6, 8, 10, 12, 14, 17)	(0, 2, 2, 2, 2, 2, 2, 3)

TABLE 4.3: The a-special representations of $2^{2a} - 3^a$ and $w(2^{2a} - 3^a)$, as well as their difference, for $4 \le a \le 8$ and $w = 341$.

a	$v(2a, 1)$	$v(2a, 341)$	$v(2a, 341) - v(2a, 1)$
4	(0, 2, 4, 6)	(0, 8, 13, 15)	(0, 6, 9, 9)
5	(0, 2, 4, 6, 8)	(0, 12, 13, 14, 15)	(0, 10, 9, 8, 7)
6	(0, 2, 4, 6, 8, 10)	(0, 10, 14, 15, 16, 17)	(0, 8, 10, 9, 8, 7)
7	(0, 2, 4, 6, 8, 10, 12)	(0, 10, 12, 16, 17, 18, 19)	(0, 8, 8, 10, 9, 8, 7)
8	(0, 2, 4, 6, 8, 10, 12, 14)	(0, 10, 12, 14, 18, 19, 20, 21)	(0, 8, 8, 8, 10, 9, 8, 7)

Suppose we have that $w \in W(a, 2a)$ for $a \in \mathbb{N}^+$, $w \notin W(a+1, 2(a+1))$, and $w \in W(a+k, 2(a+k))$ for all $k \ge 2$. That is, w appears for some a, skips a number, and then appears for every a after that skip. There are 4 such numbers less than 10^3, and they are $\{325, 397, 545, 547\}$. See Tables 4.4, 4.5 for $w = 325$ and $w = 397$. Similarly to the w with no skips, these seem to present in a parametric pattern; a leading sequence, trailing sequence, a sequence the length of the skip, and repeating term that splits the sequence the length of the skip. For example, for $w = 325$, these are $(0, 2, 3, 2, 1)$, $(7, 10)$, $(4, 7)$, and 6. So does this hold up for arbitrary w? No. Unfortunately, and as in so many cases with this problem, while there are patterns to be found, they rarely generalize in a clean way. Many w do hold up to this pattern, and for w for which there is a skip of a different length, we can find similar patterns. In fact, as the size of the w we check increases, we see sequences of increasing a for which there are several skips, of different lengths - and each (often) follows one of the patterns we see for a sequence with a single skip of the given length. That said, and while there may be some phenomenology of interest here, this is perhaps not where time is best spent. Ultimately, what we are interested in with these difference sequences is the last digit - and in particular, that it is greater than 1 when $w \ge 3$. This condition would ensure that no a-special representation of $w(2^{2a} - 3^a)$ meets the requirement of its largest power of 2 having an exponent less than $2a - 1$. We will look a bit more at predicting the largest power of 2 in a representation in a later section.

TABLE 4.4: The component-wise difference between the a-special representations of $2^{2a} - 3^a$ and $w(2^{2a} - 3^a)$ for $7 \leq a \leq 14$ and $w = 325$.

a	$v(2a, 325) - v(2a, 1)$
7	(0, 2, 3, 2, 1, 7, 10)
9	(0, 2, 3, 2, 1, 4, 7, 7, 10)
10	(0, 2, 3, 2, 1, 4, 6, 7, 7, 10)
11	(0, 2, 3, 2, 1, 4, 6, 6, 7, 7, 10)
12	(0, 2, 3, 2, 1, 4, 6, 6, 6, 7, 7, 10)
13	(0, 2, 3, 2, 1, 4, 6, 6, 6, 6, 7, 7, 10)
14	(0, 2, 3, 2, 1, 4, 6, 6, 6, 6, 6, 7, 7, 10)

TABLE 4.5: The component-wise difference between the a-special representations of $2^{2a} - 3^a$ and $w(2^{2a} - 3^a)$ for $8 \leq a \leq 15$ and $w = 397$.

a	$v(2a, 397) - v(2a, 1)$
8	(0, 1, 5, 4, 3, 3, 9, 10)
10	(0, 1, 5, 4, 3, 3, 4, 7, 9, 10)
11	(0, 1, 5, 4, 3, 3, 4, 6, 7, 9, 10)
12	(0, 1, 5, 4, 3, 3, 4, 6, 6, 7, 9, 10)
13	(0, 1, 5, 4, 3, 3, 4, 6, 6, 6, 7, 9, 10)
14	(0, 1, 5, 4, 3, 3, 4, 6, 6, 6, 6, 7, 9, 10)
15	(0, 1, 5, 4, 3, 3, 4, 6, 6, 6, 6, 6, 7, 9, 10)

The case when $b \neq 2a$...

is not a topic worth discussing here. Primarily, we would need to pull a bit of a trick to get this to work, as $2^b - 3^a$ never has an a-special representation when $b \neq 2a$. But as we saw in the previous section, these sequences - while curiously interesting in the few apparent patterns - are unlikely to sire much information of interest to us. There is perhaps a good deal of extraneous information we are attempting to understand when we try to characterize the evolution of the entire difference sequence as a increases, when we truly only care about the last element. As such, we soon move on to what we hope are greener pastures. However, there is one point of interest that we will simply observe, without digging into. Recall that in the previous section there was an approximate sequential inclusion between the sets $W(a, 2a)$ and $W(a+1, 2(a+1))$. Such an approximate inclusion is also seen between $W(a, 2a+k)$ and $W(a+1, 2(a+1)+k))$. For different $k \in \mathbb{Z}$, we see vastly different w included - but there are often several overlapping elements. See Table 4.6 for an example of this. Similarly to the previous section, these inclusions will tend to being complete given some upper bound on their elements, as a gets larger. Beyond what has already been said, little is known about the mechanics of these sets - and with that, we move onward.

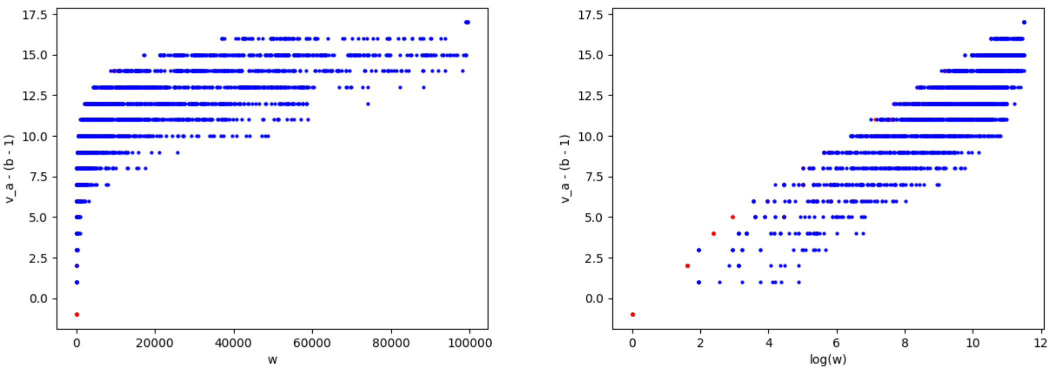
TABLE 4.6: The sets $W(a, 2a+k)$ for $k \in \{-1, 0, 1\}$, and $6 \leq a \leq 11$, for elements less than 100.

a	$W(a, 2a-1)$	$W(a, 2a)$	$W(a, 2a+1)$
6	{7, 23, 85}	{1, 5, 11, 53, 85}	{53, 85}
7	{7, 23, 29, 85}	{1, 5, 11, 19, 53, 85}	{53, 85}
8	{7, 23, 29, 37, 85}	{1, 5, 11, 19, 53, 85}	{53, 85}
9	{7, 23, 29, 37, 49, 85}	{1, 5, 11, 19, 53, 85}	{53, 67, 85}
10	{7, 23, 29, 37, 49, 65, 85}	{1, 5, 11, 19, 53, 85}	{53, 67, 85}
11	{7, 23, 29, 37, 49, 65, 85, 89}	{1, 5, 11, 19, 53, 85}	{53, 67, 85}

4.5.2 On the largest power of 2 in a k-special representation

The fundamental problem we find ourselves with is that we wish to show that for any $w \geq 3$ such that $w(2^b - 3^a)$ has an a-special representation, the largest power of 2 in that representation has an exponent greater than $b-1$. In the context of this problem, the following phrase carries very little weight, but: for every known w such that our expression has a representation, the largest power of 2 is larger than $b-1$. As we saw earlier, when $b = 2a$, the largest power of 2 had a significantly larger exponent than $b-1$. In general, we know of many cases where the largest power of 2 is 2^b, but only the trivial $w = 1, 2$ gives us a power of 2 with exponent less than b. See Figure 4.1 for the distribution of the difference between the exponent on the largest power of 2 in the representation of $w(2^b - 3^a)$ and $b-1$, as a function of w. Notice the single red point sitting below 0. This represents the trivial solution to Equation 3.2. There is a clear trend towards a larger difference between the largest power of 2 and $b-1$ with increasing w, but this is far from conclusive.

What complicates the picture a bit is that we know there are numbers with an a-special representation who have a multiple whose a-special representation has a smaller largest power of 2. For example, 27973 has the 7-special representation $(1, 3, 6, 8, 9, 10, 15)$, while $139865 (= 5 \cdot 27973)$ has the 7-special representation $(1, 8, 10, 11, 12, 13, 14)$. This fact is a bit disturbing, as it indicates that we do not get this property we are interested in for all k-special representations. Rather, we have to show there is something special about the form $w(2^b - 3^a)$ that forces the largest power of 2 to be larger than $b-1$ when $w \geq 3$ - if this is even true. It is then a bit of a shame that we cannot offer any insight into how this may be done. As we saw in the previous section, attempting to derive conditions which bound the largest power of 2 in a representation just leads us to a question about when some element appears in a Collatz orbit - almost exactly as hard a question as we started with. On that note, we will now return to the further investigation of the previously alluded to self-contained numbers.



(A) Linear

(B) Logarithmic w.r.t. w

FIGURE 4.1: Difference between the exponent on the largest power of 2 in the a-special representation of $w(2^b - 3^a)$ and $b-1$, as a function of w, for $1 \leq w \leq 10^5$, w odd, and $1 \leq a, b, \leq 20$. Red points represent integers where $b = 2a$.

Chapter 5

Self-Contained Numbers

As was mentioned previously, the numbers whose P-orbit contains an element equivalent to $-3^{-1} \mod w$ are called the self-contained numbers. This name was taken from the OEIS entry that lists them (A005184) [12], seemingly named by OEIS founder N.A. Sloane when he created the entry for the sequence. They can be thought of as the 'near-misses' for cyclicity in the Collatz process; the numbers whose orbit contains a multiple of itself. Clearly, the cyclic numbers are a subset of the self-contained numbers - in particular, those whose orbit contains a multiple that is a power of 2 times itself. Central questions relating to these numbers are then: how may we predict the quotient of w by the multiple in its orbit? How many self-contained numbers are there, and how rare are they? How might we predict whether a number is self-contained without computing its orbit?

Disappointingly, this document does not contain the answers to any of these, though we do prove a few facts about these numbers, and propose several conditions necessary for self-containedness. We present the totality of the known literature on these numbers, and come up with formulations for the Collatz conjecture and non-trivial cycles subproblem in terms of self-contained numbers. Our main contribution is a distributed computing effort that improves the upper bound on checked numbers to 10^{15}.

5.1 The Totality of Known Literature

The OEIS entry A005184 is the only known source discussing these numbers. It simply lists the numbers, and until now, the upper bound on numbers checked of 10^{11}.

5.2 Some Notation

We will introduce a bit of notation that is relevant to this section.

Notation 5.2.1. We say some $w \in \mathbb{N}^+$ is M-self contained for a Collatz map M if there exists $a \in \mathbb{N}^+$ such that $M^{(a)}(w) \equiv 0 \pmod{w}$.

Remark 5.2.1. The set of odd self-contained numbers at the end of the last chapter is then the P-self-contained numbers, and the set of odd and even is the C-self-contained numbers.

Notation 5.2.2. Let w an M-self-contained number. By $\mathrm{mult}_M(w)$ denote the largest element $x \in \mathrm{orb}_M(w)$ with $x \equiv 0 \pmod w$ for M a Collatz map. That is, $\mathrm{mult}_M(w)$ is the largest multiple of w in its orbit.

Notation 5.2.3. Let w a M-self-contained number. By $\mathrm{cont}_M(w)$ denote $\frac{\mathrm{mult}_M(w)}{w}$. That is, $\mathrm{cont}_M(w)$ is the quotient of the largest multiple of w in its orbit and w.

Notation 5.2.4. We denote

$$L_M(k, N) = \{w \in \mathbb{N}^+ : 5 \leq w \leq 10^N,\ \exists x \in \mathrm{orb}_M(w) : x \equiv -k^{-1} \pmod w\}$$

When the second parameter of L_M is not given (eg. $L_P(3)$) we take this to denote the unbounded set of such numbers.

Remark 5.2.2. The C-self-contained numbers are thus denoted by $L_C(3)$, and the P-self-contained by $L_P(3)$.

5.3 Some Facts

Now, we present a few propositions relating to self-contained numbers. These are not terribly deep, and reflect the state of our knowledge about this set of numbers.

Lemma 5.3.1. Let $w \in \mathbb{N}^+$. Then, w is C-self-contained if and only if there exists $x \in \mathrm{orb}_P(w)$ with $x \equiv -3^{-1} \pmod w$.

Proof. Suppose w is C-self contained. Then, $\mathrm{mult}_C(w) = 2^n aw$ for some $a \in \mathbb{N}^+$. Since this is the largest multiple of w in the C-orbit, we must have that it was produced by an odd step of the C map (as otherwise there would be a larger multiple. Let x be the element preceding $\mathrm{mult}_C(w)$ in $\mathrm{orb}_C(w)$. We have that $3x + 1 \equiv 0 \pmod w$, so $x \equiv -3^{-1} \pmod w$. Since x must be odd, x is also in $\mathrm{orb}_P(w)$.

Suppose there exists $x \in \mathrm{orb}_P(w)$ with $x \equiv -3^{-1} \pmod w$. Then clearly, $C(x) \equiv 0 \pmod w$, so the C-orbit contains a multiple of w. □

Proposition 5.3.1. Let $w \in \mathbb{N}^+$ a P-self-contained number. Then, there exists $n \in \mathbb{N}^+$ such that $2^{n+1}w$ is not C-self-contained, and $2^k w$ is C-self-contained for all $1 \leq k \leq n$.

Proof. Since w is P-self-contained, we have that $\mathrm{mult}_P(w) = aw$ for some $a \in \mathbb{N}^+$ with $2 \nmid a$. Then, $\mathrm{mult}_C(w) = 2^n aw$ for $n = \nu_2(3r + 1)$ for r the element in $\mathrm{orb}_P(w)$ immediately preceding $\mathrm{mult}_P(w)$. Clearly, since w maps to $2^n aw$ under C, $2^k w$ also does for any $k \geq 1$. For $2^n aw$ to be a multiple of $2^k w$, we must have $k \leq n$. Since $2^n aw$ was the maximum multiple of w in the C-orbit, it is not a multiple of $2^k w$ when $k > n$. □

Proposition 5.3.2. Let $w \in \mathbb{N}^+$ with $w \not\equiv 0 \pmod 3$. Then

$$-3^{-1} \mod w = \frac{d \cdot w - 1}{3}$$

for $d \coloneqq w \mod 3$.

Proof. The proof is self-evident. ☐

Proposition 5.3.3. For any $w \in \mathbb{N}^+$ with w P-self-contained, $\text{cont}_C(w) \not\equiv 0 \pmod 3$.

Proof. Let x be the element immediately preceding $\text{mult}_P(w)$ in the orbit of w. We have $x = qw + \frac{dw-1}{3}$ for $q \in \mathbb{N}$ and $d \coloneqq w \mod 3$. Then, $C(x) = 3qw + dw$. So, $\text{cont}_C(w) = \frac{C(x)}{w} = 3q + d$, and thus $\text{cont}_C(w) \equiv w \pmod 3$. Since $w \equiv w^{-1} \pmod 3$, we get $w \cdot \text{cont}_C(w) \equiv 1 \pmod 3$, and so $\text{cont}_C(w) \not\equiv 0 \pmod 3$ as $w \not\equiv 0 \pmod 3$. ☐

Proposition 5.3.4. For any $w \in \mathbb{N}^+$ with w C-self-contained, w is not a multiple of 3.

Proof. Since w is self-contained, there is some odd element of its orbit, x, such that $3x + 1 \equiv 0 \pmod w$. Then, $3x + 1 = aw$ for some $a \in \mathbb{Z}$. Suppose w is a multiple of 3. Clearly, $3 \mid aw$, but $3 \nmid 3x + 1$, so we have a contradiction. ☐

5.4 Computationally Improving the Upper Bound

As noted, it is difficult to say much about which numbers will contain a certain element in their orbit without actually calculating its orbit. Thus, in order to investigate which numbers are actually self-contained, we must simply perform a (semi-)naive search. In our case, we immediately sieved even numbers - as if an even number is self contained, then so is that number with all factors of 2 removed. While we did not sieve all multiples of 3, this is also a valid method that would improve efficiency non-trivially. Recall that a self-contained number cannot be a multiple of 3 by Lemma 5.3.4.

Previously, the positive integers up to 10^{11} had been checked for self-containedness. This resulted in the set of odd self-contained numbers:

$$L_P(3, 11) = \{31, 83, 293, 347, 671, 19151, 2025797\}$$

Notice that the largest element of $L_P(3, 11)$ is on the order of 10^6. It appears that there is a drought of such numbers after this point, as even searching 5 orders of magnitude higher has not recovered any more self-contained numbers. We have further improved this bound to 10^{15}, and still not found any more. Before getting too excited by the idea that there only may be finitely-many self-contained numbers, note that we have no assurance that such numbers would necessarily be small, or close together. Still, it is interesting that they simply stop showing up at a point. In this section, we will discuss the computational methods used to improve this bound, and where these may be improved upon in the future.

5.4.1 Computational methods

Initially, computations were performed rather naively in Python, with no multiprocessing. This is sufficient for checking up to about 10^6 within a few seconds. Clearly, to push further, improvements were needed. First was to parallelise the computation, as this problem lends itself very easily to such a speedup. This of course speeds up the computation by a factor of the number of threads on which it is run, but there is still the underlying slowness of a language like Python. For this reason, we chose to implement the computation in Julia. This implementation ended up being faster than our C++ implementation - though that may be down to shoddy C++ code for large integers on our part. For reference, running the computation in Julia gave an increase of about 20 times over Python. Still, our desired bound would not be doable on a single machine in a reasonable amount of time. For every order of magnitude increase in the upper bound, there was about an 11 times increase in the computation time. This is quite good actually - as it appears to be linear in time-complexity - but still increases the required resources reasonably quickly when we are trying to push 10^{15}. So, we ended up employing a distributed computing strategy, making use of Compute Canada resources to perform the computations.

In total, checking the numbers between 10^{14} and 10^{15} took 2400 48-core computers an average of 7 hours each, for a total compute time of about 90 years. Together with the calculations for integers between 10^{11} and 10^{14}, we used about 100 years of compute time. We estimate then that checking up to 10^{16} would take about 1000 compute years, and it was thus out of reach for us, given our resource allocations. In order to further improve speed, we wrote a GPU implementation using Nvidia's CUDA library. This provided a further 20 or so times speedup over the Julia implementation - although getting our hands on sufficient GPU nodes to push 10^{16} was not something we were able to do in time for it to be included in this report.

5.4.2 Further improvements

As was mentioned, the use of GPUs can significantly improve the speed at which the calculations occur, due to their inherent parallelised structure. However, the computations for large integers will be noticeably slower due to the necessity of using 64-bit types which cannot take advantage of special operations, such as fused-multiply-accumulate. Regardless, this is made up for by the large number of cores over a CPU. We also believe that further improvements can be made in the parallelisation for a GPU over our 20 times speedup, as we use a naive strategy and are not terribly familiar with programming for GPUs.

In terms of sieving, the primary methods are to remove any multiples of 2 or 3, as these either are degenerate self-contained numbers or cannot be self-contained in any case. Further sieves that assure self-contained numbers are not removed are not known.

This comes down primarily to a lack of knowledge on what such a number may or may not look like. Beyond this, it may also be prudent to sieve numbers that are equivalent to $1 \mod 3$. This comes purely from the observation that only 31 is not modularly equivalent to $2 \mod 3$, which may suggest it is the only such self-contained number. That said, this observation comes from a very small set of numbers, so it is only a tentative suggestion. If anything, it may speed up the search for the next self-contained number equivalent to $2 \mod 3$, if it exists.

5.5 A Spot of Empiricism

Unfortunately, the few propositions above represent much of what we can say about self-contained numbers. A good bit of the work on this project sought to use computational and experimental methods to identify patterns that are candidates for formalization, but very often these patterns were not clear enough to elucidate such a generalization. Nonetheless, we will discuss here several of the directions in which this experimentation went, and some of the more major observations that can be made from them. Principally, we are interested in being able to deduce *a priori* whether the P-orbit of some $w \in \mathbb{N}^+$ contains an element equivalent to $-3^{-1} \mod w$. Most interestingly, we observe an increasing rarity to the set of such numbers - which is ideally (but far from necessarily) indicative of their finiteness. We also expand our search beyond self-contained numbers to any whose C-orbit contains our element of interest. We see that the same pattern of sparsity, and seeming finiteness is exhibited here. First, we start by noting some elementary properties of the self-contained numbers we know.

5.5.1 The self-contained numbers we know

Recall our P-self-contained numbers:

$$L_P(3, 15) = \{31, 83, 293, 347, 671, 19151, 2025797\}$$

Each of our C-self-contained numbers is either in $L_P(3)$, or a power of 2 times some element of $L_P(3)$. We have 7 known P-self-contained numbers, but 15 C-self-contained numbers since both $2 \cdot 671$ and $2^2 \cdot 671$ are C-self-contained. Of the self-contained numbers we know, 671 is the only one with a larger multiple of a power of 2 than 2^1 also C-self-contained. We do not know how to predict when this may happen - nor if we should expect that any other self-contained numbers would have this property.

The only P-self-contained number not equivalent to $2 \mod 3$ is 31, which is equivalent to 1. Again, we do not know whether to expect all subsequent P-self-contained numbers to be equivalent to 2.

The set of $\text{cont}_P(w)$ for $w \in L_P(3)$ is given (in the same order as above):

$$\{5, 13, 7, 7, 11, 37, 79\}$$

The no non-trivial cycles subproblem can equivalently be stated in terms of $\text{cont}_P(w)$.

Proposition 5.5.1. The Collatz conjecture has no non-trivial cycles if and only if $\text{cont}_P(w) \neq 1$ for all $w \in L_P(3)$.

Evidently, $\text{cont}_P(w)$ is prime for all known P-self-contained numbers - however it is unlikely that trying to prove anything about these numbers in terms of primality would be particularly elucidative. It is unknown if $\text{cont}_P(w)$ can be composite - though determining this would not necessarily say anything interesting about the conjecture. Being able to say that it is always prime, however, would solve the conjecture.

5.5.2 Some almost self-contained numbers

If we take off the restriction that the element equivalent to $-3^{-1} \mod w$ must occur in the P-orbit (and thus be odd), and instead check for such elements in C-orbits, we see something interesting. First, there are quite a few more such numbers. Clearly, these are a superset of the self-contained numbers. The full set is too numerous to reasonably include here, but the first 10 element of the set are

$$L_C(3, 12) = \{5, 7, 11, 13, 19, 25, 31, 43, 47, 49, \ldots\}$$

There are 89 such numbers less than 10^{12} - including even numbers. What is perhaps interesting then is that the only even numbers in this set are C-self-contained . That is, there are no even $w \in \mathbb{N}^+$ that have an even element of their C-orbit equivalent to $-3^{-1} \mod w$. In fact, we can prove this.

Proposition 5.5.2. If $w \in L_C(3)$ and $w \notin L_P(3)$, then w is odd.

Proof. We give an outline of the proof. This is relatively obvious by arguing that the element $x \in \text{orb}_C(w)$ with $x \equiv -3^{-1} \pmod{w}$ and x even must have a different parity than $x' \in \text{orb}_C(2w)$ with $x' \equiv -3^{-1} \pmod{2w}$. Note that we need x even since $w \notin L_P(3)$. Splitting by the residue class of $w \mod 3$, we can verify in each case that such an x being in $\text{orb}_C(w)$ implies no such x' can be in $\text{orb}_C(2w)$. Further, since we have that $2w \in L_C(3)$ implies $w \in L_C(3)$, we cannot have that w is even. $\square$

This then distinguishes actual self-contained numbers from these pseudo-self-contained numbers by the fact that odd self-contained numbers have 2 times themselves also self-contained, if not also higher powers of 2. What is perhaps more interesting is that the pseudo-self-contained numbers also seem to stop appearing eventually; the largest such number less than 10^{12} is 4051594 - which is a our largest C-self-contained number. While we haven't checked as large a bound as for self-contained numbers, we see a similar distribution between these and the self-contained numbers. The fact that the pseudo-self-contained numbers also run into a drought seems to suggest that, as w gets large, it becomes quite rare that some element of your orbit is equivalent to $-3^{-1} \mod w$.

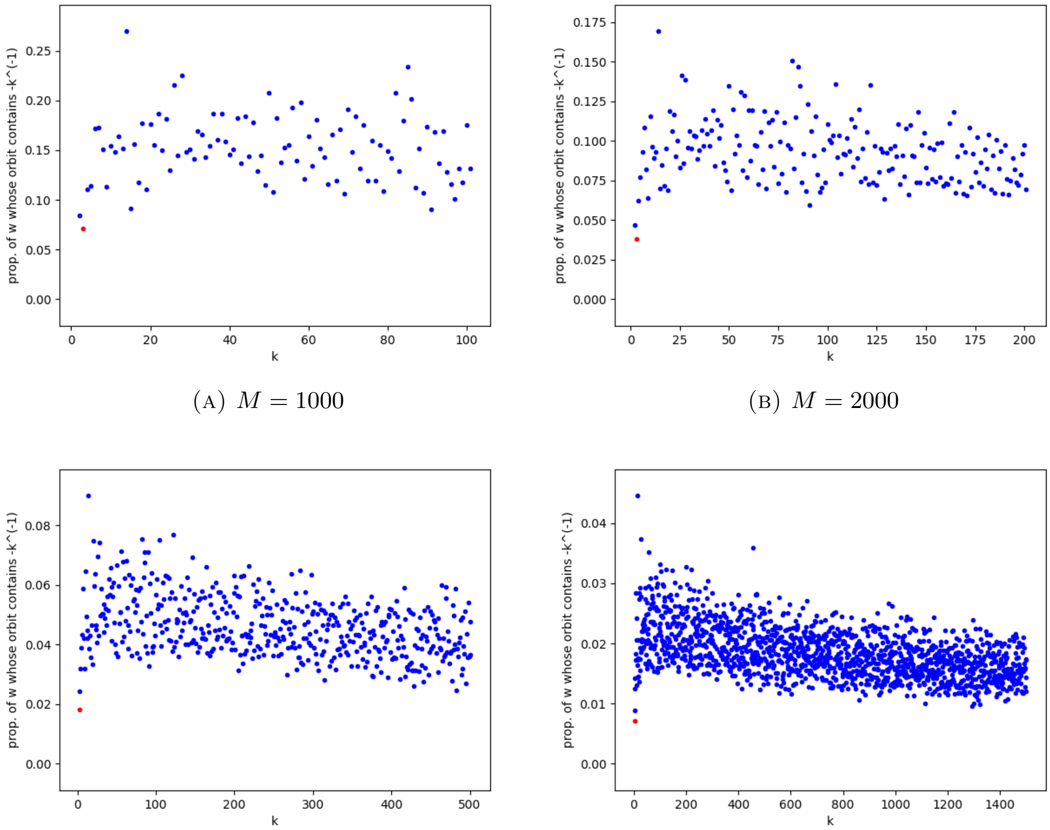
5.5.3 How common is -3^{-1}?

This all raises the question: are such elements more rare than any other? That is, are we less likely to see some element in the residue class of $-3^{-1} \mod w$ than any other of the residue classes of w? As it turns out, yes; this appears to be the case. Consider the following: For all w less than some bound, M, we find the proportion of w whose C-orbit contains the element $-k^{-1}$ out of how many have $\gcd(w, k) = 1$. Essentially, we count how often it occurs as a fraction of how often it could possibly occur. As we let M tend off to infinity, the proportion of orbits in which each $-k^{-1}$ appears should tend towards its true density. Of course, since each time M is increased we introduce new k (eg. there is no -7^{-1} when $M < 8$), each k is converging independently of every other. We thus only look at $1 \leq k \leq \frac{M}{10}$ for any given M, to give the newly present k some time to converge. A factor of 10 was chosen empirically, given the rate of convergence of newly-added k. See Figure 5.1 for an example of what this looks like. Notice that for every M, -3^{-1} is the residue class least often included in orbits. Now, if we look up to $k \leq M$, we will find that there is some other residue class which is in a smaller proportion of orbits - but in all observed circumstances, this only happens for finitely-many M, as with increasing M, the given residue class converges to a larger proportion than that of -3^{-1}.

In Figure 5.1, multiplicity within an orbit is not taken into account. If the residue class of two different elements in an orbit is $-k^{-1}$ more than once, this is still only counted as a single occurrence for the calculation of proportion. Thus, this measures the rarity of w for which a given element exists in $\text{orb}_C(w)$ (as a fraction of the w for which such an element could possibly exist). In order to measure the frequency of a particular residue class appearing in an orbit, we must consider multiplicity. In Figure 5.2, multiplicity is considered. With multiplicity, not much is changed - to the extent that you may not be able to tell the two figures apart without careful examination. Evidently, -3^{-1} is not very common - either in terms of the number of w in whose orbits it appears, or the number of times it does so across w. In both cases, the most common residue class is -14^{-1}. Currently, we are unsure as to how to interpret this in any meaningful way.

5.5.4 A closing conjecture

If we repeat the experiment we ran in an earlier section of finding all w for which there is some element of $\text{orb}_C(w)$ modularly equivalent to $-k^{-1} \mod w$ for k with $\gcd(k, w) = 1$, we see a similar pattern to what we saw with $k = 3$. That is, it appears that for most k we choose, the C-orbit of w will eventually stop containing elements in the residue class of $-k^{-1}$, as w gets sufficiently large. Recall that in the case of $k = 3$, we checked up to 10^{12} and saw that there were 89 numbers with such an element in their C-orbit - the largest of which was on the order of 10^6. See Table 5.1 for a collection of these values for other k, again checked up to 10^{12}. Most important to note are the last two columns - in particular, the difference between the largest element and the upper bound we have checked, and the relatively tiny proportion of candidate w that contain a particular



(A) $M = 1000$ (B) $M = 2000$

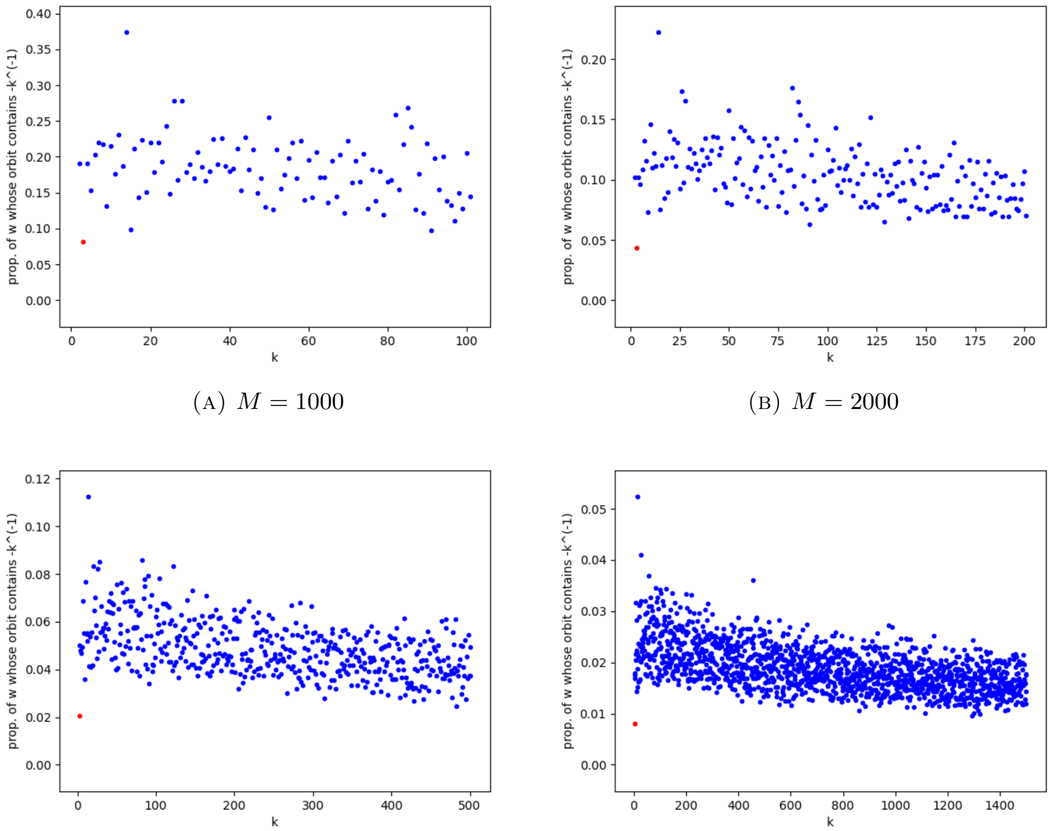
(C) $M = 5000$ (D) $M = 15000$

FIGURE 5.1: Plots of the proportion of $w \leq M$ whose C-orbit contains an element equivalent to $-k^{-1} \mod w$ for $\gcd(w,k) = 1$. Values are shown for several M. The red point corresponds to $k = 3$.

residue class in their orbit. Much like $k = 3$, in most cases, there comes some bound (much less than our upper bound) at which point we cease to see any more w with orbits intersecting the residue class of $-k^{-1}$. It is our suspicion that in the cases where we do not see this (1009, 1019, 10009, 10037, 10039), this is simply due to not checking a large enough bound. Of course, an immediate further step would to be to check to a higher bound, as we have for the $k = 3$ case. Along these lines, we will end off with a couple conjectures related to these numbers.

Conjecture 5.5.1. For every $k \in \mathbb{N}^+$ with $k \geq 3$, the natural density of $L_C(k)$ is 0. That is,

$$\lim_{n\to\infty} \frac{|L_C(k,n)|}{10^n} = 0$$



(A) $M = 1000$

(B) $M = 2000$

(C) $M = 5000$

(D) $M = 15000$

FIGURE 5.2: Plots of the proportion of $w \leq M$ whose C-orbit contains an element equivalent to $-k^{-1} \mod w$ for $\gcd(w, k) = 1$. Multiplicity within an orbit is taken into account. Values are shown for several M. The red point corresponds to $k = 3$.

This seems probable simply based on the growth rate of $L_C(k)$ we see for small numbers. Of course, this is also not so strict a condition, as we could still have $L_C(k)$ infinite - but it is certainly an inoffensive conjecture. Of course, we have only check this for relatively small k, and only up to a bound of 10^{12} - but the results are pretty uniform across the board of tested values. A much stricter, and likely much more difficult conjecture to say anything about is the following:

Conjecture 5.5.2. For every $k \in \mathbb{N}^+$ with $k \geq 3$, $|L_C(k)|$ is finite.

Again, this conjecture follows from our relatively small collection of empirical observations. To say anything convincing of its truth is quite difficult - and in fact may be more difficult than the Collatz conjecture itself. If true, it could potentially be helpful in saying something about the Collatz process - and in particular, if we knew that $L_C(3)$

was finite, this could be very useful. Of course, even if we did know that, it may prove to be entirely useless (at least in terms of an exhaustive proof) if it is still very large, or the bound on its size was unknown. One must remember than finite things can still be enormous.

With that, we have reached the end of what we can say about self-contained numbers. This stopping point is not one indicative of a lack of further directions to look in, but of the time available to do so. This part of the project especially has a penchant for devouring one's time, all the while giving little in return. Ultimately, we do not believe that this is a particularly fruitful area of research on this conjecture. Without knowing more elucidative properties of self-contained numbers there is little that can be done to analyze them theoretically. Experimentally, there is a deep well of fun to be had investigating the patterns that are just random enough to be bewildering, but just regular enough to convince you that something is going on. The fact that only 7 odd self-contained numbers are known significantly hinders our ability to make generalizations about what properties they share, or even guess at what these might be. As such, it is clear why the literature on this strange little set of numbers is so scant.

TABLE 5.1: The number of $5 \leq w \leq 10^{12}$ for which there exists $x \in \mathrm{orb}_C(w)$ with $x \equiv -k^{-1} \pmod{w}$ for various prime k. The largest known w for each k is given, as well as the number of such w found, and the proportion of such w relative to the number of integers coprime to k, less than 10^{12}.

k	$\lvert L_C(k,12)\rvert$	$\max L_C(k,12)$	Proportion of possible $w \leq 10^{12}$
2	72	$696255 \approx 10^5$	$\leq 10^{-8}$
3	89	$4051594 \approx 10^6$	$\leq 10^{-8}$
5	176	$139329 \approx 10^5$	$\leq 10^{-8}$
7	493	$13545617 \approx 10^7$	$\leq 10^{-9}$
11	327	$19756327 \approx 10^7$	$\leq 10^{-9}$
13	256	$40114101 \approx 10^7$	$\leq 10^{-9}$
17	273	$776595 \approx 10^5$	$\leq 10^{-9}$
19	1263	$36816597 \approx 10^7$	$\leq 10^{-8}$
23	391	$14785947 \approx 10^7$	$\leq 10^{-9}$
29	355	$2355789 \approx 10^6$	$\leq 10^{-9}$
31	362	$6413202 \approx 10^6$	$\leq 10^{-9}$
37	323	$235114039 \approx 10^8$	$\leq 10^{-9}$
41	597	$141512421 \approx 10^8$	$\leq 10^{-9}$
43	300	$477605 \approx 10^5$	$\leq 10^{-9}$
47	387	$15476475 \approx 10^7$	$\leq 10^{-9}$
53	588	$37311790 \approx 10^7$	$\leq 10^{-9}$
103	548	$403378601 \approx 10^8$	$\leq 10^{-7}$
1009	3394	$234416142900 \approx 10^{11}$	$\leq 10^{-8}$
1013	496	$9352017 \approx 10^6$	$\leq 10^{-9}$
1019	806	$104257576728 \approx 10^{11}$	$\leq 10^{-9}$
10007	1055	$626301280 \approx 10^8$	$\leq 10^{-8}$
10009	1121	$607406350119 \approx 10^{11}$	$\leq 10^{-8}$
10037	17223	$16266406485 \approx 10^{10}$	$\leq 10^{-7}$
10039	4614	$490352236013 \approx 10^{11}$	$\leq 10^{-8}$

Chapter 6

Conclusion

The motivation for starting this project was to investigate some of the properties of solutions to an algebraic formulation of the non-trivial cycles subproblem of the Collatz conjecture. In the course of this, we principally focused on the representation of integers by a k-special 3-smooth representation - which is in an of itself a deeply complex and interesting problem. While we were not able to say much more than other authors on the matter, we formalized a derivation of the self-contained numbers from a particular form of k-special representation. We also present some of the first elementary results on the self-contained numbers. Our main contribution is the increased bound of numbers checked for self-containedness to 10^{15}. To end out, we generalized the concept of self-containedness, and presented some conjectures on what seems to be a very sparse class of numbers, which we denoted $L_C(k)$. The empirical results presented here represent only a small portion of the amount generated throughout the course of this project. What has been stated amounts to that which we could say much of anything concrete about; the rest was often too complex to make generalizable observations - though this is also part of what made it so fascinating. In whole, the project has been a wonderful exercise in the use of computation to discover interesting patterns and results to investigate further, and with (hopefully) more analytic methods.

One doesn't decide to set aside some time to work on the Collatz conjecture with the idea in mind that they will actually solve it. One hopes, of course - but anyone short of a professional crank knows better than to imagine, with any degree of seriousness, the prospect of cracking it. Ultimately, working at a problem like this is more an exercise in masochism than anything else; a test of how little respect you have for your own time. And still, I think it is something that every young aspiring mathematician should try. With the knowledge in mind that you aren't going to solve it, or very likely even come up with anything novel, you should find some time to anguish yourself with questions far bigger than you have any right to expect to answer. Despite how disappointing it is when every 'breakthrough' you come up with was found decades ago and leads nowhere, there is near infinite intrigue to be found in delving into the inner workings of this problem. The hope then is that your curiosity is sated regularly enough that you can stick with it for at least a short while. But at the same time, you hope that you're able to let go when it's time. This is all too easy a problem to become obsessed with - and I've had my fair share of obsession with it. Perhaps more than anything, the experience of undertaking this project has given me an appreciation for the scale of even the seemingly simple questions in number theory. What so many questions come back to is the problem of understanding the interaction between the multiplicative and additive structure of the integers. It is a problem that it seems we are currently not able to answer - and may not be able to anytime soon. In my case, it took struggling against an insurmountable question for 8 months to have the sheer difficulty of this impressed upon me. For now, I will take solace in the upcoming absence of this conjecture from my life, at least for a little while. My only hope is that someone may find some utility, curiosity, or simply interest in something I've included here - but even if not, I'm just as happy.

Chapter 7

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